1. Μήκη και γωνίες δεσμών των ενώσεων UCY-4 - UCY-12, LnCAP, CeN-BDC

Πίνακας Π1-1: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-4**

Μήκη δεσμών (Å) της ένωσης UCY-4

La(1)-O(5)	2.470(4)	La(1)-O(7)	2.534(5)
La(1)-O(8)	2.481(6)	La(1)-O(3)	2.553(4)
La(1)-O(4)	2.482(4)	La(1)-O(2)	2.628(4)
La(1)-O(6)	2.502(4)	La(1)-O(4)	2.757(4)
La(1)-O(1)	2.521(4)		

Γωνίες δεσμών (º) της ένωσης UCY-4

O(5)-La(1)-O(8)	136.4(2)	O(1)-La(1)-O(7)	71.7(2)
O(5)-La(1)-O(4)	72.5(2)	O(5)-La(1)-O(3)	74.0(2)
O(8)-La(1)-O(4)	83.9(2)	O(8)-La(1)-O(3)	147.5(2)
O(5)-La(1)-O(6)	133.1(2)	O(4)-La(1)-O(3)	123.1(2)
O(8)-La(1)-O(6)	74.4(2)	O(6)-La(1)-O(3)	92.0(2)
O(4)-La(1)-O(6)	79.4(2)	O(1)-La(1)-O(3)	83.4(2)
O(5)-La(1)-O(1)	81.5(2)	O(7)-La(1)-O(3)	73.5(2)
O(8)-La(1)-O(1)	89.7(2)	O(5)-La(1)-O(2)	71.9(2)
O(4)-La(1)-O(1)	133.7(2)	O(8)-La(1)-O(2)	69.8(2)
O(6)-La(1)-O(1)	142.3(2)	O(4)-La(1)-O(2)	84.71(2)
O(5)-La(1)-O(7)	139.7(2)	O(6)-La(1)-O(2)	142.0(2)
O(8)-La(1)-O(7)	74.2(2)	O(1)-La(1)-O(2)	50.5(2)
O(4)-La(1)-O(7)	147.0(2)	O(7)-La(1)-O(2)	109.6(2)
O(6)-La(1)-O(7)	71.2(2)	O(3)-La(1)-O(2)	125.3(2)
O(1)-La(1)-O(7)	71.7(2)	O(5)-La(1)-O(4)	69.2(2)
O(4)-La(1)-O(4)	76.4(2)	O(7)-La(1)-O(4)	105.1(2)
O(6)-La(1)-O(4)	68.1(2)	O(3)-La(1)-O(4)	49.0(1)
O(1)-La(1)-O(4)	128.7(2)	O(2)-La(1)-O(4)	140.3(2)

Πίνακας Π1-2: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-5**

Μήκη δεσμών (Å) της ένωσης UCY-5

Ce(1)-O(7)	2.443(8)	Ce(1)-O(8)	2.533(7)
Ce(1)-O(4)	2.461(5)	Ce(1)-O(5)	2.534(5)
Ce(1)-O(3)	2.472(5)	Ce(1)-O(1)	2.620(5)
Ce(1)-O(6)	2.473(5)	Ce(1)-O(6)	2.741(5)
Ce(1)-O(2)	2.502(5)		

Γωνίες δεσμών (º) της ένωσης UCY-5

O(7)-Ce(1)-O(4)	135.5(2)	O(6)-Ce(1)-O(5)	123.7(2)
O(7)-Ce(1)-O(3)	75.1(2)	O(2)-Ce(1)-O(5)	83.0(2)
O(4)-Ce(1)-O(3)	133.8(2)	O(8)-Ce(1)-O(5)	73.4(2)
O(7)-Ce(1)-O(6)	83.8(2)	O(7)-Ce(1)-O(1)	69.1(2)
O(4)-Ce(1)-O(6)	72.7(2)	O(4)-Ce(1)-O(1)	71.3(2)
O(3)-Ce(1)-O(6)	80.0(2)	O(3)-Ce(1)-O(1)	142.1(2)
O(7)-Ce(1)-O(2)	89.2(3)	O(6)-Ce(1)-O(1)	84.0(2)
O(4)-Ce(1)-O(2)	80.9(2)	O(2)-Ce(1)-O(1)	50.7(2)
O(3)-Ce(1)-O(2)	142.1(2)	O(8)-Ce(1)-O(1)	110.0(2)
O(6)-Ce(1)-O(2)	133.2(2)	O(5)-Ce(1)-O(1)	125.1(2)
O(7)-Ce(1)-O(8)	74.5(2)	O(7)-Ce(1)-O(6)	140.6(2)
O(4)-Ce(1)-O(8)	139.5(2)	O(4)-Ce(1)-O(6)	69.9(2)
O(3)-Ce(1)-O(8)	70.7(2)	O(3)-Ce(1)-O(6)	67.9(2)
O(6)-Ce(1)-O(8)	147.1(2)	O(6)-Ce(1)-O(6)	76.8(2)
O(2)-Ce(1)-O(8)	71.9(2)	O(2)-Ce(1)-O(6)	128.8(2)
O(7)-Ce(1)-O(5)	147.8(2)	O(8)-Ce(1)-O(6)	104.8(2)
O(4)-Ce(1)-O(5)	74.1(2)	O(5)-Ce(1)-O(6)	49.5(2)
O(3)-Ce(1)-O(5)	92.1(2)	O(1)-Ce(1)-O(6)	140.3(2)

Πίνακας Π1-3: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-6**

Μήκη δεσμών (Å) της ένωσης UCY-6

Pr(1)-O(3)	2.436(6)	Pr(1)-O(8)	2.50(2)
Pr(1)-O(6)	2.437(6)	Pr(1)-O(4)	2.512(6)
Pr(1)-O(5)	2.439(6)	Pr(1)-O(1)	2.563(6)
Pr(1)-O(7)	2.44(2)	Pr(1)-O(3)	2.695(5)
Pr(1)-O(2)	2.489(6)		

Γωνίες δεσμών (º) της ένωσης UCY-6

O(3)-Pr(1)-O(6)	72.8(2)	O(7)-Pr(1)-O(4)	148.1(3)
O(3)-Pr(1)-O(5)	80.0(2)	O(2)-Pr(1)-O(4)	81.2(2)
O(6)-Pr(1)-O(5)	133.8(2)	O(8)-Pr(1)-O(4)	74.3(3)
O(3)-Pr(1)-O(7)	83.1(3)	O(3)-Pr(1)-O(1)	85.5(2)
O(6)-Pr(1)-O(7)	135.2(3)	O(6)-Pr(1)-O(1)	71.1(3)
O(5)-Pr(1)-O(7)	75.0(3)	O(5)-Pr(1)-O(1)	143.2(3)
O(3)-Pr(1)-O(2)	133.8(2)	O(7)-Pr(1)-O(1)	69.8(3)
O(6)-Pr(1)-O(2)	78.6(3)	O(2)-Pr(1)-O(1)	50.8(2)
O(5)-Pr(1)-O(2)	143.3(3)	O(8)-Pr(1)-O(1)	107.2(3)
O(7)-Pr(1)-O(2)	93.0(4)	O(4)-Pr(1)-O(1)	124.9(2)
O(3)-Pr(1)-O(8)	147.6(3)	O(3)-Pr(1)-O(3)	75.3(2)
O(6)-Pr(1)-O(8)	139.3(3)	O(6)-Pr(1)-O(3)	69.5(2)
O(5)-Pr(1)-O(8)	72.1(3)	O(5)-Pr(1)-O(3)	68.0(2)
O(7)-Pr(1)-O(8)	74.1(3)	O(7)-Pr(1)-O(3)	139.7(3)
O(2)-Pr(1)-O(8)	71.3(3)	O(2)-Pr(1)-O(3)	126.4(2)
O(3)-Pr(1)-O(4)	123.1(2)	O(8)-Pr(1)-O(3)	107.8(3)
O(6)-Pr(1)-O(4)	74.6(2)	O(4)-Pr(1)-O(3)	49.9(2)
O(5)-Pr(1)-O(4)	91.0(2)	O(1)-Pr(1)-O(3)	139.7(2)

Πίνακας Π1-4: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-7**

Μήκη δεσμών (Å) της ένωσης UCY-7

Sm(1)-O(3)	2.388(5)	Sm(1)-O(4)	2.462(5)
Sm(1)-O(8)	2.39(2)	Sm(1)-O(7)	2.48(2)
Sm(1)-O(5)	2.397(5)	Sm(1)-O(1)	2.539(5)
Sm(1)-O(6)	2.406(5)	Sm(1)-O(3)	2.683(5)
Sm(1)-O(2)	2.446(6)		

Γωνίες δεσμών (º) της ένωσης UCY-7

O(3)-Sm(1)-O(8)	82.7(3)	O(6)-Sm(1)-O(7)	71.0(3)
O(3)-Sm(1)-O(5)	73.7(2)	O(2)-Sm(1)-O(7)	73.0(3)
O(8)-Sm(1)-O(5)	135.3(3)	O(4)-Sm(1)-O(7)	84.7(2)
O(3)-Sm(1)-O(6)	80.2(2)	O(3)-Sm(1)-O(1)	69.5(3)
O(8)-Sm(1)-O(6)	75.2(3)	O(8)-Sm(1)-O(1)	71.0(2)
O(5)-Sm(1)-O(6)	134.4(2)	O(5)-Sm(1)-O(1)	143.1(2)
O(3)-Sm(1)-O(2)	134.3(2)	O(6)-Sm(1)-O(1)	52.0(2)
O(8)-Sm(1)-O(2)	93.1(3)	O(2)-Sm(1)-O(1)	125.8(2)
O(5)-Sm(1)-O(2)	78.3(2)	O(4)-Sm(1)-O(1)	108.1(3)
O(6)-Sm(1)-O(2)	142.5(2)	O(7)-Sm(1)-O(1)	75.7(2)
O(3)-Sm(1)-O(4)	124.3(2)	O(3)-Sm(1)-O(3)	139.7(3)
O(8)-Sm(1)-O(4)	147.1(3)	O(8)-Sm(1)-O(3)	69.7(2)
O(5)-Sm(1)-O(4)	75.3(2)	O(5)-Sm(1)-O(3)	67.9(2)
O(6)-Sm(1)-O(4)	90.2(2)	O(6)-Sm(1)-O(3)	126.2(2)
O(2)-Sm(1)-O(4)	80.8(2)	O(2)-Sm(1)-O(3)	50.3(2)
O(3)-Sm(1)-O(7)	147.3(3)	O(4)-Sm(1)-O(3)	107.4(3)
O(8)-Sm(1)-O(7)	74.5(3)	O(7)-Sm(1)-O(3)	139.6(2)
O(5)-Sm(1)-O(7)	138.7(3)	O(1)-Sm(1)-O(3)	71.0(3)

Πίνακας Π1-5: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**

Μήκη δεσμών (Å) της ένωσης UCY-8

Eu(1)-O(5)	2.366(7)	Eu(1)-O(4)	2.435(7)
Eu(1)-O(3)	2.367(7)	Eu(1)-O(1)	2.459(7)
Eu(1)-O(6)	2.405(7)	Eu(1)-O(2)	2.501(7)
Eu(1)-O(8)	2.41(2)	Eu(1)-O(3)	2.648(7)
Eu(1)-O(7)	2.426(9)		

Γωνίες δεσμών (º) της ένωσης UCY-8

O(5)-Eu(1)-O(3)	77.7(3)	O(8)-Eu(1)-O(1)	90.5(3)
O(5)-Eu(1)-O(6)	134.5(2)	O(7)-Eu(1)-O(1)	72.1(3)
O(3)-Eu(1)-O(6)	73.3(3)	O(4)-Eu(1)-O(1)	80.0(3)
O(5)-Eu(1)-O(8)	75.6(3)	O(5)-Eu(1)-O(2)	140.2(3)
O(3)-Eu(1)-O(8)	89.0(3)	O(3)-Eu(1)-O(2)	83.2(2)
O(6)-Eu(1)-O(8)	136.7(3)	O(6)-Eu(1)-O(2)	69.5(3)
O(5)-Eu(1)-O(7)	75.9(3)	O(8)-Eu(1)-O(2)	69.3(3)
O(3)-Eu(1)-O(7)	151.7(3)	O(7)-Eu(1)-O(2)	111.4(3)
O(6)-Eu(1)-O(7)	133.9(3)	O(4)-Eu(1)-O(2)	124.4(2)
O(8)-Eu(1)-O(7)	74.9(3)	O(1)-Eu(1)-O(2)	52.4(3)
O(5)-Eu(1)-O(4)	95.3(3)	O(5)-Eu(1)-O(3)	68.4(3)
O(3)-Eu(1)-O(4)	121.1(2)	O(3)-Eu(1)-O(3)	73.6(2)
O(6)-Eu(1)-O(4)	71.8(3)	O(6)-Eu(1)-O(3)	70.3(2)
O(8)-Eu(1)-O(4)	146.4(3)	O(8)-Eu(1)-O(3)	142.5(3)
O(7)-Eu(1)-O(4)	71.5(3)	O(7)-Eu(1)-O(3)	105.4(3)
O(5)-Eu(1)-O(1)	147.5(3)	O(4)-Eu(1)-O(3)	50.6(2)
O(3)-Eu(1)-O(1)	132.2(2)	O(1)-Eu(1)-O(3)	125.9(3)
O(6)-Eu(1)-O(1)	74.8(3)	O(2)-Eu(1)-O(3)	137.8(3)

Πίνακας Π1-6: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-9**

Μήκη δεσμών (Å) της ένωσης UCY-9

Gd(1)-O(5)	2.348(6)	Gd(1)-O(7)	2.39(2)
Gd(1)-O(4)	2.367(6)	Gd(1)-O(1)	2.404(7)
Gd(1)-O(8A)	2.38(7)	Gd(1)-O(3)	2.435(7)
Gd(1)-O(8)	2.39(2)	Gd(1)-O(2)	2.548(7)
Gd(1)-O(6)	2.392(6)	Gd(1)-O(4)1	2.669(6)

Γωνίες δεσμών (º) της ένωσης UCY-9

O(5)-Gd(1)-O(4)	74.3(2)	O(8)-Gd(1)-O(1)	88.9(4)
O(5)-Gd(1)-O(8A)	135.0(2)	O(6)-Gd(1)-O(1)	141.9(3)
O(4)-Gd(1)-O(8A)	76(2)	O(7)-Gd(1)-O(1)	70.8(3)
O(5)-Gd(1)-O(8)	135.0(5)	O(5)-Gd(1)-O(3)	75.2(2)
O(4)-Gd(1)-O(8)	83.8(4)	O(4)-Gd(1)-O(3)	124.8(2)
O(8A)-Gd(1)-O(8)	11(2)	O(8A)-Gd(1)-O(3)	149(2)
O(5)-Gd(1)-O(6)	134.8(2)	O(8)-Gd(1)-O(3)	146.4(4)
O(4)-Gd(1)-O(6)	79.9(2)	O(6)-Gd(1)-O(3)	90.7(2)
O(8A)-Gd(1)-O(6)	70(2)	O(7)-Gd(1)-O(3)	73.7(3)
O(8)-Gd(1)-O(6)	76.4(4)	O(1)-Gd(1)-O(3)	82.4(2)
O(5)-Gd(1)-O(7)	139.2(3)	O(5)-Gd(1)-O(2)	70.3(3)
O(4)-Gd(1)-O(7)	146.2(3)	O(4)-Gd(1)-O(2)	82.9(2)
O(8A)-Gd(1)-O(7)	77(2)	O(8A)-Gd(1)-O(2)	74(2)
O(8)-Gd(1)-O(7)	72.8(5)	O(8)-Gd(1)-O(2)	68.2(5)
O(6)-Gd(1)-O(7)	71.3(3)	O(6)-Gd(1)-O(2)	142.0(3)
O(5)-Gd(1)-O(1)	79.5(3)	O(7)-Gd(1)-O(2)	109.4(3)
O(4)-Gd(1)-O(1)	134.0(2)	O(1)-Gd(1)-O(2)	52.6(3)
O(8A)-Gd(1)-O(1)	99(2)	O(3)-Gd(1)-O(2)	126.7(2)
O(6)-Gd(1)-O(4)	68.4(2)	O(5)-Gd(1)-O(4)	69.7(2)
O(7)-Gd(1)-O(4)	108.0(3)	O(4)-Gd(1)-O(4)	75.9(2)
O(1)-Gd(1)-O(4)	128.3(3)	O(8A)-Gd(1)-O(4)	133(2)
O(3)-Gd(1)-O(4)	50.6(2)	O(8)-Gd(1)-O(4)	141.8(4)

Πίνακας Π1-7: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-10**

Μήκη δεσμών (Å) της ένωσης UCY-10

Tb(1)-O(3)1	2.324(5)	Tb(1)-O(8)	2.438(5)
Tb(1)-O(6)	2.341(5)	Tb(1)-O(2)	2.440(5)
Tb(1)-O(7)	2.365(7)	Tb(1)-O(1)	2.484(5)
Tb(1)-O(5)	2.378(4)	Tb(1)-O(3)	2.658(4)
Tb(1)-O(4)	2.409(5)		

Γωνίες δεσμών (º) της ένωσης UCY-10

O(3)1-Tb(1)-O(6)	79.2(2)	O(5)-Tb(1)-O(2)	75.3(2)
O(3)1-Tb(1)-O(7)	86.4(2)	O(4)-Tb(1)-O(2)	79.8(2)
O(6)-Tb(1)-O(7)	75.4(2)	O(8)-Tb(1)-O(2)	71.3(2)
O(3)1-Tb(1)-O(5)	73.7(2)	O(3)1-Tb(1)-O(1)	83.0(2)
O(6)-Tb(1)-O(5)	134.1(2)	O(6)-Tb(1)-O(1)	141.6(2)
O(7)-Tb(1)-O(5)	137.2(2)	O(7)-Tb(1)-O(1)	69.8(2)
O(3)1-Tb(1)-O(4)	122.8(1)	O(5)-Tb(1)-O(1)	70.5(2)
O(6)-Tb(1)-O(4)	92.3(2)	O(4)-Tb(1)-O(1)	125.8(2)
O(7)-Tb(1)-O(4)	146.2(2)	O(8)-Tb(1)-O(1)	109.2(2)
O(5)-Tb(1)-O(4)	73.0(2)	O(2)-Tb(1)-O(1)	53.1(2)
O(3)1-Tb(1)-O(8)	150.3(2)	O(3)1-Tb(1)-O(3)	74.0(2)
O(6)-Tb(1)-O(8)	74.7(2)	O(6)-Tb(1)-O(3)	67.7(2)
O(7)-Tb(1)-O(8)	73.5(2)	O(7)-Tb(1)-O(3)	140.6(2)
O(5)-Tb(1)-O(8)	135.6(2)	O(5)-Tb(1)-O(3)	69.5(2)
O(4)-Tb(1)-O(8)	72.9(2)	O(4)-Tb(1)-O(3)	51.1(2)
O(3)1-Tb(1)-O(2)	132.7(2)	O(8)-Tb(1)-O(3)	108.1(2)
O(6)-Tb(1)-O(2)	146.0(2)	O(2)-Tb(1)-O(3)	125.5(2)
O(7)-Tb(1)-O(2)	92.9(2)	O(1)-Tb(1)-O(3)	138.0(2)

Πίνακας Π1-8: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-11**

Μήκη δεσμών (Å) της ένωσης UCY-11

Dy(1)-O(4)	2.31(2)	Dy(1)-O(3)	2.40(2)
Dy(1)-O(6)	2.33(2)	Dy(1)-O(7)	2.41(2)
Dy(1)-O(8)	2.34(2)	Dy(1)-O(2)	2.49(2)
Dy(1)-O(5)	2.35(2)	Dy(1)-O(4)1	2.67(2)
Dy(1)-O(1)	2.40(2)		

Γωνίες δεσμών (º) της ένωσης UCY-11

O(4)-Dy(1)-O(6)	74.8(3)	O(5)-Dy(1)-O(7)	72.6(4)
O(4)-Dy(1)-O(8)	82.2(5)	O(1)-Dy(1)-O(7)	71.3(5)
O(6)-Dy(1)-O(8)	135.2(6)	O(3)-Dy(1)-O(7)	75.0(6)
O(4)-Dy(1)-O(5)	79.9(4)	O(4)-Dy(1)-O(2)	83.8(4)
O(6)-Dy(1)-O(5)	134.8(3)	O(6)-Dy(1)-O(2)	70.7(4)
O(8)-Dy(1)-O(5)	75.6(6)	O(8)-Dy(1)-O(2)	69.0(6)
O(4)-Dy(1)-O(1)	133.5(5)	O(5)-Dy(1)-O(2)	142.7(4)
O(6)-Dy(1)-O(1)	76.4(4)	O(1)-Dy(1)-O(2)	52.3(5)
O(8)-Dy(1)-O(1)	93.7(7)	O(3)-Dy(1)-O(2)	126.2(4)
O(5)-Dy(1)-O(1)	143.8(5)	O(7)-Dy(1)-O(2)	107.1(5)
O(4)-Dy(1)-O(3)	124.1(4)	O(4)-Dy(1)-O(4)1	74.8(4)
O(6)-Dy(1)-O(3)	74.4(4)	O(6)-Dy(1)-O(4)1	69.6(3)
O(8)-Dy(1)-O(3)	148.0(5)	O(8)-Dy(1)-O(4)1	139.4(6)
O(5)-Dy(1)-O(3)	90.4(4)	O(5)-Dy(1)-O(4)1	67.9(3)
O(1)-Dy(1)-O(3)	80.8(5)	O(1)-Dy(1)-O(4)1	126.4(5)
O(4)-Dy(1)-O(7)	146.8(4)	O(3)-Dy(1)-O(4)1	51.1(3)
O(6)-Dy(1)-O(7)	138.3(5)	O(7)-Dy(1)-O(4)1	110.2(5)
O(8)-Dy(1)-O(7)	73.4(6)	O(2)-Dy(1)-O(4)1	138.5(4)

Πίνακας Π1-9: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-12**

Μήκη δεσμών (Å) της ένωσης UCY-12

Ho(1)-O(4)	2.30(2)	Ho(1)-O(3)	2.38(2)
Ho(1)-O(7)	2.31(2)	Ho(1)-O(8)	2.39(2)
Ho(1)-O(5)	2.32(2)	Ho(1)-O(7A)	2.42(4)
Ho(1)-O(6)1	2.34(2)	Ho(1)-O(2)	2.52(2)
Ho(1)-O(1)	2.38(2)	Ho(1)-O(4)1	2.67(2)

Γωνίες δεσμών (º) της ένωσης UCY-12

O(4)-Ho(1)-O(7)	84.0(6)	O(6)-Ho(1)-O(8)	71.4(4)
O(4)-Ho(1)-O(5)	75.4(4)	O(1)-Ho(1)-O(8)	70.8(5)
O(7)-Ho(1)-O(5)	135.0(6)	O(3)-Ho(1)-O(8)	74.7(5)
O(4)-Ho(1)-O(6)	80.2(4)	O(4)-Ho(1)-O(7A)	74(2)
O(7)-Ho(1)-O(6)	78.1(7)	O(7)-Ho(1)-O(7A)	11(2)
O(5)-Ho(1)-O(6)	134.7(4)	O(5)-Ho(1)-O(7A)	134(2)
O(4)-Ho(1)-O(1)	134.1(4)	O(6)-Ho(1)-O(7A)	71(2)
O(7)-Ho(1)-O(1)	89.0(7)	O(1)-Ho(1)-O(7A)	100(2)
O(5)-Ho(1)-O(1)	78.3(4)	O(3)-Ho(1)-O(7A)	150(2)
O(6)-Ho(1)-O(1)	142.1(4)	O(8)-Ho(1)-O(7A)	78(2)
O(4)-Ho(1)-O(3)	125.6(4)	O(4)-Ho(1)-O(2)	83.0(4)
O(7)-Ho(1)-O(3)	145.4(6)	O(7)-Ho(1)-O(2)	67.8(6)
O(5)-Ho(1)-O(3)	75.7(4)	O(5)-Ho(1)-O(2)	70.3(4)
O(6)-Ho(1)-O(3)	88.9(4)	O(6)-Ho(1)-O(2)	143.3(4)
O(1)-Ho(1)-O(3)	81.9(4)	O(1)-Ho(1)-O(2)	52.7(4)
O(4)-Ho(1)-O(8)	145.1(4)	O(3)-Ho(1)-O(2)	127.1(4)
O(7)-Ho(1)-O(8)	70.8(7)	O(8)-Ho(1)-O(2)	107.9(5)
O(5)-Ho(1)-O(8)	139.5(4)	O(7A)-Ho(1)-O(2)	73(2)
O(1)-Ho(1)-O(4)	127.8(4)	O(4)-Ho(1)-O(4)	75.6(4)
O(3)-Ho(1)-O(4)	51.4(3)	O(7)-Ho(1)-O(4)	142.3(6)
O(8)-Ho(1)-O(4)	110.3(5)	O(5)-Ho(1)-O(4)	69.6(4)
O(7A)-Ho(1)-O(4)	132(2)	O(6)-Ho(1)-O(4)	67.6(4)

Πίνακας Π1-10: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **CeCAP**

Μήκη δεσμών (Å) της ένωσης CeCAP

Ce(1)-O(4)	2.4(2)	Ce(1)-O(7)	2.5(2)
Ce(1)-O(6)	2.5(2)	Ce(1)-O(5)	2.5(2)
Ce(1)-O(8)	2.5(2)	Ce(1)-O(1)	2.6(2)
Ce(1)-O(3)	2.5(2)	Ce(1)-O(6)	2.7(2)
Ce(1)-O(2)	2.5(2)		

Γωνίες δεσμών (º) της ένωσης CeCAP

O(4)-Ce(1)-O(6)	73(7)	O(8)-Ce(1)-O(5)	148(2)
O(4)-Ce(1)-O(3)	134(7)	O(2)-Ce(1)-O(5)	82(8)
O(6)-Ce(1)-O(3)	80(7)	O(7)-Ce(1)-O(5)	74(10)
O(4)-Ce(1)-O(8)	136(2)	O(4)-Ce(1)-O(1)	71(8)
O(6)-Ce(1)-O(8)	83(2)	O(6)-Ce(1)-O(1)	85(7)
O(3)-Ce(1)-O(8)	75(10)	O(3)-Ce(1)-O(1)	143(9)
O(4)-Ce(1)-O(2)	80(9)	O(8)-Ce(1)-O(1)	70(10)
O(6)-Ce(1)-O(2)	134(7)	O(2)-Ce(1)-O(1)	51(8)
O(3)-Ce(1)-O(2)	142(9)	O(7)-Ce(1)-O(1)	109(2)
O(8)-Ce(1)-O(2)	92(2)	O(5)-Ce(1)-O(1)	125(7)
O(4)-Ce(1)-O(7)	140(2)	O(4)-Ce(1)-O(6)	70(7)
O(6)-Ce(1)-O(7)	147(9)	O(6)-Ce(1)-O(6)	76(7)
O(3)-Ce(1)-O(7)	71(9)	O(3)-Ce(1)-O(6)	68(7)
O(8)-Ce(1)-O(7)	74(2)	O(8)-Ce(1)-O(6)	140(12)
O(2)-Ce(1)-O(7)	72(2)	O(2)-Ce(1)-O(6)	127(8)
O(4)-Ce(1)-O(5)	74(8)	O(7)-Ce(1)-O(6)	106(9)
O(6)-Ce(1)-O(5)	123(7)	O(5)-Ce(1)-O(6)	49(6)
O(3)-Ce(1)-O(5)	91(9)	O(1)-Ce(1)-O(6)	140(8)

Πίνακας Π1-11: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **PrCAP**

Μήκη δεσμών (Å) της ένωσης PrCAP

O(1)-Pr(1)	2.543(6)	O(5)-Pr(1)	2.678(5)
O(2)-Pr(1)	2.563(8)	O(6)-Pr(1)	2.528(5)
O(3)-Pr(1)	2.440(6)	O(7)-Pr(1)	2.480(7)
O(4)-Pr(1)	2.441(5)	O(8)-Pr(1)	2.484(8)
O(5)-Pr(1)	2.434(5)	Pr(1)-O(5)	2.678(5)

Γωνίες δεσμών (º) της ένωσης PrCAP

O(5)-Pr(1)-O(3)	73.5(2)	O(7)-Pr(1)-O(1)	73.3(3)
O(5)-Pr(1)-O(4)	78.9(2)	O(8)-Pr(1)-O(1)	92.0(4)
O(3)-Pr(1)-O(4)	133.0(2)	O(6)-Pr(1)-O(1)	83.6(2)
O(5)-Pr(1)-O(7)	148.3(3)	O(5)-Pr(1)-O(2)	84.4(3)
O(3)-Pr(1)-O(7)	137.4(3)	O(3)-Pr(1)-O(2)	70.2(3)
O(4)-Pr(1)-O(7)	73.0(3)	O(4)-Pr(1)-O(2)	143.6(3)
O(5)-Pr(1)-O(8)	84.7(3)	O(7)-Pr(1)-O(2)	110.1(3)
O(3)-Pr(1)-O(8)	138.9(3)	O(8)-Pr(1)-O(2)	73.3(3)
O(4)-Pr(1)-O(8)	73.1(3)	O(6)-Pr(1)-O(2)	123.8(2)
O(7)-Pr(1)-O(8)	73.5(3)	O(1)-Pr(1)-O(2)	48.7(3)
O(5)-Pr(1)-O(6)	122.6(2)	O(5)-Pr(1)-O(5)	74.7(2)
O(3)-Pr(1)-O(6)	72.5(2)	O(3)-Pr(1)-O(5)	67.8(2)
O(4)-Pr(1)-O(6)	92.2(2)	O(4)-Pr(1)-O(5)	68.5(2)
O(7)-Pr(1)-O(6)	73.5(3)	O(7)-Pr(1)-O(5)	107.3(3)
O(8)-Pr(1)-O(6)	146.6(2)	O(8)-Pr(1)-O(5)	139.1(4)
O(5)-Pr(1)-O(1)	131.3(2)	O(6)-Pr(1)-O(5)	50.0(2)
O(3)-Pr(1)-O(1)	78.0(2)	O(1)-Pr(1)-O(5)	128.0(2)
O(4)-Pr(1)-O(1)	145.8(2)	O(2)-Pr(1)-O(5	136.9(2)

Πίνακας Π1-12: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **NdCAP**

Μήκη δεσμών (Å) της ένωσης NdCAP

Nd(1)-O(8)	2.396(8)	Nd(1)-O(6)	2.488(9)
Nd(1)-O(1)	2.415(7)	Nd(1)-O(7)	2.502(8)
Nd(1)-O(2)	2.440(7)	Nd(1)-O(5)	2.558(9)
Nd(1)-O(3)	2.448(11)	Nd(1)-O(1)	2.657(7)
Nd(1)-O(4)	2.471(11)	O(1)-Nd(1)	2.657(7)

Γωνίες δεσμών (º) της ένωσης NdCAP

O(8)-Nd(1)-O(1)	72.5(3)	O(3)-Nd(1)-O(7)	147.2(4)
O(8)-Nd(1)-O(2)	133.2(3)	O(4)-Nd(1)-O(7)	74.1(4)
O(1)-Nd(1)-O(2)	79.3(3)	O(6)-Nd(1)-O(7)	82.1(3)
O(8)-Nd(1)-O(3)	137.0(4)	O(8)-Nd(1)-O(5)	70.4(4)
O(1)-Nd(1)-O(3)	83.2(4)	O(1)-Nd(1)-O(5)	84.3(3)
O(2)-Nd(1)-O(3)	72.8(5)	O(2)-Nd(1)-O(5)	142.9(4)
O(8)-Nd(1)-O(4)	139.4(4)	O(3)-Nd(1)-O(5)	72.3(5)
O(1)-Nd(1)-O(4)	147.6(3)	O(4)-Nd(1)-O(5)	109.5(5)
O(2)-Nd(1)-O(4)	72.2(3)	O(6)-Nd(1)-O(5)	52.0(4)
O(3)-Nd(1)-O(4)	73.9(5)	O(7)-Nd(1)-O(5)	125.9(3)
O(8)-Nd(1)-O(6)	79.2(3)	O(8)-Nd(1)-O(1)	69.6(3)
O(1)-Nd(1)-O(6)	134.1(3)	O(1)-Nd(1)-O(1)	74.6(3)
O(2)-Nd(1)-O(6)	143.6(3)	O(2)-Nd(1)-O(1)	67.3(3)
O(3)-Nd(1)-O(6)	94.4(5)	O(3)-Nd(1)-O(1)	137.0(4)
O(4)-Nd(1)-O(6)	71.5(4)	O(4)-Nd(1)-O(1)	107.2(4)
O(8)-Nd(1)-O(7)	74.6(3)	O(6)-Nd(1)-O(1)	127.4(3)
O(1)-Nd(1)-O(7)	122.2(3)	O(7)-Nd(1)-O(1)	49.8(2)
O(2)-Nd(1)-O(7)	90.8(3)	O(5)-Nd(1)-O(1)	138.8(4)

Πίνακας Π1-13: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **GdCAP**

Μήκη δεσμών (Å) της ένωσης GdCAP

Gd(1)-O(4)	2.359(5)	Gd(1)-O(6)	2.441(5)
Gd(1)-O(5)	2.362(5)	Gd(1)-O(2)	2.459(6)
Gd(1)-O(3)	2.391(5)	Gd(1)-O(1)	2.508(6)
Gd(1)-O(8)	2.423(9)	Gd(1)-O(5)	2.637(5)
Gd(1)-O(7)	2.436(7)		

Γωνίες δεσμών (º) της ένωσης GdCAP

O(4)-Gd(1)-O(5)	74.1(2)	O(8)-Gd(1)-O(2)	94.9(3)
O(4)-Gd(1)-O(3)	133.7(2)	O(7)-Gd(1)-O(2)	71.7(3)
O(5)-Gd(1)-O(3)	79.6(2)	O(6)-Gd(1)-O(2)	81.2(2)
O(4)-Gd(1)-O(8)	135.7(2)	O(4)-Gd(1)-O(1)	70.8(2)
O(5)-Gd(1)-O(8)	81.3(2)	O(5)-Gd(1)-O(1)	85.3(2)
O(3)-Gd(1)-O(8)	74.5(3)	O(3)-Gd(1)-O(1)	143.8(2)
O(4)-Gd(1)-O(7)	138.8(2)	O(8)-Gd(1)-O(1)	70.8(3)
O(5)-Gd(1)-O(7)	146.6(2)	O(7)-Gd(1)-O(1)	108.4(3)
O(3)-Gd(1)-O(7)	71.6(2)	O(6)-Gd(1)-O(1)	125.9(2)
O(8)-Gd(1)-O(7)	75.2(3)	O(2)-Gd(1)-O(1)	51.6(2)
O(4)-Gd(1)-O(6)	75.3(2)	O(4)-Gd(1)-O(5)	69.1(2)
O(5)-Gd(1)-O(6)	123.8(2)	O(5)-Gd(1)-O(5)	74.7(2)
O(3)-Gd(1)-O(6)	89.4(2)	O(3)-Gd(1)-O(5)	67.6(2)
O(8)-Gd(1)-O(6)	147.7(2)	O(8)-Gd(1)-O(5)	138.0(3)
O(7)-Gd(1)-O(6)	73.1(2)	O(7)-Gd(1)-O(5)	108.0(2)
O(4)-Gd(1)-O(2)	78.0(2)	O(6)-Gd(1)-O(5)	50.6(2)
O(5)-Gd(1)-O(2)	134.5(2)	O(2)-Gd(1)-O(5)	126.4(2)
O(3)-Gd(1)-O(2)	143.2(2)	O(1)-Gd(1)-O(5)	138.7(2)

Πίνακας Π1-14: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **CeN-BDC**

Μήκη δεσμών (Å) της ένωσης CeN-BDC

Ce(1)-O(3)	2.441(4)	Ce(1)-O(4)	2.519(4)
Ce(1)-O(5)	2.465(4)	Ce(1)-O(2)	2.543(4)
Ce(1)-O(6)	2.476(4)	Ce(1)-O(1)	2.548(4)
Ce(1)-O(7)	2.507(5)	Ce(1)-O(3)	2.753(4)
Ce(1)-O(8)	2.511(5)		

Γωνίες δεσμών (º) της ένωσης CeN-BDC

O(3)-Ce(1)-O(5)	74.1(2)	O(7)-Ce(1)-O(2)	101.1(2)
O(3)-Ce(1)-O(6)	77.0(2)	O(8)-Ce(1)-O(2)	75.4(2)
O(5)-Ce(1)-O(6)	132.9(2)	O(4)-Ce(1)-O(2)	78.4(2)
O(3)-Ce(1)-O(7)	82.8(2)	O(3)-Ce(1)-O(1)	90.4(2)
O(5)-Ce(1)-O(7)	136.2(2)	O(5)-Ce(1)-O(1)	73.5(2)
O(6)-Ce(1)-O(7)	73.9(2)	O(6)-Ce(1)-O(1)	143.0(2)
O(3)-Ce(1)-O(8)	145.8(2)	O(7)-Ce(1)-O(1)	70.0(2)
O(5)-Ce(1)-O(8)	139.9(2)	O(8)-Ce(1)-O(1)	102.8(2)
O(6)-Ce(1)-O(8)	73.6(2)	O(4)-Ce(1)-O(1)	126.8(2)
O(7)-Ce(1)-O(8)	72.7(2)	O(2)-Ce(1)-O(1)	50.5(2)
O(3) -Ce(1)-O(4)	123.2(2)	O(3)-Ce(1)-O(3)	74.6(2)
O(5)-Ce(1)-O(4)	78.0(2)	O(5)-Ce(1)-O(3)	67.9(2)
O(6)-Ce(1)-O(4)	88.1(2)	O(6)-Ce(1)-O(3)	69.0(2)
O(7)-Ce(1)-O(4)	144.6(2)	O(7)-Ce(1)-O(3)	139.9(2)
O(8)-Ce(1)-O(4)	73.0(2)	O(8)-Ce(1)-O(3)	109.7(2)
O(3)-Ce(1)-O(2)	134.0(2)	O(4)-Ce(1)-O(3)	49.2(2)
O(5)-Ce(1)-O(2)	72.1(2)	O(2)-Ce(1)-O(3)	118.4(2)
O(6)-Ce(1)-O(2)	148.5(2)	O(1)-Ce(1)-O(3)	141.1(2)

2. Μήκη και γωνίες δεσμών των τροποποιημένων ενώσεων UCY-2, UCY-3, UCY-5, UCY-8, UCY-9, EuN-BDC, CeN-BDC και GdN-BDC

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων UCY-2

Πίνακας Π2-1: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/Ακετόνη

Μήκη δεσμών (Å) της ένωσης UCY-2/Ακετόνη

Nd(1)-O(6)	2.413(5)	Nd(1)-O(7)	2.492(7)
Nd(1)-O(5)	2.414(4)	Nd(1)-O(1)	2.496(5)
Nd(1)-O(4)	2.417(5)	Nd(1)-O(2)	2.509(5)
Nd(1)-O(8)	2.459(9)	Nd(1)-O(4)	2.695(4)
Nd(1)-O(3)	2.486(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/Ακετόνη

O(6)-Nd(1)-O(5)	133.7(2)	O(8)-Nd(1)-O(1)	71.9(2)
O(6)- d(1)-O(4)	72.4(2)	O(3)-Nd(1)-O(1)	79.2(2)
O(5)-Nd(1)-O(4)	80.5(2)	O(7)-Nd(1)-O(1)	100.2(3)
O(6)-Nd(1)-O(8)	139.8(2)	O(6)-Nd(1)-O(2)	72.3(2)
O(5)-Nd(1)-O(8)	73.0(2)	O(5)-Nd(1)-O(2)	142.9(2)
O(4)-Nd(1)-O(8)	147.7(2)	O(4)-Nd(1)-O(2)	85.9(2)
O(6)-Nd(1)-O(3)	75.4(2)	O(8)-Nd(1)-O(2)	104.3(3)
O(5)-Nd(1)-O(3)	89.6(2)	O(3)-Nd(1)-O(2)	126.3(1)
O(4)-Nd(1)-O(3)	122.9(2)	O(7)-Nd(1)-O(2)	70.5(2)
O(8)-Nd(1)-O(3)	75.6(3)	O(1)-Nd(1)-O(2)	52.0(1)
O(6)-Nd(1)-O(7)	134.6(2)	O(6)-Nd(1)-O(4)	70.2(1)
O(5)-Nd(1)-O(7)	73.2(2)	O(5)-Nd(1)-O(4)	66.8(2)
O(4)-Nd(1)-O(7)	79.9(2)	O(4)-Nd(1)-O(4)	75.1(2)
O(8)-Nd(1)-O(7)	75.1(3)	O(8)-Nd(1)-O(4)	109.6(3)
O(3)-Nd(1)-O(7)	149.3(2)	O(3)-Nd(1)-O(4)	49.9(2)
O(6)-Nd(1)-O(1)	75.8(2)	O(7)-Nd(1)-O(4)	135.5(2)
O(5)-Nd(1)-O(1)	144.8(2)	O(1)-Nd(1)-O(4)	123.7(2)
O(4)-Nd(1)-O(1)	133.4(2)	O(2)-Nd(1)-O(4)	141.5(2)

Πίνακας Π2-2: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/EtOH

Μήκη δεσμών (Å) της ένωσης UCY-2/EtOH

Nd(1)-O(5)	2.413(4)	Nd(1)-O(1)	2.509(4)
Nd(1)-O(4)	2.418(4)	Nd(1)-O(8)	2.516(6)
Nd(1)-O(6)	2.434(5)	Nd(1)-O(2)	2.518(5)
Nd(1)-O(3)	2.473(5)	Nd(1)-O(4)	2.710(4)
Nd(1)-O(7)	2.498(6)		

Γωνίες δεσμών (º) της ένωσης UCY-2/EtOH

O(5)-Nd(1)-O(4)	80.4(2)	O(3)-Nd(1)-O(8)	74.7(2)
O(5)-Nd(1)-O(6)	133.2(2)	O(7)-Nd(1)-O(8)	73.7(2)
O(4)-Nd(1)-O(6)	71.6(2)	O(1)-Nd(1)-O(8)	103.9(2)
O(5)-Nd(1)-O(3)	90. (2)	O(5)-Nd(1)-O(2)	146.1(2)
O(4)-Nd(1)-O(3)	122.9(2)	O(4)-Nd(1)-O(2)	132.6(2)
O(6)-Nd(1)-O(3)	75.5(2)	O(6)-Nd(1)-O(2)	74.9(2)
O(5)-Nd(1)-O(7)	75.6(2)	O(3)-Nd(1)-O(2)	78.2(2)
O(4)-Nd(1)-O(7)	83.6(2)	O(7)-Nd(1)-O(2)	97.6(2)
O(6)-Nd(1)-O(7)	134.7(2)	O(1)-Nd(1)-O(2)	52.1(2)
O(3)-Nd(1)-O(7)	148.0(2)	O(8)-Nd(1)-O(2)	72.8(2)
O(5)-Nd(1)-O(1)	141.9(2)	O(5)-Nd(1)-O(4)	67.4(2)
O(4)-Nd(1)-O(1)	86.3(2)	O(4)-Nd(1)-O(4)	74.8(2)
O(6)-Nd(1)-O(1)	73.4(2)	O(6)-Nd(1)-O(4)	69.5(2)
O(3)-Nd(1)-O(1)	126.4(2)	O(3)-Nd(1)-O(4)	50.2(2)
O(7)-Nd(1)-O(1)	67.6(2)	O(7)-Nd(1)-O(4)	139.5(2)
O(5)-Nd(1)-O(8)	73.4(2)	O(1)-Nd(1)-O(4)	142.1(2)
O(4)-Nd(1)-O(8)	148.7(2)	O(8)-Nd(1)-O(4)	109.3(2)
O(6)-Nd(1)-O(8)	139.6(2)	O(2)-Nd(1)-O(4)	122.3(2)

Πίνακας Π2-3: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/MeOH

Μήκη δεσμών (Å) της ένωσης UCY-2/MeOH

Nd(1)-O(5)	2.404(5)	Nd(1)-O(7)	2.490(8)
Nd(1)-O(4)	2.421(6)	Nd(1)-O(2)	2.491(6)
Nd(1)-O(6)	2.430(6)	Nd(1)-O(1)	2.537(6)
Nd(1)-O(3)	2.473(7)	Nd(1)-O(4)	2.689(5)
Nd(1)-O(8)	2.483(8)		

Γωνίες δεσμών (º) της ένωσης UCY-2/MeOH

O(5)-Nd(1)-O(4)	80.0(2)	O(3)-Nd(1)-O(2)	124.6(2)
O(5)-Nd(1)-O(6)	133.1(2)	O(8)-Nd(1)-O(2)	101.9(3)
O(4)-Nd(1)-O(6)	71.8(2)	O(7)-Nd(1)-O(2)	68.1(3)
O(5)-Nd(1)-O(3)	90.7(2)	O(5)-Nd(1)-O(1)	146.2(2)
O 4)-Nd(1)-O(3)	122.8(2)	O(4)-Nd(1)-O(1)	133.4(2)
O(6)-Nd(1)-O(3)	75.1(2)	O(6)-Nd(1)-O(1)	73.7(2)
O(5)-Nd(1)-O(8)	75.4(2)	O(3)-Nd(1)-O(1)	75.7(2)
O(4)-Nd(1)-O(8)	150.4(2)	O(8)-Nd(1)-O(1)	71.1(2)
O(6)-Nd(1)-O(8)	137.8(2)	O(7)-Nd(1)-O(1)	100.1(3)
O(3)-Nd(1)-O(8)	74.3(3)	O(2)-Nd(1)-O(1)	52.4(2)
O(5)-Nd(1)-O(7)	75.8(2)	O(5)-Nd(1)-O(4)	67.2(2)
O(4)-Nd(1)-O(7)	82.8(3)	O(4)-Nd(1)-O(4)	74.3(2)
O(6)-Nd(1)-O(7)	134.1(2)	O(6)-Nd(1)-O(4)	69.4(2)
O(3)-Nd(1)-O(7)	149.0(3)	O(3)-Nd(1)-O(4)	50.7(2)
O(8)-Nd(1)-O(7)	75.3(3)	O(8)-Nd(1)-O(4)	110.2(3)
O(5)-Nd(1)-O(2)	143.1(2)	O(7)-Nd(1)-O(4)	139.0(2)
O(4)-Nd(1)-O(2)	87.9(2)	O(2)-Nd(1)-O(4)	142.0(2)
O(6)-Nd(1)-O(2)	73.2(2)	O(1)-Nd(1)-O(4)	120.4(2)

Πίνακας Π2-4: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/THF

Μήκη δεσμών (Å) της ένωσης UCY-2/THF

Nd(1)-O(4)	2.408(4)	Nd(1)-O(1)	2.511(5)
Nd(1)-O(5)	2.417(4)	Nd(1)-O(7)	2.524(6)
Nd(1)-O(6)	2.425(4)	Nd(1)-O(8)	2.537(6)
Nd(1)-O(3)	2.473(5)	Nd(1)-O(4)	2.693(4)
Nd(1)-O(2)	2.495(4)		

Γωνίες δεσμών (º) της ένωσης UCY-2/THF

O(4)-Nd(1)-O(5)	72.5(2)	O(3)-Nd(1)-O(7)	78.0(2)
O(4)-Nd(1)-O(6)	80.0(2)	O(2)-Nd(1)-O(7)	70.9(2)
O(5)-Nd(1)-O(6)	132.9(2)	O(1)-Nd(1)-O(7)	102.4(2)
O(4)-Nd(1)-O(3)	123.2(2)	O(4)-Nd(1)-O(8)	80.4(2)
O(5)-Nd(1)-O(3)	76.0(2)	O(5)-Nd(1)-O(8	134.7(2)
O(6)-Nd(1)-O(3)	88.9(2)	O(6)-Nd(1)-O(8)	74.2(2)
O(4)-Nd(1)-O(2)	134.4(2)	O(3)-Nd(1)-O(8)	148.6(2)
O(5)-Nd(1)-O(2)	77.0(2)	O(2)-Nd(1)-O(8)	98.9(2)
O(6)-Nd(1)-O(2)	144.3(2)	O(1)-Nd(1)-O(8)	70.3(2)
O(3)-Nd(1)-O(2)	79.4(2)	O(7)-Nd(1)-O(8)	72.0(2)
O(4)-Nd(1)-O(1)	86.1(2)	O(4)-Nd(1)-O(4)	74.7(2)
O(5)-Nd(1)-O(1)	72.2(2)	O(5)-Nd(1)-O(4)	69.2(2)
O(6)-Nd(1)-O(1)	143.5(2)	O(6)-Nd(1)-O(4)	66.9(2)
O(3)-Nd(1)-O(1)	126.4(2)	O(3)-Nd(1)-O(4)	50.3(2)
O(2)-Nd(1)-O(1)	52.3(2)	O(2)-Nd(1)-O(4)	124.0(2)
O(4)-Nd(1)-O(7)	145.9(2)	O(1)-Nd(1)-O(4)	140.5(2)
O(5)-Nd(1)-O(7)	141.6(2)	O(7)-Nd(1)-O(4)	113.0(2)
O(6)-Nd(1)-O(7)	73.7(2)	O(8)-Nd(1)-O(4)	136.5(2)

Πίνακας Π2-5: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/py

Μήκη δεσμών (Å) της ένωσης UCY-2/py

Nd(1)-O(4)	2.366(5)	Nd(1)-O(1)	2.485(5)
Nd(1)-O(7)	2.379(5)	Nd(1)-O(2)	2.573(5)
Nd(1)-O(8)	2.457(5)	Nd(1)-N(3)	2.673(9)
Nd(1)-O(13)	2.460(6)	Nd(1)-O(4)	2.857(5)
Nd(1)-O(3)	2.471(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/py

O(4)-Nd(1)-O(7)	74.0( )	O(13)-Nd(1)-O(2)	73.6(2)
O(4)-Nd(1)-O(8)	79.3(2)	O(3)-Nd(1)-O(2)	128.1(2)
O(7)-Nd(1)-O(8)	131.7(2)	O(1)-Nd(1)-O(2)	51.8(2)
O(4)-Nd(1)-O(13)	87.5(3)	O(4)-Nd(1)-N(3)	150.9(3)
O(7)-Nd(1)-O(13)	142.3(2)	O(7)-Nd(1)-N(3)	133.7(3)
O(8)-Nd(1)-O(13)	73.6(2)	O(8)-Nd(1)-N(3)	74.3(2)
O(4)-Nd(1)-O(3)	123.9(2)	O(13)-Nd(1)-N(3)	73.6(3)
O(7)-Nd(1)-O(3)	73.7(2)	O(3)-Nd(1)-N(3)	68.5(3)
O(8)-Nd(1)-O(3)	89.7(2)	O(1)-Nd(1)-N(3)	73.2(2)
O(13)-Nd(1)-O(3)	141.5(3)	O(2)-Nd(1)-N(3)	113.6(2)
O(4)-Nd(1)-O(1)	130.4(2)	O(4)-Nd(1)-O(4)	76.8(2)
O(7)-Nd(1)-O(1)	77.4(2)	O(7)-Nd(1)-O(4)	66.2(2)
O(8)-Nd(1)-O(1)	146.9(2)	O(8)-Nd(1)-O(4)	69.0(2)
O(13)-Nd(1)-O(1)	91.4(2)	O(13)-Nd(1)-O(4)	141.5(2)
O(3)-Nd(1)-O(1)	84.1(2)	O(3)-Nd(1)-O(4)	48.3(2)
O(4)-Nd(1)-O(2)	80.7(2)	O(1)-Nd(1)-O(4)	125.6(2)
O(7)-Nd(1)-O(2)	71.2(2)	O(2)-Nd(1)-O(4)	135.8(2)
O(8)-Nd(1)-O(2)	142.1(2)	N(3)-Nd(1)-O(4)	104.2(2)

Πίνακας Π2-6: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/BME

Μήκη δεσμών (Å) της ένωσης UCY-2/BME

Nd(1)-O(3)	2.410(4)	Nd(1)-O(1)	2.500(5)
Nd(1)-O(6)	2.414(4)	Nd(1)-O(7B)	2.51(4)
Nd(1)-O(4)	2.424(4)	Nd(1)-O(8)	2.515(5)
Nd(1)-O(5)	2.487(4)	Nd(1)-O(7A)	2.54(2)
Nd(1)-O(2)	2.492(4)	Nd(1)-O(6)	2.682(4)

Γωνίες δεσμών (º) της ένωσης UCY-2/BME

O(3)-Nd(1)-O(6)	72.2(2)	O(3)-Nd(1)-O(8)	140.4(2)
O(3)-Nd(1)-O(4)	134.1(2)	O(6)-Nd(1)-O(8)	147.4(2)
O(6)-Nd(1)-O(4)	81.7(2)	O(4)-Nd(1)-O(8)	72.6(2)
O(3 -Nd(1)-O(5)	76.7(1)	O(5)-Nd(1)-O(8)	75.6(2)
O(6)-Nd(1)-O(5)	124.2(2)	O(2)-Nd(1)-O(8)	70.4(2)
O(4)-Nd(1)-O(5)	88.5(2)	O(1)-Nd(1)-O(8)	100.7(2)
O(3)-Nd(1)-O(2)	76.3(2)	O(7B)-Nd(1)-O(8)	73.8(2)
O(6)-Nd(1)-O(2)	134.7(2)	O(3)-Nd(1)-O(7A)	135.5(5)
O(4)-Nd(1)-O(2)	142.6(2)	O(6)-Nd(1)-O(7A)	78.1(6)
O(5)-Nd(1)-O(2)	77.3(2)	O(4)-Nd(1)-O(7A)	70.7(3)
O(3)-Nd(1)-O(1)	73.9(2)	O(5)-Nd(1)-O(7A)	147.7(6)
O(6)-Nd(1)-O(1)	87.9(2)	O(2)-Nd(1)-O(7A)	104.2(4)
O(4)-Nd(1)-O(1)	143.1(2)	O(1)-Nd(1)-O(7A)	72.6(3)
O(5)-Nd(1)-O(1)	125.8(2)	O(7B)-Nd(1)-O(7A)	10.9(6)
O(2)-Nd(1)-O(1)	52.1(2)	O(8)-Nd(1)-O(7A)	74.8(6)
O(3)-Nd(1)-O(7B)	130.3(9)	O(3)-Nd(1)-O(6)	69.5(2)
O(6)-Nd(1)-O(7B)	82.8(2)	O(6)-Nd(1)-O(6)	76.0(2)
O(4)-Nd(1)-O(7B)	80.9(5)	O(4)-Nd(1)-O(6)	67.8(2)
O(5)-Nd(1)-O(7B)	149.3(2)	O(5)-Nd(1)-O(6)	49.9(2)
O(2)-Nd(1)-O(7B)	93.9(6)	O(2)-Nd(1)-O(6)	121.5(2)
O(1)-Nd(1)-O(7B)	62.6(6)	O(1)-Nd(1)-O(6)	143.0(2)
O(7B)-Nd(1)-O(6)	144.1(5)	O(7A)-Nd(1)-O(6)	133.4(3)
O(8)-Nd(1)-O(6)	110.9(2)		

Πίνακας Π2-7: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/merpdH_2

Μήκη δεσμών (Å) της ένωσης UCY-2/merpdH_2

Nd(1)-O(3)	2.390(5)	Nd(1)-O(7)	2.488(6)
Nd(1)-O(5)	2.396(4)	Nd(1)-O(8)	2.544(5)
Nd(1)-O(6)	2.404(4)	Nd(1)-O(2)	2.548(4)
Nd(1)-O(4)	2.447(5)	Nd(1)-O(3)	2.717(4)
Nd(1)-O(1)	2.482(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/merpdH_2

O(3)-Nd(1)-O(5)	79.2(2)	O(4)-Nd(1)-O(8)	143.8(2)
O(3)-Nd(1)-O(6)	72.7(2)	O(1)-Nd(1)-O(8)	67.5(2)
O(5)-Nd(1)-O(6)	133.6(2)	O(7)-Nd(1)-O(8)	70.5(2)
O(3)-Nd(1) O(4)	124.3(2)	O(3)-Nd(1)-O(2)	131.8(2)
O(5)-Nd(1)-O(4)	88.1(2)	O(5)-Nd(1)-O(2)	148.1(2)
O(6)-Nd(1)-O(4)	78.7(2)	O(6)-Nd(1)-O(2)	72.8(2)
O(3)-Nd(1)-O(1)	87.5(2)	O(4)-Nd(1)-O(2)	79.7(2)
O(5)-Nd(1)-O(1)	139.3(2)	O(1)-Nd(1)-O(2)	52.0(2)
O(6)-Nd(1)-O(1)	76.0(2)	O(7)-Nd(1)-O(2)	72.6(2)
O(4)-Nd(1)-O(1)	130.1(2)	O(8)-Nd(1)-O(2)	100.6(2)
O(3)-Nd(1)-O(7)	147.6(2)	O(3)-Nd(1)-O(3)	75.4(2)
O(5)-Nd(1)-O(7)	75.9(2)	O(5)-Nd(1)-O(3)	67.3(2)
O(6)-Nd(1)-O(7)	139.6(2)	O(6)-Nd(1)-O(3)	70.3(2)
O(4)-Nd(1)-O(7)	75.4(2)	O(4)-Nd(1)-O(3)	49.9(2)
O(1)-Nd(1)-O(7)	98.0(2)	O(1)-Nd(1)-O(3)	145.4(2)
O(3)-Nd(1)-O(8)	82.6(2)	O(7)-Nd(1)-O(3)	112.6(2)
O(5)-Nd(1)-O(8)	72.6(2)	O(8)-Nd(1)-O(3)	137.0(2)
O(6)-Nd(1)-O(8)	136.5(2)	O(2)-Nd(1)-O(3)	121.6(2)

Πίνακας Π2-8: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/2hpH$_2$

Μήκη δεσμών (Å) της ένωσης UCY-2/2hpH$_2$

Nd(1)-O(5)	2.397(4)	Nd(1)-O(2)	2.498(4)
Nd(1)-O(4)	2.407(4)	Nd(1)-O(8)	2.510(4)
Nd(1)-O(6)	2.439(3)	Nd(1)-O(1)	2.560(4)
Nd(1)-O(3)	2.478(4)	Nd(1)-O(4)	2.670(4)
Nd(1)-O(7)	2.500(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/2hpH$_2$

O(5)-Nd(1)-O(4)	70.88(13)	O(3)-Nd(1)-O(8)	79.7(2)
O(5)-Nd(1)-O(6)	134.8(2)	O(7)-Nd(1)-O(8)	71.5(2)
O(4)-Nd(1)-O(6)	81.1(2)	O(2)-Nd(1)-O(8)	92.4(2)
O(5)-Nd(1)-O(3)	81.1(2)	O(5)-Nd(1)-O(1)	7 .1(2)
O(4)-Nd(1)-O(3)	124.1(2)	O(4)-Nd(1)-O(1)	137.9(2)
O(6)-Nd(1)-O(3)	86.5(2)	O(6)-Nd(1)-O(1)	141.0(2)
O(5)-Nd(1)-O(7)	129.4(2)	O(3)-Nd(1)-O(1)	71.3(2)
O(4)-Nd(1)-O(7)	77.7(2)	O(7)-Nd(1)-O(1)	108.7(2)
O(6)-Nd(1)-O(7)	74.8(2)	O(2)-Nd(1)-O(1)	51.6(2)
O(3)-Nd(1)-O(7)	149.1(2)	O(8)-Nd(1)-O(1)	71.9(2)
O(5)-Nd(1)-O(2)	73.2(2)	O(5)-Nd(1)-O(4)1	70.1(2)
O(4)-Nd(1)-O(2)	95.5(2)	O(4)-Nd(1)-O(4)1	74.6(2)
O(6)-Nd(1)-O(2)	146.1(2)	O(6)-Nd(1)-O(4)1	68.6(2)
O(3)-Nd(1)-O(2)	121.6(2)	O(3)-Nd(1)-O(4)1	50.3(2)
O(7)-Nd(1)-O(2)	71.5(2)	O(7)-Nd(1)-O(4)1	136.7(2)
O(5)-Nd(1)-O(8)	144.8(2)	O(2)-Nd(1)-O(4)1	143.2(2)
O(4)-Nd(1)-O(8)	143.7(2)	O(8)-Nd(1)-O(4)1	116.7(2)
O(6)-Nd(1)-O(8)	72.9(2)	O(1)-Nd(1)-O(4)1	114.2(2)

Πίνακας Π2-9: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/atzH

Μήκη δεσμών (Å) της ένωσης UCY-2/atzH

Nd(1)-O(5)	2.403(4)	Nd(1)-O(2)	2.551(3)
Nd(1)-O(4)	2.411(4)	Nd(1)-O(7)	2.558(6)
Nd(1)-O(6)	2.420(4)	Nd(1)-N(2)	2.638(5)
Nd(1)-O(1)	2.484(4)	Nd(1)-O(4)	2.682(4)
Nd(1)-O(3)	2.487(4)		

Γωνίες δεσμών (º) της ένωσης UCY-2/atzH

O(5)-Nd(1)-O(4)	78.0(2)	O(1)-Nd(1)-O(7)	68.9(2)
O(5)-Nd(1)-O(6)	133.8(2)	O(3)-Nd(1)-O(7)	149.5(2)
O(4)-Nd(1)-O(6)	71.8(2)	O(2)-Nd(1)-O(7)	103.5(2)
O(5)-Nd(1)-O(1)	141.1(2)	O(5)-Nd(1)-N(2)	76.4(2)
O(4)-Nd(1)-O(1	90.1(2)	O(4)-Nd(1)-N(2)	149.9(2)
O(6)-Nd(1)-O(1)	73.8(2)	O(6)-Nd(1)-N(2)	138.2(2)
O(5)-Nd(1)-O(3)	92.3(2)	O(1)-Nd(1)-N(2)	99.9(2)
O(4)-Nd(1)-O(3)	121.3(2)	O(3)-Nd(1)-N(2)	75.5(2)
O(6)-Nd(1)-O(3)	75.3(2)	O(2)-Nd(1)-N(2)	73.1(2)
O(1)-Nd(1)-O(3)	124.8(2)	O(7)-Nd(1)-N(2)	75.3(2)
O(5)-Nd(1)-O(2)	149.1(2)	O(5)-Nd(1)-O(4)	67.3(2)
O(4)-Nd(1)-O(2)	132.6(2)	O(4)-Nd(1)-O(4)	73.1(2)
O(6)-Nd(1)-O(2)	71.2(2)	O(6)-Nd(1)-O(4)	70.9(2)
O(1)-Nd(1)-O(2)	51.5(2)	O(1)-Nd(1)-O(4)	144.1(2)
O(3)-Nd(1)-O(2)	75.6(2)	O(3)-Nd(1)-O(4)	50.5(2)
O(5)-Nd(1)-O(7)	72.8(2)	O(2)-Nd(1)-O(4)	119.7(2)
O(4)-Nd(1)-O(7)	82.3(2)	O(7)-Nd(1)-O(4)	136.4(2)
O(6)-Nd(1)-O(7)	134.0(2)	N(2)-Nd(1)-O(4)	110.5(2)

Πίνακας Π2-10: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/Cl

Μήκη δεσμών (Å) της ένωσης UCY-2/Cl

Nd(1)-O(4)	2.408(5)	Nd(1)-O(2)	2.500(5)
Nd(1)-O(5)	2.425(5)	Nd(1)-O(1)	2.534(5)
Nd(1)-O(6)	2.433(5)	Nd(1)-O(7)	2.57(8)
Nd(1)-O(8)	2.45(3)	Nd(1)-O(4)	2.660(5)
Nd(1)-O(3)	2.483(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/Cl

O(4)-Nd(1)-O(5)	71.0(2)	O(8)-Nd(1)-O(1)	77.2(7)
O(4)-Nd(1)-O(6)	81.3(2)	O(3)-Nd(1)-O(1)	75.0(2)
O(5)-Nd(1)-O(6)	133.3(2)	O(2)-Nd(1)-O(1)	52.0(2)
O(4)-Nd(1)-O(8)	144.0(2)	O(4)-Nd(1)-O(7)	76.4(2)
O(5)-Nd(1)-O(8)	145.1(2)	O(5)-Nd(1)-O(7)	131.0(2)
O(6)-Nd(1)-O(8)	70.1(7)	O(6)-Nd(1)-O(7)	73.6(2)
O(4)-Nd(1)-O(3)	123.7(2)	O(8)-Nd(1)-O(7)	75.0(2)
O(5)-Nd(1)-O(3)	81.0(2)	O(3)-Nd(1)-O(7)	148.0(2)
O(6)-Nd(1)-O(3)	84.5(2)	O(2)-Nd(1)-O(7)	71.7(2)
O(8)-Nd(1)-O(3)	76(2)	O(1)-Nd(1)-O(7)	110.4(2)
O(4)-Nd(1)-O(2)	92.1(2)	O(4)-Nd(1)-O(4)	74.4(2)
O(5)-Nd(1)-O(2)	74.1(2)	O(5)-Nd(1)-O(4)	69.6(2)
O(6)-Nd(1)-O(2)	145.2(2)	O(6)-Nd(1)-O(4)	67.2(2)
O(8)-Nd(1)-O(2)	99.1(8)	O(8)-Nd(1)-O(4)	112.0(2)
O(3)-Nd(1)-O(2)	125.9(2)	O(3)-Nd(1)-O(4)	50.0(2)
O(4)-Nd(1)-O(1)	134.0(2)	O(2)-Nd(1)-O(4)	143.6(2)
O(5)-Nd(1)-O(1)	71.8(2)	O(1)-Nd(1)-O(4)	115.7(2)
O(6)-Nd(1)-O(1)	144.8(2)	O(7)-Nd(1)-O(4)	133.8(2)

Πίνακας Π2-11: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/Im

Μήκη δεσμών (Å) της ένωσης UCY-2/Im

Nd(1)-O(4)	2.396(4)	Nd(1)-O(1)	2.533(4)
Nd(1)-O(5)	2.406(4)	Nd(1)-N(2)	2.55(2)
Nd(1)-O(3)	2.454(5)	Nd(1)-N(4)	2.588(7)
Nd(1)-O(6)	2.483(5)	Nd(1)-O(5)	2.684(5)
Nd(1)-O(2)	2.491(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/Im

O(4)-Nd(1)-O(5)	77.5(2)	O(6)-Nd(1)-N(2)	150.0(3)
O(4)-Nd(1)-O(3)	134.2(2)	O(2)-Nd(1)-N(2)	70.4(3)
O(5)-Nd(1)-O(3)	72.4(2)	O(1)-Nd(1)-N(2)	102.8(4)
O(4)-Nd(1)-O(6)	92.3(2)	O(4)-Nd(1)-N(4)	74.2(2)
O(5)-Nd(1)-O(6)	121.7(2)	O(5)-Nd(1)-N(4)	147.4(2)
O(3)-Nd(1)-O(6)	75.9(2)	O(3)-Nd(1)-N(4)	140.1(2)
O(4)-Nd(1)-O(2)	141.7(2)	O(6)-Nd(1)-N(4)	75.5(2)
O(5)-Nd(1)-O(2)	88.4(2)	O(2)-Nd(1)-N(4)	104.2(3)
O(3)-Nd(1)-O(2)	71.1(2)	O(1)-Nd(1)-N(4)	75.1(2)
O(6)-Nd(1)-O(2)	124.9(2)	N(2)-Nd(1)-N(4)	75.5(3)
O(4)-Nd(1)-O(1)	149.1(2)	O(4)-Nd(1)-O(5)	67.1(2)
O(5)-Nd(1)-O(1)	132.8(2)	O(5)-Nd(1)-O(5)	73.7(1)
O(3)-Nd(1)-O(1)	71.8(2)	O(3)-Nd(1)-O(5)	71.8(1)
O(6)-Nd(1)-O(1)	77.1(2)	O(6)-Nd(1)-O(5)	50.2(2)
O(2)-Nd(1)-O(1)	51.4(2)	O(2)-Nd(1)-O(5)	142.2(2)
O(4)-Nd(1)-N(2)	72.3(3)	O(1)-Nd(1)-O(5)	121.2(2)
O(5)-Nd(1)-N(2)	80.9(3)	N(2)-Nd(1)-O(5)	135.7(4)
O(3)-Nd(1)-N(2)	133.2(3)	N(4)-Nd(1)-O(5)	108.8(2)

Πίνακας Π2-12: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/mIma

Μήκη δεσμών (Å) της ένωσης UCY-2/mIma

Nd(1)-O(3)	2.408(5)	Nd(1)-O(7)	2.512(7)
Nd(1)-O(5)	2.419(5)	Nd(1)-O(2)	2.523(5)
Nd(1)-O(6)	2.423(6)	Nd(1)-N(2)	2.580(8)
Nd(1)-O(4)	2.477(5)	Nd(1)-O(3)	2.656(4)
Nd(1)-O(1)	2.483(5)		

Γωνίες δεσμών (º) της ένωσης UCY-2/mIma

O(3)-Nd(1)-O(5)	77.1(2)	O(4)-Nd(1)-O(2)	128.2(2)
O(3)-Nd(1)-O(6)	75.0(2)	O(1)-Nd(1)-O(2)	52.4(2)
O(5)-Nd(1)-O(6)	136.3(2)	O(7)-Nd(1)-O(2)	68.4(2)
O(3)-Nd(1)-O(4)	124.5(2)	O(3)-Nd(1)-N(2)	144.9(2)
O(5)-Nd(1)-O(4)	95.7(2)	O(5)-Nd(1)-N(2)	70.5(3)
O(6)-Nd(1)-O(4)	74.1(2)	O(6)-Nd(1)-N(2)	139.2(3)
O(3)-Nd(1)-O(1)	130.7(2)	O(4)-Nd(1)-N(2)	72.8(2)
O(5)-Nd(1)-O(1)	148.3(2)	O(1)-Nd(1)-N(2)	78.5(2)
O(6)-Nd(1)-O(1)	73.3(2)	O(7)-Nd(1)-N(2)	66.4(3)
O(4)-Nd(1)-O(1)	80.8(2)	O(2)-Nd(1)-N(2)	111.8(2)
O(3)-Nd(1)-O(7)	92.0(2)	O(3)-Nd(1)-O(3)	75.5(2)
O(5)-Nd(1)-O(7)	73.2(2)	O(5)-Nd(1)-O(3)	70.1(2)
O(6)-Nd(1)-O(7)	140.0(2)	O(6)-Nd(1)-O(3)	70.8(2)
O(4)-Nd(1)-O(7)	139.1(2)	O(4)-Nd(1)-O(3)	51.1(2)
O(1)-Nd(1)-O(7)	88.8(2)	O(1)-Nd(1)-O(3)	125.8(2)
O(3)-Nd(1)-O(2)	82.5(2)	O(7)-Nd(1)-O(3)	143.0(2)
O(5)-Nd(1)-O(2)	135.5(2)	O(2)-Nd(1)-O(3)	140.8(2)
O(6)-Nd(1)-O(2)	72.4(2)	N(2)-Nd(1)-O(3)	104.7(2)

Πίνακας Π2-13: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-2**/Im-atzH

Μήκη δεσμών (Å) της ένωσης UCY-2/Im-atzH

Nd(1)-O(3)	2.426(3)	Nd(1)-O(1)	2.516(4)
Nd(1)-O(5)	2.437(4)	Nd(1)-O(2)	2.527(4)
Nd(1)-O(7)	2.460(3)	Nd(1)-N(2)	2.587(4)
Nd(1)-O(6)	2.471(3)	Nd(1)-O(3)	2.716(3)
Nd(1)-O(4)	2.495(3)		

Γωνίες δεσμών (º) της ένωσης UCY-2/Im-atzH

O(3)-Nd(1)-O(5)	77.7(2)	O(6)-Nd(1)-O(2)	72.3(2)
O(3)-Nd(1)-O(7)	89.3(2)	O(4)-Nd(1)-O(2)	126.7(2)
O(5)-Nd(1)-O(7)	75.0(2)	O(1)-Nd(1)-O(2)	51.9(2)
O(3)-Nd(1)-O(6)	73.8(2)	O(3)-Nd(1)-N(2)	151.4(2)
O(5)-Nd(1)-O(6)	133.5(2)	O(5)-Nd(1)-N(2)	75.3(2)
O(7)-Nd(1)-O(6)	139.2(2)	O(7)-Nd(1)-N(2)	74.7(2)
O(3)-Nd(1)-O(4)	121.8(2)	O(6)-Nd(1)-N(2)	133.1(2)
O(5)-Nd(1)-O(4)	93.9(2)	O(4)-Nd(1)-N(2)	69.8(2)
O(7)-Nd(1)-O(4)	144.4(2)	O(1)-Nd(1)-N(2)	73.3(2)
O(6)-Nd(1)-O(4)	71.8(2)	O(2)-Nd(1)-N(2)	111.9(2)
O(3)-Nd(1)-O(1)	131.4(2)	O(3)-Nd(1)-O(3)	74.7(2)
O(5)-Nd(1)-O(1)	147.8(2)	O(5)-Nd(1)-O(3)	67.7(2)
O(7)-Nd(1)-O(1)	90.1(2)	O(7)-Nd(1)-O(3)	141.7(2)
O(6)-Nd(1)-O(1)	75.5(2)	O(6)-Nd(1)-O(3)	69.8(2)
O(4)-Nd(1)-O(1)	81.7(2)	O(4)-Nd(1)-O(3)	49.8(2)
O(3)-Nd(1)-O(2)	83.0(2)	O(1)-Nd(1)-O(3)	126.6(2)
O(5)-Nd(1)-O(2)	139.1(2)	O(2)-Nd(1)-O(3)	139.9(2)
O(7)-Nd(1)-O(2)	69.0(2)	N(2)-Nd(1)-O(3)	103.2(2)

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων UCY-3

Πίνακας Π2-14: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-3**/ξηρό

Μήκη δεσμών (Å) της ένωσης UCY-3/ξηρό

Cd(1)-O(1A)	2.24(2)	Cd(2)-O(8)	2.05(2)	Cd(3)-O(7)	2.38(2)
Cd(1)-O(3)	2.306(9)	Cd(2)-O(13)	2.19(2)	Cd(3)-O(4)	2.395(9)
Cd(1)-O(5)	2.32(2)	Cd(2)-O(12)	2.22(2)		
Cd(1)-O(9)	2.335(9)	Cd(2)-O(4)	2.30(2)		
Cd(1)-O(11)	2.35(2)	Cd(2)-O(10)	2.386(9)		
Cd(1)-O(2A)	2.37(2)	Cd(3)-O(14)	2.20(2)		
Cd(1)-O(1)	2.41(2)	Cd(3)-O(6)	2.22(2)		
Cd(1)-O(2)	2.55(2)	Cd(3)-O(15)	2.27(2)		
Cd(1)-O(10)	2.590(8)	Cd(3)-O(10)	2.347(8)		

Γωνίες δεσμών (º) της ένωσης UCY-3/ξηρό

O(1A)-Cd(1)-O(3)	101.1(6)	O(2A)-Cd(1)-O(10)	178.3(6)
O(1A)-Cd(1)-O(5)	122.6(6)	O(1)-Cd(1)-O(10)	134.7(5)
O(3)-Cd(1)-O(5)	81.7(4)	O(2)-Cd(1)-O(10)	125.5(4)
O(1A)-Cd(1)-O(9)	111.6(6)	O(9)-Cd(1)-O(10)	53.0(3)
O(3)-Cd(1)-O(9)	146.9(3)	O(11)-Cd(1)-O(10)	78.6(3)
O(5)-Cd(1)-O(9)	84.6(4)	O(12)-Cd(2)-O(4)	85.2(4)
O(1A)-Cd(1)-O(11)	90.1(6)	O(8)-Cd(2)-O(10)	121.3(5)
O(3)-Cd(1)-O(11)	81.2(4)	O(13)-Cd(2)-O(10)	90.6(5)
O(5)-Cd(1)-O(11)	145.4(3)	O(12)-Cd(2)-O(10)	123.8(3)
O(9)-Cd(1)-O(11)	93.8(4)	O(4)-Cd(2)-O(10)	72.9(3)
O(1A)-Cd(1)-O(2A)	20.6(5)	O(8)-Cd(2)-O(13)	97.9(8)
O(3)-Cd(1)-O(2A)	87.0(6)	O(8)-Cd(2)-O(12)	110.2(6)
O(5)-Cd(1)-O(2A)	106.0(6)	O(13)-Cd(2)-O(12)	103.9(5)
O(9)-Cd(1)-O(2A)	125.8(6)	O(8)-Cd(2)-O(4)	91.6(6)
O(11)-Cd(1)-O(2A)	102.9(6)	O(13)-Cd(2)-O(4)	163.5(5)
O(1A)-Cd(1)-O(1)	24.9(6)	O(15)-Cd(3)-O(10)	97.4(4)
O(3)-Cd(1)-O(1)	120.9(5)	O(14)-Cd(3)-O(7)	72.6(5)
O(5)-Cd(1)-O(1)	134.9(6)	O(6)-Cd(3)-O(7)	155.6(4)
O(9)-Cd(1)-O(1)	89.7(5)	O(15)-Cd(3)-O(7)	99.5(5)
O(11)-Cd(1)-O(1)	79.5(6)	O(10)-Cd(3)-O(7)	78.8(3)
O(2A)-Cd(1)-O(1)	45.2(7)	O(14)-Cd(3)-O(4)	88.5(4)
O(1A)-Cd(1)-O(2)	53.0(7)	O(6)-Cd(3)-O(4)	88.4(4)
O(3)-Cd(1)-O(2)	127.7(5)	O(15)-Cd(3)-O(4)	169.0(4)
O(5)-Cd(1)-O(2)	79.9(5)	O(10)-Cd(3)-O(4)	71.9(3)

O(9)-Cd(1)-O(2)	78.6(5)	O(7)-Cd(3)-O(4)	76.1(4)
O(11)-Cd(1)-O(2)	133.8(4)	O(14)-Cd(3)-O(6)	88.5(5)
O(2A)-Cd(1)-O(2)	52.8(7)	O(14)-Cd(3)-O(15)	99.8(5)
O(1)-Cd(1)-O(2)	55.2(7)	O(6)-Cd(3)-O(15)	98.9(5)
O(1A)-Cd(1)-O(10)	159.4(6)	O(14)-Cd(3)-O(10)	148.6(5)
O(3)-Cd(1)-O(10)	94.1(3)	O(6)-Cd(3)-O(10)	114.4(4)
O(5)-Cd(1)-O(10)	73.0(3)		

Πίνακας Π2-15: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-3**/$CHCl_3$

Μήκη δεσμών (Å) της ένωσης UCY-3/$CHCl_3$

Cd(1)-O(2A)	2.24(2)	Cd(2)-O(8)	2.10(2)	Cd(3)-O(7)	2.313(8)
Cd(1)-O(1A)	2.29(2)	Cd(2)-O(12)	2.194(6)	Cd(3)-O(10)	2.342(6)
Cd(1)-O(5)	2.293(7)	Cd(2)-O(13)	2.19(2)	Cd(3)-O(4)	2.343(6)
Cd(1)-O(3)	2.314(6)	Cd(2)-O(4)	2.307(7)		
Cd(1)-O(9)	2.314(6)	Cd(2)-O(10)	2.333(6)		
Cd(1)-O(11)	2.338(7)	Cd(2)-O(11)	2.629(6)		
Cd(1)-O(1)	2.42(2)	Cd(3)-O(15)	2.200(8)		
Cd(1)-O(10)	2.607(6)	Cd(3)-O(6)	2.238(7)		
Cd(1)-O(2)	2.62(2)	Cd(3)-O(14)	2.286(8)		

Γωνίες δεσμών (º) της ένωσης UCY-3/$CHCl_3$

O(1A)-Cd(1)-O(3)	101.1(6)	O(2A)-Cd(1)-O(10)	178.3(6)
O(1A)-Cd(1)-O(5)	122.6(6)	O(1)-Cd(1)-O(10)	134.7(5)
O(3)-Cd(1)-O(5)	81.7(4)	O(2)-Cd(1)-O(10)	125.5(4)
O(1A)-Cd(1)-O(9)	111.6(6)	O(9)-Cd(1)-O(10)	53.0(3)
O(3)-Cd(1)-O(9)	146.9(3)	O(11)-Cd(1)-O(10)	78.6(3)
O(5)-Cd(1)-O(9)	84.6(4)	O(12)-Cd(2)-O(4)	85.2(4)
O(1A)-Cd(1)-O(11)	90.1(6)	O(8)-Cd(2)-O(10)	121.3(5)
O(3)-Cd(1)-O(11)	81.2(4)	O(13)-Cd(2)-O(10)	90.6(5)
O(5)-Cd(1)-O(11)	145.4(3)	O(12)-Cd(2)-O(10)	123.8(3)
O(9)-Cd(1)-O(11)	93.8(4)	O(4)-Cd(2)-O(10)	72.9(3)
O(1A)-Cd(1)-O(2A)	20.6(5)	O(8)-Cd(2)-O(13)	97.9(8)
O(3)-Cd(1)-O(2A)	87.0(6)	O(8)-Cd(2)-O(12)	110.2(6)
O(5)-Cd(1)-O(2A)	106.0(6)	O(13)-Cd(2)-O(12)	103.9(5)
O(9)-Cd(1)-O(2A)	125.8(6)	O(8)-Cd(2)-O(4)	91.6(6)
O(11)-Cd(1)-O(2A)	102.9(6)	O(13)-Cd(2)-O(4)	163.5(5)

O(1A)-Cd(1)-O(1)	24.9(6)	O(15)-Cd(3)-O(10)	97.4(4)
O(3)-Cd(1)-O(1)	120.9(5)	O(14)-Cd(3)-O(7)	72.6(5)
O(5)-Cd(1)-O(1)	134.9(6)	O(6)-Cd(3)-O(7)	155.6(4)
O(9)-Cd(1)-O(1)	89.7(5)	O(15)-Cd(3)-O(7)	99.5(5)
O(11)-Cd(1)-O(1)	79.5(6)	O(10)-Cd(3)-O(7)	78.8(3)
O(2A)-Cd(1)-O(1)	45.2(7)	O(14)-Cd(3)-O(4)	88.5(4)
O(1A)-Cd(1)-O(2)	53.0(7)	O(6)-Cd(3)-O(4)	88.4(4)
O(3)-Cd(1)-O(2)	127.7(5)	O(15)-Cd(3)-O(4)	169.0(4)
O(5)-Cd(1)-O(2)	79.9(5)	O(10)-Cd(3)-O(4)	71.9(3)
O(9)-Cd(1)-O(2)	78.6(5)	O(7)-Cd(3)-O(4)	76.1(4)
O(11)-Cd(1)-O(2)	133.8(4)	O(14)-Cd(3)-O(6)	88.5(5)
O(2A)-Cd(1)-O(2)	52.8(7)	O(14)-Cd(3)-O(15)	99.8(5)
O(1)-Cd(1)-O(2)	55.2(7)	O(6)-Cd(3)-O(15)	98.9(5)
O(1A)-Cd(1)-O(10)	159.4(6)	O(14)-Cd(3)-O(10)	148.6(5)
O(3)-Cd(1)-O(10)	94.1(3)	O(6)-Cd(3)-O(10)	114.4(4)
O(5)-Cd(1)-O(10)	73.0(3)		

Πίνακας Π2-16: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-3**/C_6H_6

Μήκη δεσμών (Å) της ένωσης UCY-3/C_6H_6

Cd(1)-O(1)	2.227(8)	Cd(2)-O(7)	2.304(6)	Cd(2)-O(13)	2.212(6)
Cd(1)-O(1A)	2.42(2)	Cd(3)-O(8)	2.173(5)	Cd(2)-O(14)	2.312(6)
Cd(1)-O(2)	2.492(9)	Cd(3)-O(9)	2.307(5)	Cd(3)-O(15)	2.256(6)
Cd(1)-O(2A)	2.20(3)	Cd(2)-O(9)	2.377(5)		
Cd(2)-O(3)	2.231(5)	Cd(1)-O(9)	2.613(5)		
Cd(1)-O(4)	2.306(5)	Cd(1)-O(10)	2.301(5)		
Cd(2)-O(5)	2.334(5)	Cd(3)-O(11)	2.211(5)		
Cd(3)-O(5)	2.340(5)	Cd(1)-O(12)	2.398(5)		
Cd(1)-O(6)	2.305(5)	Cd(3)-O(12)	2.529(5)		

Γωνίες δεσμών (º) της ένωσης UCY-3/C_6H_6

O(2-Cd(1)-O(1)	36.0(2)	O(6)-Cd(1)-O(9)	92.4(2)
O(2A)-Cd(1)-O(10)	111(2)	O(4)-Cd(1)-O(9)	72.3(2)
O(1)-Cd(1)-O(10)	112.4(3)	O(12)-Cd(1)-O(9)	77.2(2)
O(2A)-Cd(1)-O(6)	103.0(2)	O(1A)-Cd(1)-O(9)	134.2(8)
O(1)-Cd(1)-O(6)	100.0(3)	O(2)-Cd(1)-O(9)	128.4(3)
O(10)-Cd(1)-O(6)	144.9(3)	O(13)-Cd(2)-O(3)	102.6(2)

O(2A)-Cd(1)-O(4)	92(2)	O(13)-Cd(2)-O(7)	88.9(2)
O(1)-Cd(1)-O(4)	125.8(3)	O(3)-Cd(2)-O(7)	160.0(2)
O(10)-Cd(1)-O(4)	88.8(2)	O(13)-Cd(2)-O(14)	97.6(3)
O(6)-Cd(1)-O(4)	82.7(2)	O(3)-Cd(2)-O(14)	82.4(2)
O(2A)-Cd(1)-O(12)	124.0(2)	O(7)-Cd(2)-O(14)	79.8(2)
O(1)-Cd(1)-O(12)	88.5(3)	O(13)-Cd(2)-O(5)	169.2(2)
O(10)-Cd(1)-O(12)	88.4(2)	O(3)-Cd(2)-O(5)	85.7(2)
O(6)-Cd(1)-O(12)	79.0(2)	O(7)-Cd(2)-O(5)	85.2(2)
O(4)-Cd(1)-O(12)	143.5(2)	O(14)-Cd(2)-O(5)	90.2(2)
O(2A)-Cd(1)-O(1A)	53(2)	O(13)-Cd(2)-O(9)	99.0(2)
O(1)-Cd(1)-O(1A)	25.1(7)	O(3)-Cd(2)-O(9)	110.6(2)
O(10)-Cd(1)-O(1A)	89.7(8)	O(7)-Cd(2)-O(9)	83.2(2)
O(6)-Cd(1)-O(1A)	118.3(7)	O(14)-Cd(2)-O(9)	155.9(2)
O(4)-Cd(1)-O(1A)	139.6(7)	O(5)-Cd(2)-O(9)	71.4(2)
O(12)-Cd(1)-O(1A)	76.7(7)	O(8)-Cd(3)-O(11)	107.1(2)
O(2A)-Cd(1)-O(2)	28(2)	O(8)-Cd(3)-O(15)	102.4(2)
O(1)-Cd(1)-O(2)	54.7(3)	O(11)-Cd(3)-O(15)	106.2(2)
O(10)-Cd(1)-O(2)	84.6(3)	O(8)-Cd(3)-O(9)	115.6(2)
O(6)-Cd(1)-O(2)	126.9(3)	O(11)-Cd(3)-O(9)	130.7(2)
O(4)-Cd(1)-O(2)	80.4(3)	O(15)-Cd(3)-O(9)	88.2(2)
O(12)-Cd(1)-O(2)	135.4(2)	O(8)-Cd(3)-O(5)	87.8(2)
O(1A)-Cd(1)-O(2)	59.3(7)	O(11)-Cd(3)-O(5)	86.1(2)
O(2A)-Cd(1)-O(9)	156.0(2)	O(15)-Cd(3)-O(5)	160.6(2)
O(1)-Cd(1)-O(9)	159.0(3)	O(9)-Cd(3)-O(5)	72.5(2)
O(10)-Cd(1)-O(9)	52.7(2)	O(8)-Cd(3)-O(12)	162.2(2)
		O(11)-Cd(3)-O(12)	55.1(2)
		O(15)-Cd(3)-O(12)	84.8(2)
		O(9)-Cd(3)-O(12)	80.6(2)
		O(5)-Cd(3)-O(12)	90.4(2)

Πίνακας Π2-17: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-3**/C_7H_8

Μήκη δεσμών (Å) της ένωσης UCY-3/C_7H_8

Cd(1)-O(1)	2.462(9)	Cd(3)-O(9)	2.351(6)	Cd(3)-O(15)	2.229(8)
Cd(1)-O(2)	2.26(2)	Cd(2)-O(9)	2.386(6)		
Cd(1)-O(3)	2.305(7)	Cd(1)-O(9)	2.600(5)		
Cd(2)-O(4)	2.231(7)	Cd(1)-O(10)	2.310(6)		
Cd(3)-O(5)	2.335(7)	Cd(3)-O(11)	2.257(6)		
Cd(2)-O(5)	2.339(6)	Cd(1)-O(12)	2.331(7)		

Cd(1)-O(6)	2.285(5)	Cd(3)-O(12)	2.519(6)
Cd(2)-O(7)	2.306(7)	Cd(2)-O(13)	2.289(7)
Cd(3)-O(8)	2.155(7)	Cd(2)-O(14)	2.222(7)

Γωνίες δεσμών (°) της ένωσης UCY-3/C_7H_8

O(2)-Cd(1)-O(6)	103.7(3)	O(14)-Cd(2)-O(7)	93.1(3)
O(2)-Cd(1)-O(3)	90.6(3)	O(4)-Cd(2)-O(7)	160.8(2)
O(6)-Cd(1)-O(3)	83.1(2)	O(13)-Cd(2)-O(7)	81.2(3)
O(2)-Cd(1)-O(10)	107.4(3)	O(14)-Cd(2)-O(5)	165.8(3)
O(6)-Cd(1)-O(10)	146.22(18)	O(4)-Cd(2)-O(5)	86.0(2)
O(3)-Cd(1)-O(10)	83.7(3)	O(13)-Cd(2)-O(5)	92.5(2)
O(2)-Cd(1)-O(12)	124.3(3)	O(7)-Cd(2)-O(5)	82.4(2)
O(6)-Cd(1)-O(12)	79.5(2)	O(14)-Cd(2)-O(9)	94.7(3)
O(3)-Cd(1)-O(12)	143.7(2)	O(4)-Cd(2)-O(9)	109.7(2)
O(10)-Cd(1)-O(12)	93.4(3)	O(13)-Cd(2)-O(9)	157.3(3)
O(2)-Cd(1)-O(1)	52.5(4)	O(7)-Cd(2)-O(9)	81.0(2)
O(6)-Cd(1)-O(1)	123.6(3)	O(5)-Cd(2)-O(9)	71.3(2)
O(3)-Cd(1)-O(1)	136.4(3)	O(8)-Cd(3)-O(15)	103.6(3)
O(10)-Cd(1)-O(1)	86.5(3)	O(8)-Cd(3)-O(11)	103.9(3)
O(12)-Cd(1)-O(1)	79.1(3)	O(15)-Cd(3)-O(11)	106.0(3)
O(2)-Cd(1)-O(9)	154.2(3)	O(8)-Cd(3)-O(5)	87.3(3)
O(6)-Cd(1)-O(9)	93.71(17)	O(15)-Cd(3)-O(5)	160.2(3)
O(3)-Cd(1)-O(9)	72.4(2)	O(11)-Cd(3)-O(5)	87.0(3)
O(10)-Cd(1)-O(9)	52.62(17)	O(8)-Cd(3)-O(9)	119.4(3)
O(12)-Cd(1)-O(9)	77.2(2)	O(15)-Cd(3)-O(9)	88.1(3)
O(1)-Cd(1)-O(9)	130.5(3)	O(11)-Cd(3)-O(9)	129.9(2)
O(2)-Cd(1)-C(1)	25.5(4)	O(5)-Cd(3)-O(9)	72.1(2)
O(6)-Cd(1)-C(1)	117.2(3)	O(8)-Cd(3)-O(12)	158.6(3)
O(3)-Cd(1)-C(1)	112.7(4)	O(15)-Cd(3)-O(12)	87.6(3)
O(10)-Cd(1)-C(1)	96.5(3)	O(11)-Cd(3)-O(12)	55.1(2)
O(12)-Cd(1)-C(1)	103.5(4)	O(5)-Cd(3)-O(12)	87.7(2)
O(1)-Cd(1)-C(1)	27.1(4)	O(9)-Cd(3)-O(12)	78.5(2)
O(9)-Cd(1)-C(1)	148.8(3)	O(4)-Cd(2)-O(13)	84.0(2)
O(14)-Cd(2)-O(4)	101.6(3)		
O(14)-Cd(2)-O(13)	100.2(3)		

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων UCY-5

Πίνακας Π2-18: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-5**/Ακετόνη

Μήκη δεσμών (Å) της ένωσης UCY-5/Ακετόνη

Ce(1)-O(5)	2.431(3)	Ce(1)-O(7)	2.520(4)
Ce(1)-O(3)	2.452(3)	Ce(1)-O(2)	2.529(3)
Ce(1)-O(6)	2.455(3)	Ce(1)-O(1)	2.543(3)
Ce(1)-O(8A)	2.46(2)	Ce(1)-O(8)	2.55(2)
Ce(1)-O(4)	2.518(3)	Ce(1)-O(3)	2.711(3)

Γωνίες δεσμών (º) της ένωσης UCY-5/Ακετόνη

O(5)-Ce(1)-O(3)	78.4(2)	O(8A)-Ce(1)-O(2)	66.7(3)
O(5)-Ce(1)-O(6)	133.3(2)	O(4)-Ce(1)-O(2)	125.5(2)
O(3)-Ce(1)-O(6)	71.9(2)	O(7)-Ce(1)-O(2)	107.0(2)
O(5)-Ce(1)-O(8A)	78.1(3)	O(5)-Ce(1)-O(1)	148.3(2)
O(3)-Ce(1)-O(8A)	92.2(3)	O(3)-Ce(1)-O(1)	131.8(2)
O(6)-Ce(1)-O(8A)	136.9(3)	O(6)-Ce(1)-O(1)	74.2(2)
O(5)-Ce(1)-O(4)	93.2(2)	O(8A)-Ce(1)-O(1)	89.7(3)
O(3)-Ce(1)-O(4)	121.3(2)	O(4)-Ce(1)-O(1)	79.2(2)
O(6)-Ce(1)-O(4)	73.5(2)	O(7)-Ce(1)-O(1)	73.9(2)
O(8A)-Ce(1)-O(4)	143.2(3)	O(2)-Ce(1)-O(1)	51.3(2)
O(5)-Ce(1)-O(7)	74.4(2)	O(5)-Ce(1)-O(8)	69.3(2)
O(3)-Ce(1)-O(7)	149.7(2)	O(3)-Ce(1)-O(8)	76.4(3)
O(6)-Ce(1)-O(7)	137.8(2)	O(6)-Ce(1)-O(8)	133.4(2)
O(8A)-Ce(1)-O(7)	69.4(3)	O(8A)-Ce(1)-O(8)	17.0(3)
O(4)-Ce(1)-O(7)	73.8(2)	O(4)-Ce(1)-O(8)	153.1(2)
O(5)-Ce(1)-O(2)	140.7(2)	O(7)-Ce(1)-O(8)	81.7(3)
O(3)-Ce(1)-O(2)	85.9(2)	O(2)-Ce(1)-O(8)	72.1(2)
O(6)-Ce(1)-O(2)	72.3(2)	O(1)-Ce(1)-O(8)	104.8(3)
O(5)-Ce(1)-O(3)	67.4(2)	O(7)-Ce(1)-O(3)	106.2(2)
O(3)-Ce(1)-O(3)	74.6(2)	O(2)-Ce(1)-O(3)	141.7(2)
O(6)-Ce(1)-O(3)	70.4(2)	O(1)-Ce(1)-O(3)	123.5(2)
O(8A)-Ce(1)-O(3)	144.9(3)	O(8)-Ce(1)-O(3)	131.5(3)
O(4)-Ce(1)-O(3)	49.45(9)		

Πίνακας Π2-19: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-5**/MeOH

Μήκη δεσμών (Å) της ένωσης UCY-5/MeOH

Ce(1)-O(5)	2.434(4)	Ce(1)-O(2)	2.535(4)
Ce(1)-O(3)	2.443(4)	Ce(1)-O(1)	2.557(5)
Ce(1)-O(6)	2.447(5)	Ce(1)-O(8)	2.559(6)
Ce(1)-O(4)	2.514(5)	Ce(1)-O(7)	2.68(4)
Ce(1)-O(7A)	2.534(9)	Ce(1)-O(3)	2.713(4)

Γωνίες δεσμών (º) της ένωσης UCY-5/ MeOH

O(5)-Ce(1)-O(3)	80.7(2)	O(6)-Ce(1)-O(8)	133.9(2)
O(5)-Ce(1)-O(6)	132.6(2)	O(4)-Ce(1)-O(8)	149.3(2)
O(3)-Ce(1)-O(6)	71.3(2)	O(7A)-Ce(1)-O(8)	73.5(3)
O(5)-Ce(1)-O(4)	88.4(2)	O(2)-Ce(1)-O(8)	69.0(2)
O(3)-Ce(1)-O(4)	122.5(2)	O(1)-Ce(1)-O(8)	103.1(2)
O(6)-Ce(1)-O(4)	76.3(2)	O(5)-Ce(1)-O(7)	74.0(2)
O(5)-Ce(1)-O(7A)	74.8(3)	O(3)-Ce(1)-O(7)	154(2)
O(3)-Ce(1)-O(7A)	148.0(3)	O(6)-Ce(1)-O(7)	133.0(9)
O(6)-Ce(1)-O(7A)	140.7(3)	O(4)-Ce(1)-O(7)	65.8(8)
O(4)-Ce(1)-O(7A)	77.5(3)	O(7A)-Ce(1)-O(7)	11.8(8)
O(5)-Ce(1)-O(2)	143.0(2)	O(2)-Ce(1)-O(7)	105.9(9)
O(3)-Ce(1)-O(2)	88.8(2)	O(1)-Ce(1)-O(7)	72(2)
O(6)-Ce(1)-O(2)	74.8(2)	O(8)-Ce(1)-O(7)	84.9(9)
O(4)-Ce(1)-O(2)	126.3(2)	O(5)-Ce(1)-O(3)	67.0(2)
O(7A)-Ce(1)-O(2)	98.4(3)	O(3)-Ce(1)-O(3)	74.5(2)
O(5)-Ce(1)-O(1)	146.3(2)	O(6)-Ce(1)-O(3)	69.1(1)
O(3)-Ce(1)-O(1)	132.6(2)	O(4)-Ce(1)-O(3)	49.7(2)
O(6)-Ce(1)-O(1)	73.7(2)	O(7A)-Ce(1)-O(3)	113.1(3)
O(4)-Ce(1)-O(1)	77.5(2)	O(2)-Ce(1)-O(3)	143.4(2)
O(7A)-Ce(1)-O(1)	72.4(3)	O(1)-Ce(1)-O(3)	120.3(2)
O(2)-Ce(1)-O(1)	51.4(2)	O(8)-Ce(1)-O(3)	136.3(2)
O(5)-Ce(1)-O(8)	74.3(2)	O(7)-Ce(1)-O(3)	102.9(9)
O(3)-Ce(1)-O(8)	80.2(2)		

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων UCY-8

Πίνακας Π2-20: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/Im

Μήκη δεσμών (Å) της ένωσης UCY-8/Im

Eu(1)-O(6)	2.361(6)	Eu(1)-O(5)	2.452(6)
Eu(1)-O(3)	2.378(6)	Eu(1)-O(2)	2.478(6)
Eu(1)-O(4)	2.395(6)	Eu(1)-N(2)	2.543(8)
Eu(1)-O(7)	2.420(7)	Eu(1)-O(6)	2.695(6)
Eu(1)-O(1)	2.436(6)		

Γωνίες δεσμών (º) της ένωσης UCY-8/Im

O(6)-Eu(1)-O(3)	77.4(2)	O(7)-Eu(1)-O(2)	69.6(2)
O(6)-Eu(1)-O(4)	75.3(2)	O(1)-Eu(1)-O(2)	52.8(2)
O(3)-Eu(1)-O(4)	134.2(2)	O(5)-Eu(1)-O(2)	130.9(2)
O(6)-Eu(1)-O(7)	88.4(2)	O(6)-Eu(1)-N(2)	150.3(2)
O(3)-Eu(1)-O(7)	73.9(2)	O(3)-Eu(1)-N(2)	75.1(2)
O(4)-Eu(1)-O(7)	140.2(2)	O(4)-Eu(1)-N(2)	133.1(2)
O(6)-Eu(1)-O(1)	130.4(2)	O(7)-Eu(1)-N(2)	73.6(3)
O(3)-Eu(1)-O(1)	147.5(2)	O(1)-Eu(1)-N(2)	73.7(2)
O(4)-Eu(1)-O(1)	75.9(2)	O(5)-Eu(1)-N(2)	70.7(2)
O(7)-Eu(1)-O(1)	88.7(2)	O(2)-Eu(1)-N(2)	113.8(2)
O(6)-Eu(1)-O(5)	121.3(2)	O(6)-Eu(1)-O(6)	73.2(2)
O(3)-Eu(1)-O(5)	91.8(2)	O(3)-Eu(1)-O(6)	67.4(2)
O(4)-Eu(1)-O(5)	72.5(2)	O(4)-Eu(1)-O(6)	69.8(2)
O(7)-Eu(1)-O(5)	143.9(2)	O(7)-Eu(1)-O(6)	139.8(2)
O(1)-Eu(1)-O(5)	86.4(2)	O(1)-Eu(1)-O(6)	130.5(2)
O(6)-Eu(1)-O(2)	80.0(2)	O(5)-Eu(1)-O(6)	50.1(2)
O(3)-Eu(1)-O(2)	137.2(2)	O(2)-Eu(1)-O(6)	137.5(2)
O(4)-Eu(1)-O(2)	71.9(2)	N(2)-Eu(1)-O(6)	105.6(2)

Πίνακας Π2-21: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/2-mIm

Μήκη δεσμών (Å) της ένωσης UCY-8/2-mIm

Eu(1)-O(3)	2.375(5)	Eu(1)-O(1)	2.456(5)
Eu(1)-O(6)	2.390(5)	Eu(1)-O(2)	2.464(5)
Eu(1)-O(5)	2.423(4)	Eu(1)-N(3)	2.571(6)
Eu(1)-O(4)	2.441(4)	Eu(1)-O(3)	2.686(5)
Eu(1)-O(7)	2.441(5)		

Γωνίες δεσμών (º) της ένωσης UCY-8/2-mIm

O(3)-Eu(1)-O(6)	76.7(2)	O(4)-Eu(1)-O(2)	83.3(2)
O(3)-Eu(1)-O(5)	74.4(2)	O(7)-Eu(1)-O(2)	97.4(2)
O(6)-Eu(1)-O(5)	133.4(2)	O(1)-Eu(1)-O(2)	52.8(1)
O(3)-Eu(1)-O(4)	21.2(2)	O(3)-Eu(1)-N(3)	149.6(2)
O(6)-Eu(1)-O(4)	92.7(2)	O(6)-Eu(1)-N(3)	76.3(2)
O(5)-Eu(1)-O(4)	72.7(2)	O(5)-Eu(1)-N(3)	135.4(2)
O(3)-Eu(1)-O(7)	82.7(2)	O(4)-Eu(1)-N(3)	73.8(2)
O(6)-Eu(1)-O(7)	70.4(2)	O(7)-Eu(1)-N(3)	75.3(2)
O(5)-Eu(1)-O(7)	138.9(2)	O(1)-Eu(1)-N(3)	109.8(2)
O(4)-Eu(1)-O(7)	147.6(2)	O(2)-Eu(1)-N(3)	73.7(2)
O(3)-Eu(1)-O(1)	81.8(2)	O(3)-Eu(1)-O(3)	73.5(2)
O(6)-Eu(1)-O(1)	137.7(2)	O(6)-Eu(1)-O(3)	66.1(2)
O(5)-Eu(1)-O(1)	72.2(2)	O(5)-Eu(1)-O(3)	71.0(2)
O(4)-Eu(1)-O(1)	129.6(2)	O(4)-Eu(1)-O(3)	50.3(2)
O(7)-Eu(1)-O(1)	71.0(2)	O(7)-Eu(1)-O(3)	133.9(2)
O(3)-Eu(1)-O(2)	130.7(2)	O(1)-Eu(1)-O(3)	139.9(2)
O(6)-Eu(1)-O(2)	149.6(2)	O(2)-Eu(1)-O(3)	128.2(2)
O(5)-Eu(1)-O(2)	74.1(2)	N(3)-Eu(1)-O(3)	107.5(2)

Πίνακας Π2-22: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/4(5)mIm

Μήκη δεσμών (Å) της ένωσης UCY-8/4(5)mIm

Eu(1)-O(3)	2.362(3)	Eu(1)-O(1)	2.453(3)
Eu(1)-O(7)	2.378(3)	Eu(1)-O(2)	2.488(3)
Eu(1)-O(5)	2.398(3)	Eu(1)-N(2)	2.626(4)
Eu(1)-O(4)	2.425(3)	Eu(1)-O(3)	2.730(3)
Eu(1)-O(6)	2.446(3)		

Γωνίες δεσμών (º) της ένωσης UCY-8/4(5)mIm

O(3)-Eu(1)-O(7)	87.7(2)	O(4)-Eu(1)-O(2)	130.2(2)
O(3)-Eu(1)-O(5)	77.8(2)	O(6)-Eu(1)-O(2)	72.0(2)
O(7)-Eu(1)-O(5)	75.9(2)	O(1)-Eu(1)-O(2)	53.0(2)
O(3)-Eu(1)-O(4)	121.99(9)	O(3)-Eu(1)-N(2)	149.0(2)
O(7)-Eu(1)-O(4)	144.2(2)	O(7)-Eu(1)-N(2)	73.3(2)
O(5)-Eu(1)-O(4)	90.4(2)	O(5)-Eu(1)-N(2)	74.0(2)
O(3)-Eu(1)-O(6)	75.0(2)	O(4)-Eu(1)-N(2)	71.2(2)
O(7)-Eu(1)-O(6)	139.7(2)	O(6)-Eu(1)-N(2)	134.7(2)
O(5)-Eu(1)-O(6)	132.5(2)	O(1)-Eu(1)-N(2)	75.5(2)
O(4)-Eu(1)-O(6)	72.7(2)	O(2)-Eu(1)-N(2)	113.7(2)
O(3)-Eu(1)-O(1)	130.3(2)	O(3)-Eu(1)-O(3)	73.8(2)
O(7)-Eu(1)-O(1)	90.8(2)	O(7)-Eu(1)-O(3)	141.0(2)
O(5)-Eu(1)-O(1)	149.1(2)	O(5)-Eu(1)-O(3)	66.86(9)
O(4)-Eu(1)-O(1)	84.3(2)	O(4)-Eu(1)-O(3)	49.91(9)
O(6)-Eu(1)-O(1)	74.64(9)	O(6)-Eu(1)-O(3)	68.56(9)
O(3)-Eu(1)-O(2)	80.4(2)	O(1)-Eu(1)-O(3)	127.41(9)
O(7)-Eu(1)-O(2)	69.2(2)	O(2)-Eu(1)-O(3)	137.15(9)
O(5)-Eu(1)-O(2)	139.3(2)	N(2)-Eu(1)-O(3)	105.9(2)

Πίνακας Π2-23: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/bzIm

Μήκη δεσμών (Å) της ένωσης UCY-8/bzIm

Eu(1)-O(4)	2.355(4)	Eu(1)-O(7)	2.456(6)
Eu(1)-O(6)	2.373(4)	Eu(1)-O(1)	2.473(5)
Eu(1)-O(5)	2.395(4)	Eu(1)-O(2)	2.479(4)
Eu(1)-O(3)	2.430(4)	Eu(1)-O(4)	2.670(4)
Eu(1)-O(8)	2.432(5)		

Γωνίες δεσμών (º) της ένωσης UCY-8/bzIm

O(4)-Eu(1)-O(6)	79.1(2)	O(3)-Eu(1)-O(1)	127.4(2)
O(4)-Eu(1)-O(5)	73.4(2)	O(8)-Eu(1)-O(1)	70.0(2)
O(6)-Eu(1)-O(5)	134.3(2)	O(7)-Eu(1)-O(1)	107.1(2)
O(4)-Eu(1)-O(3)	122.8(2)	O(4)-Eu(1)-O(2)	131.4(2)
O(6)-Eu(1)-O(3)	93.2(2)	O(6)-Eu(1)-O(2)	147.0(2)
O(5)-Eu(1)-O(3)	73.1(2)	O(5)-Eu(1)-O(2)	75.0(2)
O(4)-Eu(1)-O(8)	85.4(2)	O(3)-Eu(1)-O(2)	80.5(2)
O(6)-Eu(1)-O(8)	71.9(2)	O(8)-Eu(1)-O(2)	95.3(2)
O(5)-Eu(1)-O(8)	138.9(2)	O(7)-Eu(1)-O(2)	70.7(2)
O(3)-Eu(1)-O(8)	145.8(2)	O(1)-Eu(1)-O(2)	52.7(2)
O(4)-Eu(1)-O(7)	152.1(2)	O(4)-Eu(1)-O(4)	74.6(2)
O(6)-Eu(1)-O(7)	76.5(2)	O(6)-Eu(1)-O(4)	68.5(2)
O(5)-Eu(1)-O(7)	134.2(2)	O(5)-Eu(1)-O(4)	69.4(2)
O(3)-Eu(1)-O(7)	72.1(2)	O(3)-Eu(1)-O(4)	50.6(2)
O(8)-Eu(1)-O(7)	74.4(2)	O(8)-Eu(1)-O(4)	138.2(2)
O(4)-Eu(1)-O(1)	83.0(2)	O(7)-Eu(1)-O(4)	108.1(2)
O(6)-Eu(1)-O(1)	138.9(2)	O(1)-Eu(1)-O(4)	140.1(2)
O(5)-Eu(1)-O(1)	72.8(2)	O(2)-Eu(1)-O(4)	125.5(2)

Πίνακας Π2-24: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8/**etmIm

Μήκη δεσμών (Å) της ένωσης UCY-8/etmIm

Eu(1)-O(5)	2.351(6)	Eu(1)-O(7)	2.497(7)
Eu(1)-O(4)	2.368(5)	Eu(1)-O(2)	2.544(6)
Eu(1)-O(6)	2.382(6)	Eu(1)-N(2)	2.584(8)
Eu(1)-O(3)	2.405(5)	Eu(1)-O(4)	2.730(5)
Eu(1)-O(1)	2.459(6)		

Γωνίες δεσμών (º) της ένωσης UCY-8/etmIm

O(5)-Eu(1)-O(4)	79.7(2)	O(3)-Eu(1)-O(2)	81.3(2)
O(5)-Eu(1)-O(6)	132.7(2)	O(1)-Eu(1)-O(2)	52.5(2)
O(4)-Eu(1)-O(6)	72.2(2)	O(7)-Eu(1)-O(2)	100.3(2)
O(5)-Eu(1)-O(3)	89.0(2)	O(5)-Eu(1)-N(2)	76.3(2)
O(4)-Eu(1)-O(3)	124.0(2)	O(4)-Eu(1)-N(2)	148.5(2)
O(6)-Eu(1)-O(3)	76.8(2)	O(6)-Eu(1)-N(2)	139.3(2)
O(5)-Eu(1)-O(1)	138.9(2)	O(3)-Eu(1)-N(2)	76.0(2)
O(4)-Eu(1)-O(1)	83.7(2)	O(1)-Eu(1)-N(2)	101.3(2)
O(6)-Eu(1)-O(1)	75.1(2)	O(7)-Eu(1)-N(2)	74.1(2)
O(3)-Eu(1)-O(1)	130.9(2)	O(2)-Eu(1)-N(2)	72.9(2)
O(5)-Eu(1)-O(7)	73.2(2)	O(5)-Eu(1)-O(4)	66.1(2)
O(4)-Eu(1)-O(7)	79.6(2)	O(4)-Eu(1)-O(4)	74.7(2)
O(6)-Eu(1)-O(7)	134.7(2)	O(6)-Eu(1)-O(4)	70.2(2)
O(3)-Eu(1)-O(7)	147.9(2)	O(3)-Eu(1)-O(4)	51.0(2)
O(1)-Eu(1)-O(7)	66.9(2)	O(1)-Eu(1)-O(4)	143.1(2)
O(5)-Eu(1)-O(2)	149.1(2)	O(7)-Eu(1)-O(4)	134.8(2)
O(4)-Eu(1)-O(2)	129.7(2)	O(2)-Eu(1)-O(4)	124.7(2)
O(6)-Eu(1)-O(2)	73.5(2)	N(2)-Eu(1)-O(4)	112.8(2)

Πίνακας Π2-25: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8/**Ima

Μήκη δεσμών (Å) της ένωσης UCY-8/Ima

Eu(1)-O(1)	2.457(5)	Eu(1)-O(5)	2.415(5)
Eu(1)-O(2)	2.447(5)	Eu(1)-O(6)	2.375(5)
Eu(1)-O(3)	2.423(5)	Eu(1)-O(7)	2.452(7)
Eu(1)-O(4)	2.362(5)	Eu(1)-N(2)	2.589(8)
Eu(1)-O(4)	2.643(5)		

Γωνίες δεσμών (º) της ένωσης UCY-8/Ima

O(4)-Eu(1)-O(6)	76.9(2)	O(3)-Eu(1)-O(1)	128.3(2)
O(4)-Eu(1)-O(5)	74.9(2)	O(2)-Eu(1)-O(1)	53.3(2)
O(6)-Eu(1)-O(5)	136.2(2)	O(7)-Eu(1)-O(1)	68.6(2)
O(4)-Eu(1)-O(3)	123.8(2)	O(4)-Eu(1)-N(2)	146.6(2)
O(6)-Eu(1)-O(3)	96.2(2)	O(6)-Eu(1)-N(2)	71.6(2)
O(5)-Eu(1)-O(3)	73.2(2)	O(5)-Eu(1)-N(2)	137.2(2)
O(4)-Eu(1)-O(2)	131.2(2)	O(3)-Eu(1)-N(2)	71.6(2)
O(6)-Eu(1)-O(2)	147.2(2)	O(2)-Eu(1)-N(2)	76.7(2)
O(5)-Eu(1)-O(2)	74.8(2)	O(7)-Eu(1)-N(2)	67.1(3)
O(3)-Eu(1)-O(2)	81.6(2)	O(1)-Eu(1)-N(2)	113.9(3)
O(4)-Eu(1)-O(7)	93.9(3)	O(4)-Eu(1)-O(4)	74.9(2)
O(6)-Eu(1)-O(7)	74.5(2)	O(6)-Eu(1)-O(4)	69.6(2)
O(5)-Eu(1)-O(7)	140.0(2)	O(5)-Eu(1)-O(4)	71.1(2)
O(3)-Eu(1)-O(7)	138.5(3)	O(3)-Eu(1)-O(4)	51.4(2)
O(2)-Eu(1)-O(7)	85.5(3)	O(2)-Eu(1)-O(4)	127.8(2)
O(4)-Eu(1)-O(1)	81.1(2)	O(7)-Eu(1)-O(4)	143.8(2)
O(6)-Eu(1)-O(1)	135.1(2)	O(1)-Eu(1)-O(4)	139.7(2)
O(5)-Eu(1)-O(1)	71.7(2)	N(2)-Eu(1)-O(4)	103.7(2)

Πίνακας Π2-26: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8/**mIma

Μήκη δεσμών (Å) της ένωσης UCY-8/mIma

Eu(1)-O(1)	2.469(4)	Eu(1)-O(5)	2.379(4)
Eu(1)-O(2)	2.467(4)	Eu(1)-O(6)	2.364(4)
Eu(1)-O(3)	2.426(4)	Eu(1)-O(7)	2.483(7)
Eu(1)-O(4)	2.352(4)	Eu(1)-N(2)	2.517(7)
Eu(1)-O(4)	2.693(4)		

Γωνίες δεσμών (º) της ένωσης UCY-8/mIma

O(4)-Eu(1)-O(6)	79.2(2)	O(3)-Eu(1)-O(7)	142.6(2)
O(4)-Eu(1)-O(5)	73.8(2)	O(2)-Eu(1)-O(7)	68.2(2)
O(6)-Eu(1)-O(5)	134.5(2)	O(1)-Eu(1)-O(7)	95.0(2)
O(4)-Eu(1)-O(3)	124.7(2)	O(4)-Eu(1)-N(2)	145.4(2)
O(6)-Eu(1)-O(3)	90.4(2)	O(6)-Eu(1)-N(2)	71.4(2)
O(5)-Eu(1)-O(3)	76.4(2)	O(5)-Eu(1)-N(2)	140.6(2)
O(4)-Eu(1)-O(2)	85.3(2)	O(3)-Eu(1)-N(2)	74.3(2)
O(6)-Eu(1)-O(2)	140.3(2)	O(2)-Eu(1)-N(2)	105.7(2)
O(5)-Eu(1)-O(2)	73.1(12)	O(1)-Eu(1)-N(2)	74.8(2)
O(3)-Eu(1)-O(2)	127.9(2)	O(7)-Eu(1)-N(2)	68.6(2)
O(4)-Eu(1)-O(1)	133.0(2)	O(4)-Eu(1)-O(4)	75.3(2)
O(6)-Eu(1)-O(1)	146.2(2)	O(6)-Eu(1)-O(4)	68.0(2)
O(5)-Eu(1)-O(1)	74.1(2)	O(5)-Eu(1)-O(4)	70.1(2)
O(3)-Eu(1)-O(1)	78.7(2)	O(3)-Eu(1)-O(4)	51.0(2)
O(2)-Eu(1)-O(1)	52.8(2)	O(2)-Eu(1)-O(4)	141.9(2)
O(4)-Eu(1)-O(7)	86.4(2)	O(1)-Eu(1)-O(4)	123.1(2)
O(6)-Eu(1)-O(7)	74.4(2)	O(7)-Eu(1)-O(4)	140.5(2)
O(5)-Eu(1)-O(7)	137.7(2)	N(2)-Eu(1)-O(4)	108.9(2)

Πίνακας Π2-27: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8/**atzH

Μήκη δεσμών (Å) της ένωσης UCY-8/atzH

Eu(1)-O(3)	2.357(4)	Eu(1)-O(2)	2.455(4)
Eu(1)-O(6)	2.364(4)	Eu(1)-O(1)	2.515(4)
Eu(1)-O(5)	2.383(4)	Eu(1)-N(3)	2.606(5)
Eu(1)-O(7)	2.426(5)	Eu(1)-O(3)	2.669(4)
Eu(1)-O(4)	2.431(4)		

Γωνίες δεσμών (º) της ένωσης UCY-8/atzH

O(3)-Eu(1)-O(6)	79(2)	O(7)-Eu(1)-O(1)	102.0(2)
O(3)-Eu(1)-O(5)	73.3(2)	O(4)-Eu(1)-O(1)	79.3(2)
O(6)-Eu(1)-O(5)	133.7(2)	O(2)-Eu(1)-O(1)	52.5(2)
O(3)-Eu(1)-O(7)	81.2(2)	O(3)-Eu(1)-N(3)	148.5(2)
O(6)-Eu(1)-O(7)	71.6(2)	O(6)-Eu(1)-N(3)	75.5(2)
O(5)-Eu(1)-O(7)	136.7(2)	O(5)-Eu(1)-N(3)	138.2(2)
O(3)-Eu(1)-O(4)	122.6(2)	O(7)-Eu(1)-N(3)	73.5(2)
O(6)-Eu(1)-O(4)	90.2(2)	O(4)-Eu(1)-N(3)	75.8(2)
O(5)-Eu(1)-O(4)	75.3(2)	O(2)-Eu(1)-N(3)	103.0(2)
O(7)-Eu(1)-O(4)	147.3(2)	O(1)-Eu(1)-N(3)	73.2(2)
O(3)-Eu(1)-O(2)	85.4(2)	O(3)-Eu(1)-O(3)	73.9(2)
O(6)-Eu(1)-O(2)	140.6(2)	O(6)-Eu(1)-O(3)	67.0(2)
O(5)-Eu(1)-O(2)	73.1(2)	O(5)-Eu(1)-O(3)	70.1(2)
O(7)-Eu(1)-O(2)	70.4(2)	O(7)-Eu(1)-O(3)	134.8(2)
O(4)-Eu(1)-O(2)	128.2(2)	O(4)-Eu(1)-O(3)	50.5(2)
O(3)-Eu(1)-O(1)	131.5(2)	O(2)-Eu(1)-O(3)	141.6(2)
O(6)-Eu(1)-O(1)	148.5(2)	O(1)-Eu(1)-O(3)	122.8(2)
O(5)-Eu(1)-O(1)	72.3(2)	N(3)-Eu(1)-O(3)	111.6(2)

Πίνακας Π2-28: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8/**2hpH_2

Μήκη δεσμών (Å) της ένωσης UCY-8/2hpH$_2$

Eu(1)-O(1)	2.465(6)	Eu(1)-O(5)	2.366(6)
Eu(1)-O(2)	2.471(6)	Eu(1)-O(6)	2.382(5)
Eu(1)-O(3)	2.426(5)	Eu(1)-O(7)	2.52(4)
Eu(1)-O(4)	2.360(6)	Eu(1)-O(7A)	2.38(2)
Eu(1)-O(4)	2.627(6)	Eu(1)-O(8)	2.451(7)

Γωνίες δεσμών (º) της ένωσης UCY-8/2hpH$_2$

O(4)-Eu(1)-O(5)	72.2(2)	O(3)-Eu(1)-O(8)	77.6(3)
O(4)-Eu(1)-O(6)	80.7(2)	O(7A)-Eu(1)-O(8)	70(2)
O(5)-Eu(1)-O(6)	134.1(2)	O(7)-Eu(1)-O(8)	72.2(7)
O(4)-Eu(1)-O(3)	124.1(2)	O(4)-Eu(1)-O(1)	136.8(2)
O(5)-Eu(1)-O(3)	78.3(2)	O(5)-Eu(1)-O(1)	74.4(2)
O(6)-Eu(1)-O(3)	87.8(2)	O(6)-Eu(1)-O(1)	142.4(2)
O(4)-Eu(1)-O(7A)	80(2)	O(3)-Eu(1)-O(1)	73.5(2)
O(5)-Eu(1)-O(7A)	134.9(9)	O(7A)-Eu(1)-O(1)	105.9(9)
O(6)-Eu(1)-O(7A)	72.4(9)	O(7)-Eu(1)-O(1)	104.2(9)
O(3)-Eu(1)-O(7A)	146.3(2)	O(8)-Eu(1)-O(1)	72.1(2)
O(4)-Eu(1)-O(7)	79.6(7)	O(4)-Eu(1)-O(2)	91.2(2)
O(5)-Eu(1)-O(7)	132.0(8)	O(5)-Eu(1)-O(2)	72.8(3)
O(6)-Eu(1)-O(7)	75.5(9)	O(6)-Eu(1)-O(2)	145.2(2)
O(3)-Eu(1)-O(7)	148.7(7)	O(3)-Eu(1)-O(2)	123.7(2)
O(7A)-Eu(1)-O(7)	3(2)	O(7A)-Eu(1)-O(2)	72.9(9)
O(4)-Eu(1)-O(8)	144.7(2)	O(7)-Eu(1)-O(2)	69.7(9)
O(5)-Eu(1)-O(8)	143.1(2)	O(8)-Eu(1)-O(2)	98.3(3)
O(6)-Eu(1)-O(8)	72.2(2)	O(1)-Eu(1)-O(2)	52.8(2)
O(4)-Eu(1)-O(4)	74.3(2)	O(7A)-Eu(1)-O(4)	135.5(9)
O(5)-Eu(1)-O(4)	69.4(2)	O(7)-Eu(1)-O(4)	137.7(9)
O(6)-Eu(1)-O(4)	67.9(2)	O(8)-Eu(1)-O(4)	113.9(3)
O(3)-Eu(1)-O(4)	51.0(2)	O(1)-Eu(1)-O(4)	117.7(2)
O(2)-Eu(1)-O(4)	142.1(3)		

Πίνακας Π2-29: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8/**2hmp

Μήκη δεσμών (Å) της ένωσης UCY-8/2hmp

Eu(1)-N(2)	2.59(2)	Eu(1)-O(4)	2.660(7)
Eu(1)-O(1)	2.496(8)	Eu(1)-O(5)	2.364(8)
Eu(1)-O(2)	2.439(6)	Eu(1)-O(6)	2.382(7)
Eu(1)-O(3)	2.404(8)	Eu(1)-O(7)	2.429(8)
Eu(1)-O(4)	2.369(7)	Eu(1)-O(6)	2.382(7)
		Eu(1)-O(4)	2.660(7)

Γωνίες δεσμών (º) της ένωσης UCY-8/2hmp

O(6)-Eu(1)-O(1)	138.2(3)	O(7)-Eu(1)-O(1)	68.2(3)
O(5)-Eu(1)-O(4)	75.2(3)	O(2)-Eu(1)-O(1)	53.6(3)
O(5)-Eu(1)-O(6)	135.3(3)	O(5)-Eu(1)-N(2)	143.3(3)
O(4)-Eu(1)-O(6)	77.5(3)	O(4)-Eu(1)-N(2)	141.3(3)
O(5)-Eu(1)-O(3)	76.3(3)	O(6)-Eu(1)-N(2)	69.0(3)
O(4)-Eu(1)-O(3)	124.6(3)	O(3)-Eu(1)-N(2)	76.2(3)
O(6)-Eu(1)-O(3)	91.4(3)	O(7)-Eu(1)-N(2)	63.0(3)
O(5)-Eu(1)-O(7)	138.3(3)	O(2)-Eu(1)-N(2)	75.8(3)
O(4)-Eu(1)-O(7)	90.9(3)	O(1)-Eu(1)-N(2)	110.4(3)
O(6)-Eu(1)-O(7)	76.0(3)	O(5)-Eu(1)-O(4)	69.9(2)
O(3)-Eu(1)-O(7)	139.2(3)	O(4)-Eu(1)-O(4)	75.4(3)
O(5)-Eu(1)-O(2)	77.2(2)	O(6)-Eu(1)-O(4)	69.5(3)
O(4)-Eu(1)-O(2)	133.4(2)	O(3)-Eu(1)-O(4)	50.4(2)
O(6)-Eu(1)-O(2)	144.7(3)	O(7)-Eu(1)-O(4)	144.8(3)
O(3)-Eu(1)-O(2)	83.0(2)	O(2)-Eu(1)-O(4)	127.3(2)
O(7)-Eu(1)-O(2)	85.6(3)	O(1)-Eu(1)-O(4)	138.6(3)
O(5)-Eu(1)-O(1)	71.0(3)	N(2)-Eu(1)-O(4)	108.9(3)
O(4)-Eu(1)-O(1)	82.1(3)	O(3)-Eu(1)-O(1)	129.9(2)
		O(7)-Eu(1)-O(1)	104.6(3)

Πίνακας Π2-30: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/merpdH_2

Μήκη δεσμών (Å) της ένωσης UCY-8/merpdH_2

Eu(1)-O(4)	2.353(6)	Eu(1)-O(7)	2.45(2)
Eu(1)-O(6)	2.356(7)	Eu(1)-O(2)	2.464(7)
Eu(1)-O(5)	2.364(6)	Eu(1)-O(1)	2.503(7)
Eu(1)-O(9)	2.41(2)	Eu(1)-O(4)	2.716(7)
Eu(1)-O(3)	2.417(7)		

Γωνίες δεσμών (º) της ένωσης UCY-8/merpdH_2

O(4)-Eu(1)-O(6)	74.1(2)	O(9)-Eu(1)-O(2)	69.5(4)
O(4)-Eu(1)-O(5)	79.9(2)	O(3)-Eu(1)-O(2)	129.1(2)
O(6)-Eu(1)-O(5)	133.1(2)	O(7)-Eu(1)-O(2)	102.9(4)
O(4)-E (1)-O(9)	82.6(4)	O(4)-Eu(1)-O(1)	132.7(2)
O(6)-Eu(1)-O(9)	137.2(4)	O(6)-Eu(1)-O(1)	73.7(2)
O(5)-Eu(1)-O(9)	74.6(4)	O(5)-Eu(1)-O(1)	146.4(3)
O(4)-Eu(1)-O(3)	124.6(2)	O(9)-Eu(1)-O(1)	98.7(4)
O(6)-Eu(1)-O(3)	77.3(3)	O(3)-Eu(1)-O(1)	80.1(3)
O(5)-Eu(1)-O(3)	86.7(2)	O(7)-Eu(1)-O(1)	72.5(3)
O(9)-Eu(1)-O(3)	144.1(4)	O(2)-Eu(1)-O(1)	52.4(3)
O(4)-Eu(1)-O(7)	146.9(3)	O(4)-Eu(1)-O(4)	75.5(2)
O(6)-Eu(1)-O(7)	138.9(4)	O(6)-Eu(1)-O(4)	69.3(2)
O(5)-Eu(1)-O(7)	74.2(3)	O(5)-Eu(1)-O(4)	66.8(2)
O(9)-Eu(1)-O(7)	71.1(6)	O(9)-Eu(1)-O(4)	138.1(4)
O(3)-Eu(1)-O(7)	74.5(5)	O(3)-Eu(1)-O(4)	50.1(2)
O(4)-Eu(1)-O(2)	85.5(2)	O(7)-Eu(1)-O(4)	111.4(4)
O(6)-Eu(1)-O(2)	73.3(3)	O(2)-Eu(1)-O(4)	141.4(3)
O(5)-Eu(1)-O(2)	142.7(3)	O(1)-Eu(1)-O(4)	122.4(3)

Πίνακας Π2-31: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/py

Μήκη δεσμών (Å) της ένωσης UCY-8/py

Eu(1)-N(2)	2.633(6)	Eu(1)-O(7)	2.420(5)
Eu(2)-N(4)	2.679(5)	Eu(2)-O(8)	2.533(5)
Eu(1)-O(1)	2.429(5)	Eu(2)-O(9)	2.443(5)
Eu(1)-O(2)	2.552(5)	Eu(2)-O(10)	2.357(4)
Eu(1)-O(3)	2.408(4)	Eu(2)-O(10)	2.712(5)
Eu(1)-O(4)	2.298(5)	Eu(2)-O(11)	2.450(4)
Eu(1)-O(4)	3.071(5)	Eu(1)-O(12)	2.325(4)
Eu(2)-O(5)	2.365(4)	Eu(2)-O(14)	2.409(5)
Eu(2)-O(6)	2.405(4)	Eu(1)-O(13)	2.397(4)
		Eu(2)-O(10)	2.357(4)

Γωνίες δεσμών (°) της ένωσης UCY-8/py

O(4)-Eu(1)-O(13)	79.1(2)	O(7)-Eu(1)-O(2)	74.8(2)
O(12)-Eu(1)-O(13)	128.5(2)	O(1)-Eu(1)-O(2)	52.3(2)
O(4)-Eu(1)-O(3)	124.5(2)	O(4)-Eu(1)-N(2)	150.6(2)
O(12)-Eu(1)-O(3)	73.7(2)	O(12)-Eu(1)-N(2)	131.9(2)
O(13)-Eu(1)-O(3)	84.4(2)	O(13)-Eu(1)-N(2)	76.1(2)
O(4)-Eu(1)-O(7)	85.5(2)	O(3)-Eu(1)-N(2)	68.4(2)
O(12)-Eu(1)-O(7)	144.6(2)	O(7)-Eu(1)-N(2)	73.4(2)
O(13)-Eu(1)-O(7)	75.9(2)	O(1)-Eu(1)-N(2)	72.5(2)
O(3)-Eu(1)-O(7)	140.2(2)	O(2)-Eu(1)-N(2)	114.7(2)
O(4)-Eu(1)-O(1)	128.9(2)	O(4)-Eu(1)-C(1)	103.1(2)
O(12)-Eu(1)-O(1)	78.4(2)	O(12)-Eu(1)-C(1)	72.2(2)
O(13)-Eu(1)-O(1)	148.2(2)	O(13)-Eu(1)-C(1)	158.3(2)
O(3)-Eu(1)-O(1)	88.9(2)	O(3)-Eu(1)-C(1)	110.6(2)
O(7)-Eu(1)-O(1)	90.1(2)	O(7)-Eu(1)-C(1)	82.7(2)
O(4)-Eu(1)-O(2)	77.7(2)	O(1)-Eu(1)-C(1)	26.2(2)
O(12)-Eu(1)-O(2)	71.7(2)	O(2)-Eu(1)-C(1)	26.1(2)
O(13)-Eu(1)-O(2)	143.7(2)	N(2)-Eu(1)-C(1)	94.4(2)
O(3)-Eu(1)-O(2)	131.9(2)	O(4)-Eu(1)-O(4)	79.4(2)
O(12)-Eu(1)-O(4)	62.8(2)	O(1)-Eu(1)-O(4)	125.2(2)
O(13)-Eu(1)-O(4)	68.6(2)	O(2)-Eu(1)-O(4)	132.6(2)
O(3)-Eu(1)-O(4)	45.4(2)	N(2)-Eu(1)-O(4)	105.5(2)
O(7)-Eu(1)-O(4)	143.4(2)	C(1)-Eu(1)-O(4)	133.2(2)

Πίνακας Π2-32: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/2mpy

Μήκη δεσμών (Å) της ένωσης UCY-8/2mpy

Eu(1)-O(4)	2.337(6)	Eu(1)-O(2)	2.444(7)
Eu(1)-O(6)	2.361(6)	Eu(1)-O(7)	2.47(2)
Eu(1)-O(5)	2.381(6)	Eu(1)-O(1)	2.495(7)
Eu(1)-O(8)	2.418(9)	Eu(1)-O(4)	2.748(7)
Eu(1)-O(3)	2.422(6)		

Γωνίες δεσμών (º) της ένωσης UCY-8/2mpy

O(4)-Eu(1)-O(6)	74.1(2)	O(8)-Eu(1)-O(7)	73.7(4)
O(4)-Eu(1)-O(5)	78.9(2)	O(3)-Eu(1)-O(7)	71.9(4)
O(6)-Eu(1)-O(5)	133.4(2)	O(2)-Eu(1)-O(7)	71.8(3)
O(4)-Eu(1)-O(8)	83.5(3)	O(4)-Eu(1)-O(1)	84.4(2)
O(6)-Eu(1)-O(8)	136.6(3)	O(6)-Eu(1)-O(1)	70.8(3)
O(5)-Eu(1)-O(8)	75.0(3)	O(5)-Eu(1)-O(1)	143.0(2)
O(4)-Eu(1)-O(3)	124.3(2)	O(8)-Eu(1)-O(1)	70.4(3)
O(6)-Eu(1)-O(3)	76.5(2)	O(3)-Eu(1)-O(1)	127.6(2)
O(5)-Eu(1)-O(3)	88.8(2)	O(2)-Eu(1)-O(1)	52.3(2)
O(8)-Eu(1)-O(3)	144.9(3)	O(7)-Eu(1)-O(1)	108.4(3)
O(4)-Eu(1)-O(2)	133.9(2)	O(4)-Eu(1)-O(4)	75.4(2)
O(6)-Eu(1)-O(2)	76.8(2)	O(6)-Eu(1)-O(4)	68.7(2)
O(5)-Eu(1)-O(2)	144.9(2)	O(5)-Eu(1)-O(4)	68.1(2)
O(8)-Eu(1)-O(2)	94.2(3)	O(8)-Eu(1)-O(4)	140.2(3)
O(3)-Eu(1)-O(2)	81.3(2)	O(3)-Eu(1)-O(4)	49.9(2)
O(4)-Eu(1)-O(7)	147.5(3)	O(2)-Eu(1)-O(4)	124.7(2)
O(6)-Eu(1)-O(7)	138.0(3)	O(7)-Eu(1)-O(4)	108.2(3)
O(5)-Eu(1)-O(7)	73.2(3)	O(1)-Eu(1)-O(4)	138.3(2)

Πίνακας Π2-33: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/Im-atzH

Μήκη δεσμών (Å) της ένωσης UCY-8/Im-atzH

Eu(1)-O(1)	2.462(6)	Eu(1)-O(5)	2.427(5)
Eu(1)-O(2)	2.483(6)	Eu(1)-O(6)	2.395(6)
Eu(1)-O(3)	2.437(7)	Eu(1)-O(7)	2.418(7)
Eu(1)-O(4)	2.371(6)	Eu(1)-N(2)	2.551(9)
Eu(1)-O(4)	2.697(6)		

Γωνίες δεσμών (º) της ένωσης UCY-8/Im-atzH

O(4)-Eu(1)-O(6)	77.8(2)	O(5)-Eu(1)-O(2)	71.8(2)
O(4)-Eu(1)-O(7)	88.7(2)	O(3)-Eu(1)-O(2)	128.1(2)
O(6)-Eu(1)-O(7)	75.4(2)	O(1)-Eu(1)-O(2)	52.6(2)
O(4)-Eu(1)-O(5)	74.8(2)	O(4)-Eu(1)-N(2)	150.3(2)
O(6)-Eu(1)-O(5)	134.0(2)	O(6)-Eu(1)-N(2)	74.7(2)
O(7)-Eu(1)-O(5)	139.0(2)	O(7)-Eu(1)-N(2)	73.7(3)
O(4)-Eu(1)-O(3)	122.3(2)	O(5)-Eu(1)-N(2)	133.7(2)
O(6)-Eu(1)-O(3)	93.4(2)	O(3)-Eu(1)-N(2)	70.9(2)
O(7)-Eu(1)-O(3)	144.5(2)	O(1)-Eu(1)-N(2)	73.5(2)
O(5)-Eu(1)-O(3)	71.8(2)	O(2)-Eu(1)-N(2)	112.8(2)
O(4)-Eu(1)-O(1)	131.0(2)	O(4)-Eu(1)-O(4)	74.4(2)
O(6)-Eu(1)-O(1)	147.3(2)	O(6)-Eu(1)-O(4)	68.2(2)
O(7)-Eu(1)-O(1)	88.5(2)	O(7)-Eu(1)-O(4)	142.2(2)
O(5)-Eu(1)-O(1)	75.8(2)	O(5)-Eu(1)-O(4)	69.3(2)
O(3)-Eu(1)-O(1)	83.3(2)	O(3)-Eu(1)-O(4)	50.2(2)
O(4)-Eu(1)-O(2)	81.1(2)	O(1)-Eu(1)-O(4)	128.1(2)
O(6)-Eu(1)-O(2)	138.4(2)	O(2)-Eu(1)-O(4)	138.1(2)
O(7)-Eu(1)-O(2)	68.6(2)	N(2)-Eu(1)-O(4)	105.0(2)

Πίνακας Π2-34: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/bpy

Μήκη δεσμών (Å) της ένωσης UCY-8/bpy

Eu(1)-O(5)	2.368(3)	Eu(1)-O(7)	2.472(4)
Eu(1)-O(3)	2.386(4)	Eu(1)-O(2)	2.483(4)
Eu(1)-O(4)	2.407(3)	Eu(1)-O(5)	2.647(3)
Eu(1)-O(6)	2.410(4)	Eu(1)-N(2)	2.667(4)
Eu(1)-O(1)	2.440(4)		

Γωνίες δεσμών (º) της ένωσης UCY-8/bpy

O(5)-Eu(1)-O(3)	71.2(2)	O(6)-Eu(1)-O(2)	78.6(2)
O(5)-Eu(1)-O(4)	84.6(2)	O(1)-Eu(1)-O(2)	53.2(2)
O(3)-Eu(1)-O(4)	133.7(2)	O(7)-Eu(1)-O(2)	112.0(2)
O(5)-Eu(1)-O(6)	126.4(2)	O(5)-Eu(1)-O(5)	75.6(2)
O(3)-Eu(1)-O(6)	82.7(2)	O(3)-Eu(1)-O(5)	70.4(2)
O(4)-Eu(1)-O(6)	82.0(2)	O(4)-Eu(1)-O(5)	65.6(2)
O(5)-Eu(1)-O(1)	89.3(2)	O(6)-Eu(1)-O(5)	51.4(2)
O(3)-Eu(1)-O(1)	79.9(2)	O(1)-Eu(1)-O(5)	149.6(2)
O(4)-Eu(1)-O(1)	140.1(2)	O(7)-Eu(1)-O(5)	128.1(2)
O(6)-Eu(1)-O(1)	131.7(2)	O(2)-Eu(1)-O(5)	119.7(2)
O(5)-Eu(1)-O(7)	74.2(2)	O(5)-Eu(1)-N(2)	145.4(2)
O(3)-Eu(1)-O(7)	133.9(2)	O(3)-Eu(1)-N(2)	142.3(3)
O(4)-Eu(1)-O(7)	70.3(2)	O(4)-Eu(1)-N(2)	74.3(2)
O(6)-Eu(1)-O(7)	143.2(2)	O(6)-Eu(1)-N(2)	77.6(3)
O(1)-Eu(1)-O(7)	70.1(2)	O(1)-Eu(1)-N(2)	89.6(3)
O(5)-Eu(1)-O(2)	131.2(2)	O(7)-Eu(1)-N(2)	72.9(3)
O(3)-Eu(1)-O(2)	72.2(2)	O(2)-Eu(1)-N(2)	72.5(3)
O(4)-Eu(1)-O(2)	144.0(2)	O(5)-Eu(1)-N(2)	117.7(2)

Πίνακας Π2-35: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/bpa

Μήκη δεσμών (Å) της ένωσης UCY-8/bpa

Eu(1)-O(6)	2.353(6)	Eu(1)-O(1)	2.496(7)
Eu(1)-O(3)	2.357(7)	Eu(1)-N(3)	2.54(2)
Eu(1)-O(4)	2.393(6)	Eu(1)-O(7)	2.60(2)
Eu(1)-O(5)	2.408(6)	Eu(1)-O(6)	2.622(6)
Eu(1)-O(2)	2.430(7)		

Γωνίες δεσμών (º) της ένωσης UCY-8/bpa

O(6)-Eu(1)-O(3)	72.8(2)	O(5)-Eu(1)-N(3)	81.7(3)
O(6)-Eu(1)-O(4)	82.9(2)	O(2)-Eu(1)-N(3)	86.2(3)
O(3)-Eu(1)-O(4)	133.9(2)	O(1)-Eu(1)-N(3)	72.7(3)
O(6)-Eu(1)-O(5)	126.0(2)	O(6)-Eu(1)-O(7)	70.7(3)
O(3)-Eu(1)-O(5)	81.1(2)	O(3)-Eu(1)-O(7)	130.5(3)
O(4)-Eu(1)-O(5)	82.6(2)	O(4)-Eu(1)-O(7)	72.3(3)
O(6)-Eu(1)-O(2)	89.7(3)	O(5)-Eu(1)-O(7)	148.2(3)
O(3)-Eu(1)-O(2)	84.0(3)	O(2)-Eu(1)-O(7)	63.8(4)
O(4)-Eu(1)-O(2)	135.4(3)	O(1)-Eu(1)-O(7)	108.2(4)
O(5)-Eu(1)-O(2)	133.9(3)	N(3)-Eu(1)-O(7)	72.7(4)
O(6)-Eu(1)-O(1)	132.3(2)	O(6)-Eu(1)-O(6)	75.4(2)
O(3)-Eu(1)-O(1)	74.5(3)	O(3)-Eu(1)-O(6)	69.5(2)
O(4)-Eu(1)-O(1)	143.9(2)	O(4)-Eu(1)-O(6)	66.7(2)
O(5)-Eu(1)-O(1)	81.0(2)	O(5)-Eu(1)-O(6)	51.1(2)
O(2)-Eu(1)-O(1)	53.0(3)	O(2)-Eu(1)-O(6)	152.4(3)
O(6)-Eu(1)-N(3)	140.9(3)	O(1)-Eu(1)-O(6)	122.7(3)
O(3)-Eu(1)-N(3)	144.8(3)	N(3)-Eu(1)-O(6)	120.0(3)
O(4)-Eu(1)-N(3)	73.4(3)	O(7)-Eu(1)-O(6)	129.1(3)

Πίνακας Π2-36: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-8**/bpe

Μήκη δεσμών (Å) της ένωσης UCY-8/bpe

Eu(1)-O(4)	2.347(4)	Eu(1)-O(1)	2.518(4)
Eu(1)-O(6)	2.351(4)	Eu(1)-N(3)	2.547(5)
Eu(1)-O(3)	2.388(4)	Eu(1)-O(6)	2.604(4)
Eu(1)-O(5)	2.423(4)	Eu(1)-O(7)	2.639(5)
Eu(1)-O(2)	2.424(4)		

Γωνίες δεσμών (º) της ένωσης UCY-8/bpe

O(4)-Eu(1)-O(6)	73.1(2)	O(5)-Eu(1)-N(3)	80.5(2)
O(4)-Eu(1)-O(3)	134.7(2)	O(2)-Eu(1)-N(3)	86.9(2)
O(6)-Eu(1)-O(3)	81.2(2)	O(1)-Eu(1)-N(3)	72.8(2)
O(4)-Eu(1)-O(5)	81.9(2)	O(4)-Eu(1)-O(6)	70.3(2)
O(6)-Eu(1)-O(5)	125.7(2)	O(6)-Eu(1)-O(6)	74.6(2)
O(3)-Eu(1)-O(5)	83.8(2)	O(3)-Eu(1)-O(6)	67.1(2)
O(4)-Eu(1)-O(2)	82.5(2)	O(5)-Eu(1)-O(6)	51.6(2)
O(6)-Eu(1)-O(2)	91.4(2)	O(2)-Eu(1)-O(6)	152.0(2)
O(3)-Eu(1)-O(2)	135.6(2)	O(1)-Eu(1)-O(6)	122.1(2)
O(5)-Eu(1)-O(2)	132.5(2)	N(3)-Eu(1)-O(6)	119.2(2)
O(4)-Eu(1)-O(1)	73.8(2)	O(4)-Eu(1)-O(7)	130.4(2)
O(6)-Eu(1)-O(1)	133.6(2)	O(6)-Eu(1)-O(7)	71.7(2)
O(3)-Eu(1)-O(1)	144.4(2)	O(3)-Eu(1)-O(7)	71.5(2)
O(5)-Eu(1)-O(1)	79.9(2)	O(5)-Eu(1)-O(7)	147.7(2)
O(2)-Eu(1)-O(1)	52.7(2)	O(2)-Eu(1)-O(7)	64.7(2)
O(4)-Eu(1)-N(3)	144.3(2)	O(1)-Eu(1)-O(7)	108.5(2)
O(6)-Eu(1)-N(3)	141.4(2)	N(3)-Eu(1)-O(7)	72.8(2)
O(3)-Eu(1)-N(3)	73.4(2)	O(6)-Eu(1)-O(7)	129.5(2)

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων UCY-9

Πίνακας Π2-37: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **UCY-9**/Ακετόνη

Μήκη δεσμών (Å) της ένωσης UCY-9/Ακετόνη

Gd(1)-O(2)	2.337(5)	Gd(1)-O(3)	2.452(6)
Gd(1)-O(6)	2.366(5)	Gd(1)-O(7)	2.464(7)
Gd(1)-O(5)	2.374(5)	Gd(1)-O(4)	2.471(6)
Gd(1)-O(1)	2.416(6)	Gd(1)-O(2)	2.682(5)
Gd(1)-O(8)	2.442(8)		

Γωνίες δεσμών (º) της ένωσης UCY-9/Ακετόνη

O(2)-Gd(1)-O(6)	80.7(2)	O(1)-Gd(1)-O(7)	148.6(2)
O(2)-Gd(1)-O(5)	73.2(2)	O(8)-Gd(1)-O(7)	74.2(3)
O(6)-Gd(1)-O(5)	133.5(2)	O(3)-Gd(1)-O(7)	102.9(3)
O(2)-Gd(1)-O(1)	124.0(2)	O(2)-Gd(1)-O(4)	85.4(2)
O(6)-Gd(1)-O(1)	87.6(2)	O(6)-Gd(1)-O(4)	143.2(2)
O(5)-Gd(1)-O(1)	76.7(2)	O(5)-Gd(1)-O(4)	72.5(2)
O(2)-Gd(1)-O(8)	146.0(2)	O(1)-Gd(1)-O(4)	127.9(2)
O(6)-Gd(1)-O(8)	73.2(2)	O(8)-Gd(1)-O(4)	102.7(3)
O(5)-Gd(1)-O(8)	140.8(2)	O(3)-Gd(1)-O(4)	53.2(2)
O(1)-Gd(1)-O(8)	76.8(3)	O(7)-Gd(1)-O(4)	71.0(2)
O(2)-Gd(1)-O(3)	133.8(2)	O(2)-Gd(1)-O(2)	74.6(2)
O(6)-Gd(1)-O(3)	144.5(2)	O(6)-Gd(1)-O(2)	66.4(2)
O(5)-Gd(1)-O(3)	75.1(2)	O(5)-Gd(1)-O(2)	69.9(2)
O(1)-Gd(1)-O(3)	78.9(2)	O(1)-Gd(1)-O(2)	50.9(2)
O(8)-Gd(1)-O(3)	71.8(2)	O(8)-Gd(1)-O(2)	112.7(3)
O(2)-Gd(1)-O(7)	77.6(3)	O(3)-Gd(1)-O(2)	123.4(2)
O(6)-Gd(1)-O(7)	72.7(2)	O(7)-Gd(1)-O(2)	133.3(2)
O(5)-Gd(1)-O(7)	134.5(2)	O(4)-Gd(1)-O(2)	141.1(2)

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων EuN-BDC

Πίνακας Π2-38: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/Im

Μήκη δεσμών (Å) της ένωσης EuN-BDC/Im

Eu(01)-N(4)	2.531(7)	Eu(01)-O(3)	2.729(5)
Eu(01)-N(6)	2.473(7)	Eu(01)-O(4)	2.446(5)
Eu(01)-O(1)	2.487(6)	Eu(01)-O(5)	2.378(5)
Eu(01)-O(2)	2.496(6)	Eu(01)-O(6)	2.365(5)
Eu(01)-O(3)	2.358(5)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/Im

O(3)-Eu(01)-O(6)	76.1(2)	O(4)-Eu(01)-O(2)	124.1(2)
O(3)-Eu(01)-O(5)	75.6(2)	N(6)-Eu(01)-O(2)	69.8(2)
O(6)-Eu(01)-O(5)	133.2(2)	O(1)-Eu(01)-O(2)	52.1(2)
O(3)-Eu(01)-O(4)	123.7(2)	O(3)-Eu(01)-N(4)	145.2(2)
O(6)-Eu(01)-O(4)	91.2(2)	O(6)-Eu(01)-N(4)	73.5(2)
O(5)-Eu(01)-O(4)	74.8(2)	O(5)-Eu(01)-N(4)	138.8(2)
O(3)-Eu(01)-N(6)	82.9(2)	O(4)-Eu(01)-N(4)	73.8(2)
O(6)-Eu(01)-N(6)	75.5(2)	N(6)-Eu(01)-N(4)	73.4(3)
O(5)-Eu(01)-N(6)	135.7(2)	O(1)-Eu(01)-N(4)	74.4(2)
O(4)-Eu(01)-N(6)	147.0(2)	O(2)-Eu(01)-N(4)	105.7(2)
O(3)-Eu(01)-O(1)	135.7(2)	O(3)-Eu(01)-O(3)	74.7(2)
O(6)-Eu(01)-O(1)	147.6(2)	O(6)-Eu(01)-O(3)	68.9(1)
O(5)-Eu(01)-O(1)	72.5(2)	O(5)-Eu(01)-O(3)	68.1(1)
O(4)-Eu(01)-O(1)	75.8(2)	O(4)-Eu(01)-O(3)	50.1(2)
N(6)-Eu(01)-O(1)	99.2(2)	N(6)-Eu(01)-O(3)	141.4(2)
O(3)-Eu(01)-O(2)	89.0(2)	O(1)-Eu(01)-O(3)	118.8(2)
O(6)-Eu(01)-O(2)	143.6(2)	O(2)-Eu(01)-O(3)	139.0(2)
O(5)-Eu(01)-O(2)	71.6(2)	N(4)-Eu(01)-O(3)	109.0(2)

Πίνακας Π2-39: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/2-mIm

Μήκη δεσμών (Å) της ένωσης EuN-BDC/2-mIm

Eu(01)-N(5)	2.50(2)	Eu(01)-O(4)	2.684(6)
Eu(01)-O(1)	2.495(6)	Eu(01)-O(5)	2.348(7)
Eu(01)-O(2)	2.459(7)	Eu(01)-O(6)	2.379(7)
Eu(01)-O(3)	2.432(7)	Eu(01)-O(7)	2.45(2)
Eu(01)-O(4)	2.363(7)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/2-mIm

O(5)-Eu(01)-O(4)	77.0(2)	O(3)-Eu(01)-O(1)	76.8(2)
O(5)-Eu(01)-O(6)	133.8(2)	O(7)-Eu(01)-O(1)	101.0(4)
O(4)-Eu(01)-O(6)	75.0(2)	O(2)-Eu(01)-O(1)	52.0(2)
O(5)-Eu(01)-O(3)	91.2(3)	O(5)-Eu(01)-N(5)	75.5(3)
O(4)-Eu(01)-O(3)	124.3(2)	O(4)-Eu(01)-N(5)	145.5(3)
O(6)-Eu(01)-O(3)	75.6(3)	O(6)-Eu(01)-N(5)	139.4(3)
O(5)-Eu(01)-O(7)	73.5(4)	O(3)-Eu(01)-N(5)	76.8(4)
O(4)-Eu(01)-O(7)	80.4(3)	O(7)-Eu(01)-N(5)	72.1(4)
O(6)-Eu(01)-O(7)	135.0(4)	O(2)-Eu(01)-N(5)	99.6(4)
O(3)-Eu(01)-O(7)	147.9(4)	O(1)-Eu(01)-N(5)	72.5(3)
O(5)-Eu(01)-O(2)	141.0(3)	O(5)-Eu(01)-O(4)	69.5(2)
O(4)-Eu(01)-O(2)	88.8(2)	O(4)-Eu(01)-O(4)	75.1(2)
O(6)-Eu(01)-O(2)	74.0(3)	O(6)-Eu(01)-O(4)	68.2(2)
O(3)-Eu(01)-O(2)	126.0(2)	O(3)-Eu(01)-O(4)	50.2(2)
O(7)-Eu(01)-O(2)	68.3(4)	O(7)-Eu(01)-O(4)	139.2(3)
O(5)-Eu(01)-O(1)	147.6(3)	O(2)-Eu(01)-O(4)	141.5(3)
O(4)-Eu(01)-O(1)	134.5(2)	O(1)-Eu(01)-O(4)	119.5(2)
O(6)-Eu(01)-O(1)	72.6(2)	N(5)-Eu(01)-O(4)	113.5(4)

Πίνακας Π2-40: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/4-mIm

Μήκη δεσμών (Å) της ένωσης EuN-BDC/4-mIm

Eu(01)-O(4)	2.343(8)	Eu(01)-O(1)	2.48(2)
Eu(01)-O(5)	2.368(8)	Eu(01)-O(2)	2.493(9)
Eu(01)-O(6)	2.395(8)	Eu(01)-N(5)	2.51(2)
Eu(01)-O(3)	2.447(9)	Eu(01)-O(4)	2.758(9)
Eu(01)-O(7)	2.47(2)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/4-mIm

O(4)-Eu(01)-O(5)	77.1(3)	O(3)-Eu(01)-O(2)	80.9(3)
O(4)-Eu(01)-O(6)	75.7(3)	O(7)-Eu(01)-O(2)	94.9(5)
O(5)-Eu(01)-O(6)	132.7(3)	O(1)-Eu(01)-O(2)	51.4(3)
O(4)-Eu(01)-O(3)	124.2(3)	O(4)-Eu(01)-N(5)	145.9(5)
O(5)-Eu(01)-O(3)	90.1(4)	O(5)-Eu(01)-N(5)	73.6(4)
O(6)-Eu(01)-O(3)	74.7(3)	O(6)-Eu(01)-N(5)	138.0(5)
O(4)-Eu(01)-O(7)	83.2(4)	O(3)-Eu(01)-N(5)	73.2(5)
O(5)-Eu(01)-O(7)	76.0(5)	O(7)-Eu(01)-N(5)	73.3(5)
O(6)-Eu(01)-O(7)	136.6(4)	O(1)-Eu(01)-N(5)	107.9(4)
O(3)-Eu(01)-O(7)	146.1(4)	O(2)-Eu(01)-N(5)	74.8(4)
O(4)-Eu(01)-O(1)	85.0(3)	O(4)-Eu(01)-O(4)	75.4(3)
O(5)-Eu(01)-O(1)	141.9(4)	O(5)-Eu(01)-O(4)	68.3(3)
O(6)-Eu(01)-O(1)	72.3(4)	O(6)-Eu(01)-O(4)	67.8(3)
O(3)-Eu(01)-O(1)	127.5(3)	O(3)-Eu(01)-O(4)	49.8(3)
O(7)-Eu(01)-O(1)	68.5(4)	O(7)-Eu(01)-O(4)	141.5(5)
O(4)-Eu(01)-O(2)	132.6(3)	O(1)-Eu(01)-O(4)	138.7(3)
O(5)-Eu(01)-O(2)	148.4(3)	O(2)-Eu(01)-O(4)	123.1(3)
O(6)-Eu(01)-O(2)	74.0(3)	N(5)-Eu(01)-O(4)	108.6(4)

Πίνακας Π2-41: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/bzIm

Μήκη δεσμών (Å) της ένωσης EuN-BDC/bzIm

Eu(01)-N(5)	2.532(10)	Eu(01)-O(4)	2.688(6)
Eu(01)-O(1)	2.455(6)	Eu(01)-O(5)	2.354(6)
Eu(01)-O(2)	2.498(6)	Eu(01)-O(6)	2.371(5)
Eu(01)-O(3)	2.471(6)	Eu(01)-O(7)	2.402(7)
Eu(01)-O(4)	2.362(6)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/bzIm

O(5)-Eu(01)-O(4)	76.5(2)	O(7)-Eu(01)-O(2)	69.7(3)
O(5)-Eu(01)-O(6)	134.3(2)	O(1)-Eu(01)-O(2)	52.2(2)
O(4)-Eu(01)-O(6)	75.7(2)	O(3)-Eu(01)-O(2)	125.6(2)
O(5)-Eu(01)-O(7)	74.2(3)	O(5)-Eu(01)-N(5)	73.5(2)
O(4)-Eu(01)-O(7)	85.5(3)	O(4)-Eu(01)-N(5)	146.6(2)
O(6)-Eu(01)-O(7)	137.8(3)	O(6)-Eu(01)-N(5)	136.9(3)
O(5)-Eu(01)-O(1)	146.5(2)	O(7)-Eu(01)-N(5)	72.6(3)
O(4)-Eu(01)-O(1)	134.0(2)	O(1)-Eu(01)-N(5)	73.3(2)
O(6)-Eu(01)-O(1)	75.5(2)	O(3)-Eu(01)-N(5)	72.4(3)
O(7)-Eu(01)-O(1)	92.4(3)	O(2)-Eu(01)-N(5)	109.8(3)
O(5)-Eu(01)-O(3)	93.6(2)	O(5)-Eu(01)-O(4)	69.6(2)
O(4)-Eu(01)-O(3)	124.2(2)	O(4)-Eu(01)-O(4)	75.6(2)
O(6)-Eu(01)-O(3)	73.5(2)	O(6)-Eu(01)-O(4)	68.8(2)
O(7)-Eu(01)-O(3)	144.9(3)	O(7)-Eu(01)-O(4)	142.1(3)
O(1)-Eu(01)-O(3)	79.8(2)	O(1)-Eu(01)-O(4)	124.4(2)
O(5)-Eu(01)-O(2)	140.3(2)	O(3)-Eu(01)-O(4)	50.2(2)
O(4)-Eu(01)-O(2)	84.7(2)	O(2)-Eu(01)-O(4)	138.5(2)
O(6)-Eu(01)-O(2)	71.2(2)	N(5)-Eu(01)-O(4)	106.6(2)

Πίνακας Π2-42: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/hmIm

Μήκη δεσμών (Å) της ένωσης EuN-BDC/hmIm

Eu(01)-O(3)	2.349(6)	Eu(01)-O(4)	2.465(6)
Eu(01)-O(5)	2.368(6)	Eu(01)-O(1)	2.482(6)
Eu(01)-O(6)	2.372(7)	Eu(01)-N(4)	2.52(1)
Eu(01)-O(8)	2.41(2)	Eu(01)-O(3)	2.731(6)
Eu(01)-O(2)	2.464(6)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/hmIm

O(3)-Eu(01)-O(5)	76.2(2)	O(8)-Eu(01)-O(1)	96.8(4)
O(3)-Eu(01)-O(6)	75.9(2)	O(2)-Eu(01)-O(1)	52.4(2)
O(5)-Eu(01)-O(6)	133.3(2)	O(4)-Eu(01)-O(1)	79.0(2)
O(3)-Eu(01)-O(8)	83.4(4)	O(3)-Eu(01)-N(4)	145.5(3)
O(5)-Eu(01)-O(8)	74.4(4)	O(5)-Eu(01)-N(4)	73.9(3)
O(6)-Eu(01)-O(8)	137.3(4)	O(6)-Eu(01)-N(4)	138.2(3)
O(3)-Eu(01)-O(2)	85.5(2)	O(8)-Eu(01)-N(4)	72.3(4)
O(5)-Eu(01)-O(2)	141.0(3)	O(2)-Eu(01)-N(4)	107.4(3)
O(6)-Eu(01)-O(2)	72.0(3)	O(4)-Eu(01)-N(4)	73.4(3)
O(8)-Eu(01)-O(2)	69.4(4)	O(1)-Eu(01)-N(4)	74.8(3)
O(3)-Eu(01)-O(4)	124.4(2)	O(3)-Eu(01)-O(3)	75.4(2)
O(5)-Eu(01)-O(4)	91.3(3)	O(5)-Eu(01)-O(3)	69.2(3)
O(6)-Eu(01)-O(4)	74.9(3)	O(6)-Eu(01)-O(3)	68.0(2)
O(8)-Eu(01)-O(4)	145.3(3)	O(8)-Eu(01)-O(3)	141.2(4)
O(2)-Eu(01)-O(4)	127.1(2)	O(2)-Eu(01)-O(3)	138.7(3)
O(3)-Eu(01)-O(1)	133.5(2)	O(4)-Eu(01)-O(3)	49.9(2)
O(5)-Eu(01)-O(1)	148.7(2)	O(1)-Eu(01)-O(3)	121.3(2)
O(6)-Eu(01)-O(1)	73.0(2)	N(4)-Eu(01)-O(3)	108.9(3)

Πίνακας Π2-43: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/Ima

Μήκη δεσμών (Å) της ένωσης EuN-BDC/Ima

Eu(01)-O(5)	2.356(5)	Eu(01)-O(1)	2.468(5)
Eu(01)-O(4)	2.359(5)	Eu(01)-N(4)	2.515(8)
Eu(01)-O(6)	2.369(5)	Eu(01)-O(7)	2.59(2)
Eu(01)-O(3)	2.422(5)	Eu(01)-O(4)	2.675(5)
Eu(01)-O(2)	2.458(6)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/Ima

O(5)-Eu(01)-O(4)	75.2(2)	O(3)-Eu(01)-N(4)	69.9(2)
O(5)-Eu(01)-O(6)	135.6(2)	O(2)-Eu(01)-N(4)	110.4(3)
O(4)-Eu(01)-O(6)	76.4(2)	O(1)-Eu(01)-N(4)	76.2(2)
O(5)-Eu(01)-O(3)	93.4(2)	O(5)-Eu(01)-O(7)	72.3(3)
O(4)-Eu(01)-O(3)	126.2(2)	O(4)-Eu(01)-O(7)	92.4(3)
O(6)-Eu(01)-O(3)	77.0(2)	O(6)-Eu(01)-O(7)	142.1(3)
O(5)-Eu(01)-O(2)	134.9(2)	O(3)-Eu(01)-O(7)	134.6(3)
O(4)-Eu(01)-O(2)	83.2(2)	O(2)-Eu(01)-O(7)	69.5(3)
O(6)-Eu(01)-O(2)	73.3(2)	O(1)-Eu(01)-O(7)	88.4(3)
O(3)-Eu(01)-O(2)	130.8(2)	N(4)-Eu(01)-O(7)	64.8(3)
O(5)-Eu(01)-O(1)	148.0(2)	O(5)-Eu(01)-O(4)	71.2(2)
O(4)-Eu(01)-O(1)	132.4(2)	O(4)-Eu(01)-O(4)	76.2(2)
O(6)-Eu(01)-O(1)	74.4(2)	O(6)-Eu(01)-O(4)	69.4(2)
O(3)-Eu(01)-O(1)	82.1(2)	O(3)-Eu(01)-O(4)	50.8(2)
O(2)-Eu(01)-O(1)	52.7(2)	O(2)-Eu(01)-O(4)	140.6(2)
O(5)-Eu(01)-N(4)	72.5(2)	O(1)-Eu(01)-O(4)	125.1(2)
O(4)-Eu(01)-N(4)	144.8(2)	N(4)-Eu(01)-O(4)	105.8(2)
O(6)-Eu(01)-N(4)	138.1(2)	O(7)-Eu(01)-O(4)	143.4(3)

Πίνακας Π2-44: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/mIma

Μήκη δεσμών (Å) της ένωσης EuN-BDC/mIma

Eu(01)-O(1)	2.406(7)	Eu(01)-O(5)	2.63(2)
Eu(01)-O(2)	2.326(7)	Eu(01)-O(6)	2.451(6)
Eu(01)-O(3)	2.697(6)	Eu(01)-O(7)	2.436(6)
Eu(01)-O(4)	2.375(6)	Eu(01)-N(4)	2.55(2)
Eu(01)-O(4)	2.371(6)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/mIma

O(4)-Eu(01)-O(6)	79.0(2)	O(3)-Eu(01)-N(4)	79.2(5)
O(4)-Eu(01)-O(5)	76.4(2)	O(1)-Eu(01)-N(4)	92.0(5)
O(6)-Eu(01)-O(5)	135.1(2)	O(2)-Eu(01)-N(4)	71.6(6)
O(4)-Eu(01)-O(3)	127.4(2)	O(4)-Eu(01)-O(7)	75.1(4)
O(6)-Eu(01)-O(3)	83.4(3)	O(6)-Eu(01)-O(7)	70.3(5)
O(5)-Eu(01)-O(3)	82.6(3)	O(5)-Eu(01)-O(7)	135.5(5)
O(4)-Eu(01)-O(1)	90.0(2)	O(3)-Eu(01)-O(7)	141.8(5)
O(6)-Eu(01)-O(1)	140.0(3)	O(1)-Eu(01)-O(7)	69.7(5)
O(5)-Eu(01)-O(1)	77.0(3)	O(2)-Eu(01)-O(7)	105.8(5)
O(3)-Eu(01)-O(1)	131.2(2)	N(4)-Eu(01)-O(7)	67.2(6)
O(4)-Eu(01)-O(2)	137.0(2)	O(4)-Eu(01)-O(4)	76.7(2)
O(6)-Eu(01)-O(2)	142.9(2)	O(6)-Eu(01)-O(4)	68.7(2)
O(5)-Eu(01)-O(2)	74.4(2)	O(5)-Eu(01)-O(4)	69.4(2)
O(3)-Eu(01)-O(2)	78.9(2)	O(3)-Eu(01)-O(4)	50.7(2)
O(1)-Eu(01)-O(2)	53.1(2)	O(1)-Eu(01)-O(4)	145.8(2)
O(4)-Eu(01)-N(4)	138.8(6)	O(2)-Eu(01)-O(4)	120.0(2)
O(6)-Eu(01)-N(4)	73.3(5)	N(4)-Eu(01)-O(4)	118.8(5)
O(5)-Eu(01)-N(4)	143.8(6)	O(7)-Eu(01)-O(4)	133.6(5)

Πίνακας Π2-45: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/atzH

Μήκη δεσμών (Å) της ένωσης EuN-BDC/atzH

Eu(01)-O(4)	2.356(5)	Eu(01)-O(3)	2.456(6)
Eu(01)-O(6)	2.381(6)	Eu(01)-O(2)	2.456(5)
Eu(01)-O(5)	2.388(6)	Eu(01)-O(1)	2.477(6)
Eu(01)-N(4)	2.44(2)	Eu(01)-O(4)	2.667(6)
Eu(01)-O(7)	2.41(2)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/atzH

O(4)-Eu(01)-O(6)	77.6(2)	N(4)-Eu(01)-O(2)	72.6(3)
O(4)-Eu(01)-O(5)	75.5(2)	O(7)-Eu(01)-O(2)	91.4(4)
O(6)-Eu(01)-O(5)	135.2(2)	O(3)-Eu(01)-O(2)	78.7(2)
O(4)-Eu(01)-N(4)	148.0(3)	O(4)-Eu(01)-O(1)	85.2(2)
O(6)-Eu(01)-N(4)	73.2(3)	O(6)-Eu(01)-O(1)	140.7(3)
O(5)-Eu(01)-N(4)	135.6(3)	O(5)-Eu(01)-O(1)	71.1(3)
O(4)-Eu(01)-O(7)	87.4(3)	N(4)-Eu(01)-O(1)	109.7(4)
O(6)-Eu(01)-O(7)	74.9(4)	O(7)-Eu(01)-O(1)	69.3(4)
O(5)-Eu(01)-O(7)	137.8(4)	O(3)-Eu(01)-O(1)	124.7(2)
N(4)-Eu(01)-O(7)	72.8(4)	O(2)-Eu(01)-O(1)	52.3(2)
O(4)-Eu(01)-O(3)	124.2(2)	O(4)-Eu(01)-O(4)	75.5(2)
O(6)-Eu(01)-O(3)	93.8(3)	O(6)-Eu(01)-O(4)	70.0(2)
O(5)-Eu(01)-O(3)	73.3(2)	O(5)-Eu(01)-O(4)	69.0(2)
N(4)-Eu(01)-O(3)	71.1(3)	N(4)-Eu(01)-O(4)	105.7(3)
O(7)-Eu(01)-O(3)	143.9(4)	O(7)-Eu(01)-O(4)	143.4(4)
O(4)-Eu(01)-O(2)	134.2(2)	O(3)-Eu(01)-O(4)	50.5(2)
O(6)-Eu(01)-O(2)	145.5(2)	O(2)-Eu(01)-O(4)	123.6(2)
O(5)-Eu(01)-O(2)	75.2(2)	O(1)-Eu(01)-O(4)	138.8(3)

Πίνακας Π2-46: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/Im-atzH

Μήκη δεσμών (Å) της ένωσης EuN-BDC/Im-atzH

Eu(01)-O(3)	2.355(7)	Eu(01)-O(1)	2.484(8)
Eu(01)-N(6)	2.41(2)	Eu(01)-O(2)	2.498(7)
Eu(01)-O(6)	2.383(6)	Eu(01)-N(4)	2.55(2)
Eu(01)-O(5)	2.388(6)	Eu(01)-O(3)	2.786(7)
Eu(01)-O(4)	2.440(7)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/Im-atzH

O(3)-Eu(01)-N(6)	83.2(4)	O(5)-Eu(01)-O(2)	73.2(3)
O(3)-Eu(01)-O(6)	75.9(2)	O(4)-Eu(01)-O(2)	77.6(3)
N(6)-Eu(01)-O(6)	74.6(5)	O(1)-Eu(01)-O(2)	52.0(3)
O(3)-Eu(01)-O(5)	75.0(2)	O(3)-Eu(01)-N(4)	145.6(3)
N(6)-Eu(01)-O(5)	137.7(4)	N(6)-Eu(01)-N(4)	72.5(5)
O(6)-Eu(01)-O(5)	131.5(2)	O(6)-Eu(01)-N(4)	74.4(3)
O(3)-Eu(01)-O(4)	123.6(2)	O(5)-Eu(01)-N(4)	138.9(4)
N(6)-Eu(01)-O(4)	145.2(4)	O(4)-Eu(01)-N(4)	73.3(4)
O(6)-Eu(01)-O(4)	89.8(3)	O(1)-Eu(01)-N(4)	106.0(4)
O(5)-Eu(01)-O(4)	75.4(3)	O(2)-Eu(01)-N(4)	74.6(3)
O(3)-Eu(01)-O(1)	88.0(3)	O(3)-Eu(01)-O(3)	74.9(2)
N(6)-Eu(01)-O(1)	71.0(4)	N(6)-Eu(01)-O(3)	140.0(5)
O(6)-Eu(01)-O(1)	143.5(3)	O(6)-Eu(01)-O(3)	67.8(2)
O(5)-Eu(01)-O(1)	72.4(3)	O(5)-Eu(01)-O(3)	67.7(2)
O(4)-Eu(01)-O(1)	125.9(3)	O(4)-Eu(01)-O(3)	49.6(2)
O(3)-Eu(01)-O(2)	134.7(2)	O(1)-Eu(01)-O(3)	139.4(3)
N(6)-Eu(01)-O(2)	99.6(5)	O(2)-Eu(01)-O(3)	119.7(3)
O(6)-Eu(01)-O(2)	148.7(3)	N(4)-Eu(01)-O(3)	108.7(3)

Πίνακας Π2-47: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/py

Μήκη δεσμών (Å) της ένωσης EuN-BDC/py

Eu(1)-O(4)	2.351(5)	Eu(1)-O(1)	2.486(6)
Eu(1)-O(6)	2.361(5)	Eu(1)-O(7)	2.54(3)
Eu(1)-O(5)	2.359(5)	Eu(1)-N(4)	2.545(14)
Eu(1)-O(3)	2.425(5)	Eu(1)-O(4)	2.723(6)
Eu(1)-O(2)	2.429(5)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/py

O(4)-Eu(1)-O(6)	77.7(2)	O(3)-Eu(1)-O(7)	139.7(5)
O(4)-Eu(1)-O(5)	75.4(2)	O(2)-Eu(1)-O(7)	93.9(6)
O(6)-Eu(1)-O(5)	133.8(2)	O(1)-Eu(1)-O(7)	71.6(5)
O(4)-Eu(1)-O(3)	124.3(2)	O(4)-Eu(1)-N(4)	146.6(3)
O(6)-Eu(1)-O(3)	90.3(3)	O(6)-Eu(1)-N(4)	72.3(3)
O(5)-Eu(1)-O(3)	75.3(2)	O(5)-Eu(1)-N(4)	137.1(3)
O(4)-Eu(1)-O(2)	134.1(2)	O(3)-Eu(1)-N(4)	70.9(3)
O(6)-Eu(1)-O(2)	146.0(2)	O(2)-Eu(1)-N(4)	73.8(3)
O(5)-Eu(1)-O(2)	75.2(2)	O(1)-Eu(1)-N(4)	109.1(4)
O(3)-Eu(1)-O(2)	80.3(2)	O(7)-Eu(1)-N(4)	69.2(6)
O(4)-Eu(1)-O(1)	85.1(2)	O(4)-Eu(1)-O(4)	75.7(2)
O(6)-Eu(1)-O(1)	140.6(3)	O(6)-Eu(1)-O(4)	68.0(2)
O(5)-Eu(1)-O(1)	72.9(3)	O(5)-Eu(1)-O(4)	69.4(2)
O(3)-Eu(1)-O(1)	128.3(2)	O(3)-Eu(1)-O(4)	49.9(2)
O(2)-Eu(1)-O(1)	52.8(2)	O(2)-Eu(1)-O(4)	124.0(2)
O(4)-Eu(1)-O(7)	88.1(6)	O(1)-Eu(1)-O(4)	140.8(3)
O(6)-Eu(1)-O(7)	72.6(5)	O(7)-Eu(1)-O(4)	139.7(5)
O(5)-Eu(1)-O(7)	141.9(5)	N(4)-Eu(1)-O(4)	105.6(4)

Πίνακας Π2-48: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/2hmp

Μήκη δεσμών (Å) της ένωσης EuN-BDC/2hmp

Eu(01)-O(4)	2.343(6)	Eu(01)-O(1)	2.476(5)
Eu(01)-O(6)	2.380(5)	Eu(01)-O(7)	2.487(6)
Eu(01)-O(5)	2.376(6)	Eu(01)-N(4)	2.533(8)
Eu(01)-O(3)	2.422(6)	Eu(01)-O(4)	2.688(5)
Eu(01)-O(2)	2.456(5)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/2hmp

O(4)-Eu(01)-O(6)	80.0(2)	O(3)-Eu(01)-O(7)	137.6(2)
O(4)-Eu(01)-O(5)	75.2(2)	O(2)-Eu(01)-O(7)	73.6(2)
O(6)-Eu(01)-O(5)	134.2(2)	O(1)-Eu(01)-O(7)	109.3(2)
O(4)-Eu(01)-O(3)	127.2(2)	O(4)-Eu(01)-N(4)	137.7(2)
O(6)-Eu(01)-O(3)	78.7(2)	O(6)-Eu(01)-N(4)	73.7(2)
O(5)-Eu(01)-O(3)	86.4(2)	O(5)-Eu(01)-N(4)	145.3(2)
O(4)-Eu(01)-O(2)	93.2(2)	O(3)-Eu(01)-N(4)	79.4(2)
O(6)-Eu(01)-O(2)	145.0(2)	O(2)-Eu(01)-N(4)	90.0(2)
O(5)-Eu(01)-O(2)	74.9(2)	O(1)-Eu(01)-N(4)	72.9(2)
O(3)-Eu(01)-O(2)	129.4(2)	O(7)-Eu(01)-N(4)	64.0(3)
O(4)-Eu(01)-O(1)	138.4(2)	O(4)-Eu(01)-O(4)	76.6(2)
O(6)-Eu(01)-O(1)	141.5(2)	O(6)-Eu(01)-O(4)	67.0(2)
O(5)-Eu(01)-O(1)	73.2(2)	O(5)-Eu(01)-O(4)	70.2(2)
O(3)-Eu(01)-O(1)	77.0(2)	O(3)-Eu(01)-O(4)	50.6(2)
O(2)-Eu(01)-O(1)	52.8(2)	O(2)-Eu(01)-O(4)	144.9(2)
O(4)-Eu(01)-O(7)	76.6(2)	O(1)-Eu(01)-O(4)	116.0(2)
O(6)-Eu(01)-O(7)	71.5(2)	O(7)-Eu(01)-O(4)	133.6(2)
O(5)-Eu(01)-O(7)	135.9(2)	N(4)-Eu(01)-O(4)	120.2(2)
O(4)-Eu(01)-O(6)	80.0(2)	O(3)-Eu(01)-O(7)	137.6(2)
O(4)-Eu(01)-O(5)	75.2(2)	O(2)-Eu(01)-O(7)	73.6(2)
O(6)-Eu(01)-O(5)	134.2(2)	O(1)-Eu(01)-O(7)	109.3(2)
O(4)-Eu(01)-O(3)	127.2(2)	O(4)-Eu(01)-N(4)	137.7(2)

Πίνακας Π2-49: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/2hp

Μήκη δεσμών (Å) της ένωσης EuN-BDC/2hp

Eu(1)-O(1)	2.453(6)	Eu(1)-O(5)	2.362(6)
Eu(1)-O(2)	2.500(6)	Eu(1)-O(6)	2.365(6)
Eu(1)-O(3)	2.427(6)	Eu(1)-O(7)	2.400(9)
Eu(1)-O(4)	2.345(6)	Eu(1)-O(8)	2.477(8)
Eu(1)-O(4)	2.692(6)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/2hp

O(4)-Eu(1)-O(5)	76.9(2)	O(7)-Eu(1)-O(8)	71.4(3)
O(4)-Eu(1)-O(6)	77.0(2)	O(3)-Eu(1)-O(8)	70.3(3)
O(5)-Eu(1)-O(6)	135.1(2)	O(1)-Eu(1)-O(8)	69.8(2)
O(4)-Eu(1)-O(7)	86.3(3)	O(4)-Eu(1)-O(2)	83.1(2)
O(5)-Eu(1)-O(7)	74.8(3)	O(5)-Eu(1)-O(2)	140.3(3)
O(6)-Eu(1)-O(7)	138.5(3)	O(6)-Eu(1)-O(2)	70.5(3)
O(4)-Eu(1)-O(3)	126.1(2)	O(7)-Eu(1)-O(2)	69.9(3)
O(5)-Eu(1)-O(3)	91.4(3)	O(3)-Eu(1)-O(2)	127.8(2)
O(6)-Eu(1)-O(3)	75.6(2)	O(1)-Eu(1)-O(2)	51.8(2)
O(7)-Eu(1)-O(3)	141.4(3)	O(8)-Eu(1)-O(2)	109.1(3)
O(4)-Eu(1)-O(1)	133.6(2)	O(4)-Eu(1)-O(4)	76.7(2)
O(5)-Eu(1)-O(1)	144.3(2)	O(5)-Eu(1)-O(4)	70.1(2)
O(6)-Eu(1)-O(1)	77.7(2)	O(6)-Eu(1)-O(4)	68.6(2)
O(7)-Eu(1)-O(1)	87.6(3)	O(7)-Eu(1)-O(4)	143.6(3)
O(3)-Eu(1)-O(1)	83.3(2)	O(3)-Eu(1)-O(4)	50.3(7)
O(4)-Eu(1)-O(8)	147.9(3)	O(1)-Eu(1)-O(4)	127.3(2)
O(5)-Eu(1)-O(8)	75.1(3)	O(8)-Eu(1)-O(4)	107.8(2)
O(6)-Eu(1)-O(8)	134.8(3)	O(2)-Eu(1)-O(4)	137.4(3)

Πίνακας Π2-50: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/2mpy

Μήκη δεσμών (Å) της ένωσης EuN-BDC/2mpy

Eu(01)-N(4)	2.50(2)	Eu(01)-O(4)	2.756(6)
Eu(01)-O(1)	2.437(6)	Eu(01)-O(5)	2.357(6)
Eu(01)-O(2)	2.461(6)	Eu(01)-O(6)	2.362(6)
Eu(01)-O(3)	2.388(7)	Eu(01)-O(8)	2.47(2)
Eu(01)-O(4)	2.349(7)	Eu(01)-O(7)	2.51(2)

Γωνίες δεσμών (º) της ένωσης EuN-BDC/2mpy

O(4)-Eu(01)-O(5)	76.0(2)	O(3)-Eu(01)-O(8)	70.3(4)
O(4)-Eu(01)-O(6)	78.2(2)	O(1)-Eu(01)-O(8)	97.5(3)
O(5)-Eu(01)-O(6	134.7(2)	O(2)-Eu(01)-O(8)	69.3(3)
O(4)-Eu(01)-O(3)	127.0(2)	O(4)-Eu(01)-N(4)	127.8(6)
O(5)-Eu(01)-O(3)	83.4(2)	O(5)-Eu(01)-N(4)	149.0(6)
O(6)-Eu(01)-O(3)	83.2(2)	O(6)-Eu(01)-N(4)	74.9(6)
O(4)-Eu(01)-O(1)	88.7(2)	O(3)-Eu(01)-N(4)	93.2(7)
O(5)-Eu(01)-O(1)	76.7(2)	O(1)-Eu(01)-N(4)	83.6(6)
O(6)-Eu(01)-O(1)	139.1(2)	O(2)-Eu(01)-N(4)	74.4(6)
O(3)-Eu(01)-O(1)	133.1(2)	O(8)-Eu(01)-N(4)	23.0(6)
O(4)-Eu(01)-O(2)	136.0(2)	O(4)-Eu(01)-O(7)	78.4(3)
O(5)-Eu(01)-O(2)	74.6(2)	O(5)-Eu(01)-O(7)	136.6(3)
O(6)-Eu(01)-O(2)	144.4(2)	O(6)-Eu(01)-O(7)	71.2(3)
O(3)-Eu(01)-O(2)	80.8(2)	O(3)-Eu(01)-O(7)	139.7(3)
O(1)-Eu(01)-O(2)	53.1(2)	O(1)-Eu(01)-O(7)	68.2(3)
O(4)-Eu(01)-O(8)	146.1(3)	O(2)-Eu(01)-O(7)	102.0(3)
O(5)-Eu(01)-O(8)	137.9(3)	O(8)-Eu(01)-O(7)	73.2(4)
O(6)-Eu(01)-O(8)	75.4(3)	N(4)-Eu(01)-O(7)	50.8(7)
O(4)-Eu(01)-O(4)	77.5(2)	O(2)-Eu(01)-O(4)	120.3(2)
O(5)-Eu(01)-O(4)	69.6(2)	O(8)-Eu(01)-O(4)	111.5(3)
O(6)-Eu(01)-O(4)	68.8(2)	N(4)-Eu(01)-O(4)	129.5(6)
O(3)-Eu(01)-O(4)	49.5(2)	O(7)-Eu(01)-O(4)	136.6(3)
O(1)-Eu(01)-O(4)	145.7(2)		

Πίνακας Π2-51: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **EuN-BDC**/bpy

Μήκη δεσμών (Å) της ένωσης EuN-BDC/bpy

Eu(1)-O(4)	2.319(5)	Eu(1)-O(7)	2.438(7)
Eu(1)-O(5)	2.351(5)	Eu(1)-O(2)	2.497(6)
Eu(1)-O(6)	2.371(5)	Eu(1)-N(4)	2.612(9)
Eu(1)-O(3)	2.396(6)	Eu(1)-O(4)	2.858(6)
Eu(1)-O(1)	2.426(6)		

Γωνίες δεσμών (º) της ένωσης EuN-BDC/bpy

O(4)-Eu(1)-O(5)	76.2(2)	O(6)-Eu(1)-N(4)	74.7(2)
O(4)-Eu(1)-O(6)	78.2(2)	O(3)-Eu(1)-N(4)	67.6(2)
O(5)-Eu(1)-O(6)	132.2(2)	O(1)-Eu(1)-N(4)	70.6(2)
O(4)-Eu(1)-O(3)	125.5(2)	O(7)-Eu(1)-N(4)	73.8(3)
O(5)-Eu(1)-O(3)	77.2(2)	O(2)-Eu(1)-N(4)	107.9(3)
O(6)-Eu(1)-O(3)	86.1(2)	O(4)-Eu(1)-O(4)	77.4(2)
O(4)-Eu(1)-O(1)	133.9(2)	O(5)-Eu(1)-O(4)	67.7(2)
O(5)-Eu(1)-O(1)	77.2(2)	O(6)-Eu(1)-O(4)	67.7(2)
O(6)-Eu(1)-O(1)	145.2(2)	O(3)-Eu(1)-O(4)	48.5(2)
O(3)-Eu(1)-O(1)	83.3(2)	O(1)-Eu(1)-O(4)	124.4(2)
O(4)-Eu(1)-O(7)	84.5(3)	O(7)-Eu(1)-O(4)	140.2(2)
O(5)-Eu(1)-O(7)	140.9(3)	O(2)-Eu(1)-O(4)	141.0(2)
O(6)-Eu(1)-O(7)	74.1(3)	N(4)-Eu(1)-O(4)	105.4(2)
O(3)-Eu(1)-O(2)	131.4(2)	O(3)-Eu(1)-O(7)	140.1(3)
O(1)-Eu(1)-O(2)	52.4(2)	O(1)-Eu(1)-O(7)	93.5(3)
O(7)-Eu(1)-O(2)	70.0(3)	O(4)-Eu(1)-O(2)	84.4(2)
O(4)-Eu(1)-N(4)	148.9(2)	O(5)-Eu(1)-O(2)	74.5(2)
O(5)-Eu(1)-N(4)	134.2(2)	O(6)-Eu(1)-O(2)	141.3(2)

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων CeN-BDC

Πίνακας Π2-52: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **CeN-BDC**/Ακετόνη

Μήκη δεσμών (Å) της ένωσης CeN-BDC/Ακετόνη

Ce(1)-O(4)	2.436(5)	Ce(1)-O(1)	2.530(5)
Ce(1)-O(6)	2.443(5)	Ce(1)-O(2)	2.541(5)
Ce(1)-O(5)	2.449(5)	Ce(1)-O(7)	2.545(6)
Ce(1)-O(3)	2.514(5)	Ce(1)-O(4)	2.726(5)
Ce(1)-O(8)	2.528(6)		

Γωνίες δεσμών (º) της ένωσης CeN-BDC/Ακετόνη

O(4)-Ce(1)-O(6)	76.7(2)	O(3)-Ce(1)-O(2)	81.7(2)
O(4)-Ce(1)-O(5)	74.5(2)	O(8)-Ce(1)-O(2)	74.6(2)
O(6)-Ce(1)-O(5)	133.2(2)	O(1)-Ce(1)-O(2)	51.1(2)
O(4)-Ce(1)-O(3)	123.5(2)	O(4)-Ce(1)-O(7)	83.4(2)
O(6)-Ce(1)-O(3)	91.2(2)	O(6)-Ce(1)-O(7)	71.7(3)
O(5)-Ce(1)-O(3)	75.5(2)	O(5)-Ce(1)-O(7)	138.5(2)
O(4)-Ce(1)-O(8)	146.8(2)	O(3)-Ce(1)-O(7)	144.6(2)
O(6)-Ce(1)-O(8)	74.3(2)	O(8)-Ce(1)-O(7)	72.5(3)
O(5)-Ce(1)-O(8)	138.4(2)	O(1)-Ce(1)-O(7)	70.8(3)
O(3)-Ce(1)-O(8)	73.2(2)	O(2)-Ce(1)-O(7)	97.0(3)
O(4)-Ce(1)-O(1)	85.2(2)	O(4)-Ce(1)-O(4)	75.1(2)
O(6)-Ce(1)-O(1)	139.8(2)	O(6)-Ce(1)-O(4)	69.4(1)
O(5)-Ce(1)-O(1)	72.7(2)	O(5)-Ce(1)-O(4)	68.0(2)
O(3)-Ce(1)-O(1)	128.3(2)	O(3)-Ce(1)-O(4)	49.4(2)
O(8)-Ce(1)-O(1)	107.1(2)	O(8)-Ce(1)-O(4)	108.7(2)
O(4)-Ce(1)-O(2)	132.1(2)	O(1)-Ce(1)-O(4)	139.4(2)
O(6)-Ce(1)-O(2)	148.9(2)	O(2)-Ce(1)-O(4)	123.4(2)
O(5)-Ce(1)-O(2)	74.3(2)	O(7)-Ce(1)-O(4)	138.9(2)

Μήκη δεσμών και γωνίες δεσμών των τροποποιημένων ενώσεων GdN-BDC

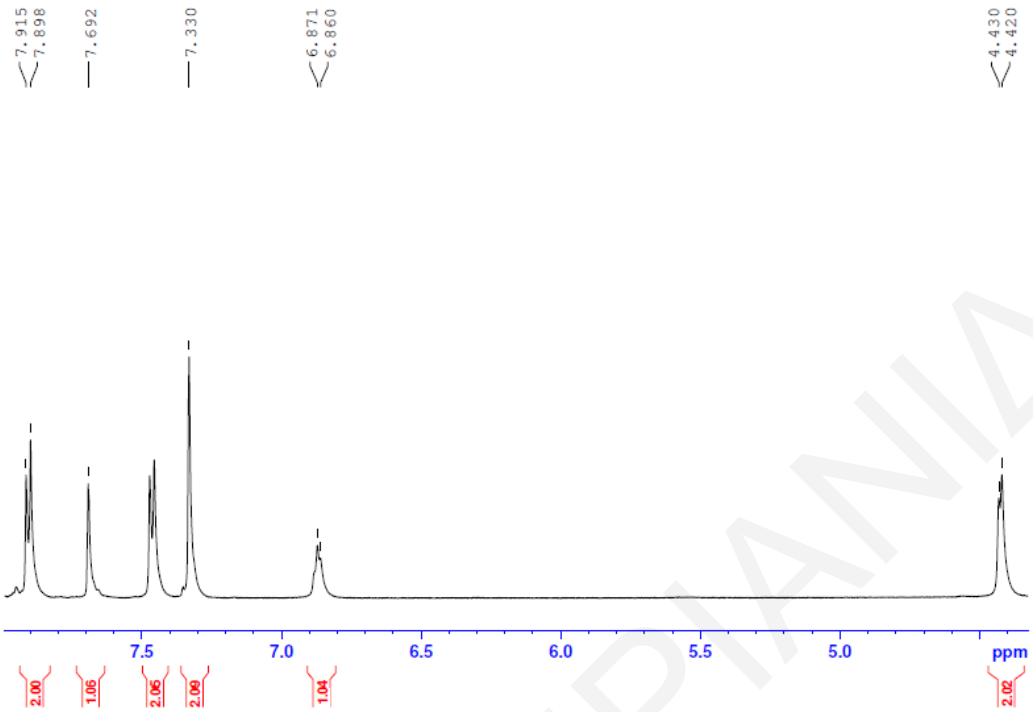
Πίνακας Π2-52: Μήκη δεσμών (Å) και γωνίες (˚) για την ένωση **GdN-BDC**/Ακετόνη

Μήκη δεσμών (Å) της ένωσης GdN-BDC/Ακετόνη

Gd(1)-O(4)	2.32(2)	Gd(1)-O(7)	2.44(2)
Gd(1)-O(6)	2.34(2)	Gd(1)-O(8)	2.45(2)
Gd(1)-O(5)	2.360(9)	Gd(1)-O(1)	2.465(9)
Gd(1)-O(3)	2.415(9)	Gd(1)-O(4)	2.703(9)
Gd(1)-O(2)	2.43(2)		

Γωνίες δεσμών (º) της ένωσης GdN-BDC/Ακετόνη

O(4)-Gd(1)-O(6)	76.0(3)	O(3)-Gd(1)-O(8)	143.3(5)
O(4)-Gd(1)-O(5)	78.2(4)	O(2)-Gd(1)-O(8)	71.4(5)
O(6)-Gd(1)-O(5)	133.8(4)	O(7)-Gd(1)-O(8)	71.0(6)
O(4)-Gd(1)-O(3)	125.0(3)	O(4)-Gd(1)-O(1)	133.6(3)
O(6)-Gd(1)-O(3)	76.6(4)	O(6)-Gd(1)-O(1)	74.0(3)
O(5)-Gd(1)-O(3)	88.1(4)	O(5)-Gd(1)-O(1)	146.5(4)
O(4)-Gd(1)-O(2)	84.7(4)	O(3)-Gd(1)-O(1)	80.6(3)
O(6)-Gd(1)-O(2)	73.1(4)	O(2)-Gd(1)-O(1)	53.1(3)
O(5)-Gd(1)-O(2)	141.0(4)	O(7)-Gd(1)-O(1)	72.8(4)
O(3)-Gd(1)-O(2)	129.8(3)	O(8)-Gd(1)-O(1)	99.5(6)
O(4)-Gd(1)-O(7)	145.4(4)	O(4)-Gd(1)-O(4)	75.1(3)
O(6)-Gd(1)-O(7)	138.5(4)	O(6)-Gd(1)-O(4)	67.9(3)
O(5)-Gd(1)-O(7)	73.8(4)	O(5)-Gd(1)-O(4)	68.7(3)
O(3)-Gd(1)-O(7)	74.1(5)	O(3)-Gd(1)-O(4)	50.5(3)
O(2)-Gd(1)-O(7)	104.8(5)	O(2)-Gd(1)-O(4)	139.3(4)
O(4)-Gd(1)-O(8)	81.3(5)	O(7)-Gd(1)-O(4)	111.9(4)
O(6)-Gd(1)-O(8)	139.2(5)	O(8)-Gd(1)-O(4)	137.0(5)
O(5)-Gd(1)-O(8)	71.6(5)	O(1)-Gd(1)-O(4)	122.8(3)



Εικόνα Π1: *Φάσμα ^{1}H NMR του υποκαταστάτη* ***H_3CAP****.*

Κρυσταλλογραφικά δεδομένα των ενώσεων που απομονώθηκαν στην παρούσα εργασία (CIF files)

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 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    29.0739(10)
_cell_length_b                    14.5356(5)
_cell_length_c                    13.5095(5)
_cell_angle_alpha                 90.0
_cell_angle_beta                  100.097(5)
_cell_angle_gamma                 90.0
_cell_volume                      5620.8(4)
_cell_formula_units_Z             8
_cell_measurement_temperature     100(2)
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_cell_measurement_reflns_used   5672
_cell_measurement_theta_min     2.9807
_cell_measurement_theta_max     25.0628

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_exptl_crystal_colour             'colorless'
_exptl_crystal_size_max           0.1
_exptl_crystal_size_mid           0.08
_exptl_crystal_size_min           0.04
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.402
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2352
_exptl_absorpt_coefficient_mu     1.563
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min    0.72619
_exptl_absorpt_correction_T_max   1.00000
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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_diffrn_ambient_temperature       100(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'SuperNova (Mo) X-ray
Source'
_diffrn_radiation_monochromator   'mirror'
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Atlas'
_diffrn_measurement_method        '\w scans'
_diffrn_detector_area_resol_mean  10.4223
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_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             12896
_diffrn_reflns_av_R_equivalents   0.0429
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_diffrn_reflns_limit_k_min        -17
_diffrn_reflns_limit_k_max        13
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_diffrn_reflns_limit_l_max        15
_diffrn_reflns_theta_min          3.06
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_reflns_number_total              4946
_reflns_number_gt                 4306
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_computing_data_collection        'CrysAlis CCD'
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1997)'
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1997)'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0883P)^2^+21.2011P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4946
_refine_ls_number_parameters      311
_refine_ls_number_restraints      77
_refine_ls_R_factor_all           0.0526
_refine_ls_R_factor_gt            0.0473
_refine_ls_wR_factor_ref          0.1485
_refine_ls_wR_factor_gt           0.1438
_refine_ls_goodness_of_fit_ref    1.084
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_refine_ls_shift/su_max           0.001
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1 d . . .
O1 O 0.39617(14) 0.1834(3) 0.4880(4) 0.0617(13) Uani 1 1
d . . .
O2 O 0.38215(14) 0.3310(3) 0.5015(4) 0.0533(11) Uani 1 1
d . . .
O3 O 0.29421(12) 0.0667(3) 0.4462(3) 0.0447(10) Uani 1 1
d . . .
O4 O 0.23180(12) 0.1481(2) 0.4627(3) 0.0399(9) Uani 1 1 d . . .
O5 O 0.29710(13) 0.2601(3) 0.3652(3) 0.0455(9) Uani 1 1 d . . .
O6 O 0.27278(13) 0.1744(4) 0.6768(3) 0.0560(12) Uani 1 1
d . . .
O7 O 0.35934(19) 0.0832(4) 0.6480(5) 0.0780(14) Uani 1 1 d
U . .
O8 O 0.3615(2) 0.2858(4) 0.7000(5) 0.0805(17) Uani 1 1 d U . .
N1 N 0.59992(15) 0.4182(4) 0.3513(4) 0.0465(12) Uani 1 1
d . . .
N2 N 0.3841(3) 0.0153(7) 0.8106(7) 0.106(2) Uani 1 1 d U . .
N3 N 0.3826(4) 0.3863(8) 0.8285(8) 0.130(3) Uani 1 1 d U . .
```

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C1 C 0.40701(19) 0.2668(4) 0.4806(5) 0.0442(14) Uani 1 1
d . . .
C2 C 0.4521(2) 0.2865(4) 0.4447(5) 0.0471(15) Uani 1 1 d . . .
C3 C 0.4813(3) 0.2149(5) 0.4260(8) 0.075(3) Uani 1 1 d . . .
H3 H 0.4729 0.1543 0.4359 0.090 Uiso 1 1 calc R . .
C4 C 0.5226(3) 0.2336(5) 0.3928(8) 0.080(3) Uani 1 1 d . . .
H4 H 0.5414 0.1854 0.3784 0.097 Uiso 1 1 calc R . .
C5 C 0.5361(2) 0.3231(5) 0.3809(5) 0.0541(16) Uani 1 1 d . . .
C6 C 0.5083(2) 0.3944(5) 0.4009(6) 0.0605(18) Uani 1 1 d . . .
H6 H 0.5174 0.4549 0.3935 0.073 Uiso 1 1 calc R . .
C7 C 0.4661(2) 0.3754(5) 0.4325(6) 0.0591(18) Uani 1 1 d . . .
H7 H 0.4471 0.4237 0.4456 0.071 Uiso 1 1 calc R . .
C8 C 0.5830(2) 0.3393(5) 0.3562(6) 0.0569(17) Uani 1 1 d D . .
H16 H 0.605(3) 0.290(5) 0.351(8) 0.12(4) Uiso 1 1 d D . .
C9 C 0.25119(17) 0.0769(3) 0.4306(4) 0.0363(12) Uani 1 1
d . . .
C10 C 0.22054(17) 0.0048(4) 0.3736(4) 0.0367(12) Uani 1 1
d . . .
C11 C 0.17373(17) -0.0029(4) 0.3832(5) 0.0406(13) Uani 1 1
d . . .
H11 H 0.1606 0.0389 0.4223 0.049 Uiso 1 1 calc R . .
C12 C 0.14661(18) -0.0743(4) 0.3330(4) 0.0403(12) Uani 1 1
d . . .
C13 C 0.16476(17) -0.1310(4) 0.2676(4) 0.0375(12) Uani 1 1
d . . .
H13 H 0.1459 -0.1753 0.2311 0.045 Uiso 1 1 calc R . .
C14 C 0.21171(17) -0.1219(4) 0.2559(4) 0.0371(12) Uani 1 1
d . . .
C15 C 0.23962(17) -0.0547(4) 0.3111(4) 0.0377(12) Uani 1 1
d . . .
H15 H 0.2710 -0.0498 0.3060 0.045 Uiso 1 1 calc R . .
C16 C 0.26944(19) 0.3167(4) 0.3157(4) 0.0423(13) Uani 1 1
d . . .
C17 C 0.3687(4) 0.0890(9) 0.7503(9) 0.114(3) Uani 1 1 d U . .
C18 C 0.3767(6) -0.0763(10) 0.7537(13) 0.163(4) Uani 1 1 d
U . .
H18A H 0.3878 -0.1259 0.7985 0.245 Uiso 1 1 calc R . .
H18B H 0.3936 -0.0757 0.6987 0.245 Uiso 1 1 calc R . .
H18C H 0.3440 -0.0847 0.7282 0.245 Uiso 1 1 calc R . .
C19 C 0.3977(5) 0.0270(10) 0.9191(9) 0.132(3) Uani 1 1 d U . .
H19A H 0.4075 -0.0312 0.9494 0.199 Uiso 1 1 calc R . .
H19B H 0.3716 0.0497 0.9465 0.199 Uiso 1 1 calc R . .
H19C H 0.4231 0.0701 0.9328 0.199 Uiso 1 1 calc R . .
C20 C 0.3498(5) 0.3246(11) 0.7601(11) 0.125(3) Uani 1 1 d U . .
C21 C 0.3665(5) 0.4354(10) 0.9006(11) 0.138(4) Uani 1 1 d U . .
H21A H 0.3911 0.4731 0.9358 0.207 Uiso 1 1 calc R . .
H21B H 0.3558 0.3940 0.9471 0.207 Uiso 1 1 calc R . .
H21C H 0.3410 0.4738 0.8700 0.207 Uiso 1 1 calc R . .
C22 C 0.4287(5) 0.3986(10) 0.8009(11) 0.144(4) Uani 1 1 d U . .
H22A H 0.4322 0.3566 0.7479 0.215 Uiso 1 1 calc R . .
H22B H 0.4525 0.3867 0.8583 0.215 Uiso 1 1 calc R . .
H22C H 0.4317 0.4606 0.7783 0.215 Uiso 1 1 calc R . .

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0.00072(10)
O1 0.034(2) 0.047(3) 0.114(4) 0.000(3) 0.041(2) 0.001(2)
O2 0.037(2) 0.047(2) 0.085(3) -0.010(2) 0.036(2) -0.0089(18)
O3 0.0265(18) 0.037(2) 0.075(3) -0.0075(19) 0.0206(18) -
0.0020(15)
O4 0.0298(18) 0.0331(19) 0.062(2) -0.0033(17) 0.0241(17) -
0.0028(15)
O5 0.036(2) 0.055(2) 0.052(2) 0.008(2) 0.0224(18) 0.0046(19)
O6 0.029(2) 0.083(3) 0.062(3) 0.028(2) 0.0232(19) 0.007(2)
O7 0.060(3) 0.082(3) 0.092(3) 0.012(3) 0.015(2) 0.027(2)
O8 0.085(3) 0.086(3) 0.070(3) 0.005(2) 0.010(3) -0.014(3)
N1 0.028(2) 0.055(3) 0.062(3) -0.010(2) 0.023(2) -0.011(2)
N2 0.105(4) 0.108(4) 0.103(3) 0.017(3) 0.015(3) 0.002(4)
N3 0.141(4) 0.121(5) 0.126(5) -0.014(4) 0.018(4) -0.001(4)
C1 0.028(3) 0.051(3) 0.058(4) -0.006(3) 0.019(3) -0.005(3)
C2 0.031(3) 0.052(4) 0.063(4) -0.008(3) 0.022(3) -0.011(2)
C3 0.050(4) 0.046(4) 0.143(8) -0.002(4) 0.059(5) -0.004(3)
C4 0.055(4) 0.053(4) 0.148(9) -0.018(5) 0.057(5) -0.006(3)
C5 0.049(3) 0.050(4) 0.072(4) -0.014(3) 0.034(3) -0.011(3)
C6 0.048(4) 0.047(4) 0.094(5) -0.012(4) 0.035(4) -0.010(3)
C7 0.042(3) 0.055(4) 0.087(5) -0.012(3) 0.029(3) -0.006(3)
C8 0.042(3) 0.059(4) 0.077(5) -0.011(3) 0.031(3) -0.005(3)
C9 0.032(3) 0.026(2) 0.057(3) -0.002(2) 0.023(2) -0.002(2)
C10 0.029(2) 0.032(3) 0.053(3) 0.002(2) 0.019(2) -0.001(2)
C11 0.030(3) 0.036(3) 0.063(4) 0.000(3) 0.027(2) -0.002(2)
C12 0.028(3) 0.046(3) 0.053(3) -0.003(3) 0.022(2) -0.001(2)
C13 0.031(3) 0.036(3) 0.050(3) -0.002(2) 0.021(2) -0.006(2)
C14 0.029(3) 0.040(3) 0.048(3) 0.000(2) 0.021(2) -0.002(2)
C15 0.022(2) 0.042(3) 0.053(3) 0.002(2) 0.018(2) 0.001(2)
C16 0.033(3) 0.052(3) 0.048(3) 0.007(3) 0.022(2) 0.003(3)
C17 0.106(5) 0.129(4) 0.109(4) 0.020(4) 0.018(4) 0.003(4)
C18 0.178(6) 0.145(4) 0.170(6) -0.022(4) 0.036(5) 0.002(5)
C19 0.138(6) 0.139(5) 0.118(4) 0.014(4) 0.015(4) -0.001(4)
C20 0.132(5) 0.127(5) 0.119(5) -0.008(4) 0.028(4) 0.007(4)
C21 0.148(6) 0.136(6) 0.127(5) -0.011(4) 0.019(4) 0.004(4)
C22 0.140(4) 0.143(6) 0.147(6) 0.000(5) 0.021(4) 0.001(4)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
```

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 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

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La1 O8 2.481(6) . ?
La1 O4 2.482(4) 7_556 ?
La1 O6 2.502(4) . ?
La1 O1 2.521(4) . ?
La1 O7 2.534(5) . ?
La1 O3 2.553(4) . ?
La1 O2 2.628(4) . ?
La1 O4 2.757(4) . ?
La1 C1 2.928(6) . ?
La1 C9 3.027(5) . ?
La1 La1 4.1206(8) 7_556 ?
O1 C1 1.261(8) . ?
O2 C1 1.243(7) . ?
O3 C9 1.240(6) . ?
O4 C9 1.289(6) . ?
O4 La1 2.482(4) 7_556 ?
O5 C16 1.257(7) . ?
O6 C16 1.256(7) 7_556 ?
O7 C17 1.363(13) . ?
O8 C20 1.091(15) . ?
N1 C8 1.254(8) . ?
N1 C12 1.426(7) 3 ?
N2 C17 1.373(14) . ?
N2 C19 1.460(14) . ?
N2 C18 1.534(16) . ?
N3 C21 1.356(16) . ?
N3 C22 1.463(17) . ?
N3 C20 1.503(17) . ?
C1 C2 1.504(8) . ?
C2 C7 1.373(9) . ?
C2 C3 1.393(9) . ?
C3 C4 1.381(10) . ?
C3 H3 0.9300 . ?
C4 C5 1.377(10) . ?
C4 H4 0.9300 . ?
C5 C6 1.370(9) . ?
C5 C8 1.478(8) . ?
C6 C7 1.395(9) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.96(2) . ?
C9 C10 1.499(7) . ?
C10 C15 1.390(8) . ?
C10 C11 1.394(7) . ?
C11 C12 1.404(8) . ?
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C11 H11 0.9300 . ?
C12 C13 1.379(8) . ?
C12 N1 1.426(7) 3_445 ?
C13 C14 1.408(7) . ?
C13 H13 0.9300 . ?
C14 C15 1.399(8) . ?
C14 C16 1.490(8) 4_545 ?
C15 H15 0.9300 . ?
C16 O6 1.256(7) 7_556 ?
C16 C14 1.490(8) 4 ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
C21 H21A 0.9600 . ?
C21 H21B 0.9600 . ?
C21 H21C 0.9600 . ?
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C22 H22B 0.9600 . ?
C22 H22C 0.9600 . ?

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O5 La1 O8 136.36(17) . . ?
O5 La1 O4 72.53(14) . 7_556 ?
O8 La1 O4 83.93(18) . 7_556 ?
O5 La1 O6 133.11(13) . . ?
O8 La1 O6 74.4(2) . . ?
O4 La1 O6 79.38(14) 7_556 . ?
O5 La1 O1 81.49(16) . . ?
O8 La1 O1 89.7(2) . . ?
O4 La1 O1 133.66(14) 7_556 . ?
O6 La1 O1 142.28(16) . . ?
O5 La1 O7 139.65(17) . . ?
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O4 La1 O7 146.96(16) 7_556 . ?
O6 La1 O7 71.15(16) . . ?
O1 La1 O7 71.66(18) . . ?
O5 La1 O3 73.96(15) . . ?
O8 La1 O3 147.53(16) . . ?
O4 La1 O3 123.08(12) 7_556 . ?
O6 La1 O3 91.99(15) . . ?
O1 La1 O3 83.40(14) . . ?
O7 La1 O3 73.52(18) . . ?
O5 La1 O2 71.88(15) . . ?
O8 La1 O2 69.75(18) . . ?
O4 La1 O2 84.71(12) 7_556 . ?
O6 La1 O2 142.02(16) . . ?
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O1 La1 O2 50.47(14) . . ?
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O3 La1 O2 125.31(13) . . ?
O5 La1 O4 69.20(13) . . ?
O8 La1 O4 140.13(19) . . ?
O4 La1 O4 76.38(12) 7_556 . ?
O6 La1 O4 68.14(13) . . ?
O1 La1 O4 128.70(14) . . ?
O7 La1 O4 105.09(16) . . ?
O3 La1 O4 49.01(11) . . ?
O2 La1 O4 140.26(14) . . ?
O5 La1 C1 74.88(16) . . ?
O8 La1 C1 79.1(2) . . ?
O4 La1 C1 109.10(15) 7_556 . ?
O6 La1 C1 151.21(16) . . ?
O1 La1 C1 25.37(16) . . ?
O7 La1 C1 91.02(18) . . ?
O3 La1 C1 104.72(15) . . ?
O2 La1 C1 25.11(15) . . ?
O4 La1 C1 140.06(15) . . ?
O5 La1 C9 69.66(15) . . ?
O8 La1 C9 152.54(18) . . ?
O4 La1 C9 100.45(13) 7_556 . ?
O6 La1 C9 79.76(15) . . ?
O1 La1 C9 105.59(15) . . ?
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O2 La1 C9 137.39(14) . . ?
O4 La1 C9 25.21(12) . . ?
C1 La1 C9 123.51(16) . . ?
O5 La1 La1 65.27(9) . 7_556 ?
O8 La1 La1 116.73(17) . 7_556 ?
O4 La1 La1 40.55(8) 7_556 7_556 ?
O6 La1 La1 68.89(9) . 7_556 ?
O1 La1 La1 146.52(13) . 7_556 ?
O7 La1 La1 132.76(13) . 7_556 ?
O3 La1 La1 83.68(8) . 7_556 ?
O2 La1 La1 117.32(10) . 7_556 ?
O4 La1 La1 35.82(8) . 7_556 ?
C1 La1 La1 135.23(13) . 7_556 ?
C9 La1 La1 60.26(10) . 7_556 ?
C1 O1 La1 95.7(3) . . ?
C1 O2 La1 91.1(3) . . ?
C9 O3 La1 100.0(3) . . ?
C9 O4 La1 158.4(4) . 7_556 ?
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C17 O7 La1 120.6(6) . . ?
C20 O8 La1 132.8(10) . . ?
C8 N1 C12 118.3(5) . 3 ?
C17 N2 C19 120.5(11) . . ?
C17 N2 C18 112.2(10) . . ?
C19 N2 C18 126.5(11) . . ?
C21 N3 C22 124.5(12) . . ?
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C22 N3 C20 115.3(12) . . ?
O2 C1 O1 122.7(5) . . ?
O2 C1 C2 120.3(5) . . ?
O1 C1 C2 116.9(5) . . ?
O2 C1 La1 63.8(3) . . ?
O1 C1 La1 58.9(3) . . ?
C2 C1 La1 175.5(4) . . ?
C7 C2 C3 118.7(6) . . ?
C7 C2 C1 120.7(6) . . ?
C3 C2 C1 120.6(5) . . ?
C4 C3 C2 120.2(6) . . ?
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C2 C3 H3 119.9 . . ?
C5 C4 C3 120.4(7) . . ?
C5 C4 H4 119.8 . . ?
C3 C4 H4 119.8 . . ?
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C6 C5 C8 121.6(6) . . ?
C4 C5 C8 118.0(6) . . ?
C5 C6 C7 119.5(6) . . ?
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N1 C8 H16 114(6) . . ?
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C11 C12 N1 116.4(5) . 3_445 ?
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C13 C14 C16 119.4(5) . 4_545 ?
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C14 C15 H15 119.9 . . ?
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O6 C16 C14 117.8(5) 7_556 4 ?
O5 C16 C14 117.6(5) . 4 ?
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N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
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H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
O8 C20 N3 121.3(14) . . ?
N3 C21 H21A 109.5 . . ?
N3 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
N3 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
N3 C22 H22A 109.5 . . ?
N3 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
N3 C22 H22C 109.5 . . ?
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H22B C22 H22C 109.5 . . ?

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 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
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 'x+1/2, -y+1/2, z-1/2'

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Diffraction)'

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Atlas'
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 MERCURY (Bruno et al. 2002)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O1 O 0.38127(17) 0.3309(4) 0.0018(5) 0.0489(14) Uani 1 1
d . . .
O2 O 0.39513(18) 0.1838(4) -0.0122(6) 0.0579(17) Uani 1 1
d . . .
O3 O 0.27290(17) 0.1734(4) 0.1744(4) 0.0515(15) Uani 1 1
d . . .
O4 O 0.29748(17) 0.2605(4) -0.1345(4) 0.0409(12) Uani 1 1
d . . .
O5 O 0.29442(16) 0.0681(3) -0.0547(4) 0.0408(12) Uani 1 1
d . . .
O6 O 0.26837(16) 0.3515(3) 0.0372(4) 0.0372(11) Uani 1 1
d . . .
O7 O 0.3609(3) 0.2845(5) 0.1963(6) 0.0744(19) Uani 1 1 d DU . .
O8 O 0.3586(2) 0.0827(5) 0.1471(6) 0.0721(18) Uani 1 1 d DU . .
N1 N 0.5992(2) 0.4185(5) -0.1501(5) 0.0418(15) Uani 1 1 d . . .
N2 N 0.3826(4) 0.3840(9) 0.3285(10) 0.124(4) Uani 1 1 d DU . .
N3 N 0.3832(4) 0.0130(7) 0.3105(8) 0.100(3) Uani 1 1 d DU . .
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C1 C 0.4060(2) 0.2669(5) -0.0192(6) 0.0381(17) Uani 1 1 d . . .
C2 C 0.4517(2) 0.2862(5) -0.0541(6) 0.0400(17) Uani 1 1 d . . .
C3 C 0.4801(3) 0.2153(6) -0.0746(9) 0.065(3) Uani 1 1 d . . .
H3 H 0.4707 0.1549 -0.0681 0.078 Uiso 1 1 calc R . .
C4 C 0.5228(3) 0.2329(7) -0.1049(11) 0.083(4) Uani 1 1 d . . .
H4 H 0.5418 0.1844 -0.1174 0.099 Uiso 1 1 calc R . .
C5 C 0.5367(3) 0.3214(6) -0.1164(7) 0.051(2) Uani 1 1 d . . .
C6 C 0.5077(3) 0.3948(6) -0.0996(8) 0.055(2) Uani 1 1 d . . .
H6 H 0.5165 0.4551 -0.1092 0.066 Uiso 1 1 calc R . .
C7 C 0.4648(3) 0.3749(6) -0.0675(7) 0.054(2) Uani 1 1 d . . .
H7 H 0.4453 0.4228 -0.0555 0.065 Uiso 1 1 calc R . .
C8 C 0.5828(3) 0.3396(6) -0.1456(7) 0.049(2) Uani 1 1 d D . .
C9 C 0.2305(2) 0.1817(5) 0.1834(6) 0.0393(17) Uani 1 1 d . . .
C10 C 0.2114(2) 0.1213(5) 0.2554(5) 0.0336(15) Uani 1 1 d . . .
C11 C 0.1648(2) 0.1314(5) 0.2672(5) 0.0345(15) Uani 1 1 d . . .
H11 H 0.1462 0.1765 0.2316 0.041 Uiso 1 1 calc R . .
C12 C 0.1463(2) 0.0733(5) 0.3327(6) 0.0355(16) Uani 1 1 d . . .
C13 C 0.1737(2) 0.0025(5) 0.3837(6) 0.0354(16) Uani 1 1 d . . .
H13 H 0.1607 -0.0382 0.4241 0.043 Uiso 1 1 calc R . .
C14 C 0.2203(2) -0.0061(4) 0.3730(5) 0.0313(14) Uani 1 1
d . . .
C15 C 0.2392(2) 0.0543(5) 0.3098(5) 0.0325(15) Uani 1 1 d . . .
H15 H 0.2706 0.0495 0.3042 0.039 Uiso 1 1 calc R . .
C16 C 0.2508(2) 0.0784(4) -0.0710(5) 0.0314(14) Uani 1 1
d . . .
C17 C 0.3479(5) 0.3272(11) 0.2662(10) 0.127(4) Uani 1 1 d
DU . .
C18 C 0.3614(6) 0.4361(12) 0.3997(12) 0.141(5) Uani 1 1 d
DU . .
H18A H 0.3305 0.4132 0.4004 0.212 Uiso 1 1 calc R . .
H18B H 0.3597 0.4996 0.3805 0.212 Uiso 1 1 calc R . .
H18C H 0.3800 0.4300 0.4656 0.212 Uiso 1 1 calc R . .
C19 C 0.4285(5) 0.3974(12) 0.3023(13) 0.134(5) Uani 1 1 d
DU . .
H19A H 0.4332 0.3534 0.2521 0.202 Uiso 1 1 calc R . .
H19B H 0.4520 0.3895 0.3610 0.202 Uiso 1 1 calc R . .
H19C H 0.4305 0.4583 0.2762 0.202 Uiso 1 1 calc R . .
C20 C 0.3674(5) 0.0870(9) 0.2412(6) 0.109(4) Uani 1 1 d DU . .
C21 C 0.3778(7) -0.0723(10) 0.2534(13) 0.148(5) Uani 1 1 d
DU . .
H21A H 0.3881 -0.1228 0.2975 0.223 Uiso 1 1 calc R . .
H21B H 0.3963 -0.0697 0.2012 0.223 Uiso 1 1 calc R . .
H21C H 0.3455 -0.0807 0.2241 0.223 Uiso 1 1 calc R . .
C22 C 0.3988(6) 0.0256(13) 0.4177(9) 0.140(6) Uani 1 1 d DU . .
H22A H 0.4076 -0.0326 0.4485 0.210 Uiso 1 1 calc R . .
H22B H 0.3738 0.0515 0.4468 0.210 Uiso 1 1 calc R . .
H22C H 0.4251 0.0664 0.4287 0.210 Uiso 1 1 calc R . .
H16 H 0.592(6) 0.274(3) -0.151(14) 0.168 Uiso 1 1 d D . .

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O2 0.038(3) 0.039(3) 0.109(5) 0.000(3) 0.048(3) -0.002(2)
O3 0.028(3) 0.071(4) 0.060(4) 0.029(3) 0.022(2) 0.006(3)
O4 0.032(3) 0.049(3) 0.047(3) 0.008(3) 0.019(2) 0.004(2)
O5 0.026(2) 0.029(2) 0.072(4) -0.008(2) 0.021(2) -0.0024(19)
O6 0.031(2) 0.026(2) 0.060(3) -0.004(2) 0.023(2) -0.0030(19)
O7 0.080(4) 0.072(4) 0.070(3) 0.008(3) 0.009(3) -0.015(3)
O8 0.057(3) 0.080(4) 0.080(3) 0.005(3) 0.012(3) 0.020(3)
N1 0.028(3) 0.050(4) 0.053(4) -0.005(3) 0.022(3) -0.009(3)
N2 0.129(5) 0.117(5) 0.121(5) -0.008(4) 0.011(4) -0.002(4)
N3 0.101(5) 0.101(5) 0.099(4) 0.009(4) 0.017(4) 0.002(4)
C1 0.024(3) 0.041(4) 0.055(5) -0.003(3) 0.021(3) -0.003(3)
C2 0.025(3) 0.047(4) 0.052(4) -0.005(4) 0.019(3) -0.009(3)
C3 0.046(5) 0.044(5) 0.116(9) -0.002(5) 0.048(5) -0.002(4)
C4 0.049(5) 0.055(6) 0.161(12) -0.022(7) 0.064(7) -0.007(4)
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C9 0.032(4) 0.040(4) 0.051(4) 0.007(4) 0.021(3) 0.006(3)
C10 0.030(3) 0.032(3) 0.043(4) 0.000(3) 0.019(3) -0.001(3)
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C12 0.024(3) 0.035(4) 0.052(4) 0.000(3) 0.020(3) 0.001(3)
C13 0.028(3) 0.028(3) 0.056(4) 0.003(3) 0.021(3) -0.001(3)
C14 0.029(3) 0.021(3) 0.048(4) 0.002(3) 0.020(3) 0.001(2)
C15 0.019(3) 0.035(4) 0.048(4) 0.000(3) 0.017(3) -0.001(3)
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C17 0.129(6) 0.126(6) 0.127(6) -0.006(4) 0.023(4) 0.003(4)
C18 0.147(6) 0.141(7) 0.135(6) -0.005(4) 0.026(5) 0.003(5)
C19 0.135(5) 0.132(7) 0.135(7) 0.002(5) 0.021(4) 0.002(4)
C20 0.106(6) 0.116(5) 0.104(5) 0.009(4) 0.019(4) 0.000(4)
C21 0.158(7) 0.137(6) 0.152(7) -0.016(5) 0.032(5) 0.003(5)
C22 0.143(7) 0.140(8) 0.138(7) 0.001(5) 0.025(5) -0.003(5)

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 All esds (except the esd in the dihedral angle between two
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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
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P=(Fo^2^+2Fc^2^)/3'
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d . . .
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O7 O 0.1418(5) 0.2841(7) 0.8028(10) 0.118(3) Uani 1 1 d DU . .
O8 O 0.1401(4) 0.0823(7) 0.8561(9) 0.113(3) Uani 1 1 d DU . .
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H3 H 0.0313 0.1510 1.0795 0.109 Uiso 1 1 calc R . .
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C11 C 0.2612(3) -0.0542(6) 1.1932(6) 0.0387(18) Uani 1 1
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d . . .
H13 H 0.3561 -0.1722 1.2758 0.048 Uiso 1 1 calc R . .
C14 C 0.3542(3) -0.0737(6) 1.1672(7) 0.049(2) Uani 1 1 d . . .
C15 C 0.3271(3) -0.0031(6) 1.1190(7) 0.045(2) Uani 1 1 d . . .
H15 H 0.3404 0.0394 1.0802 0.055 Uiso 1 1 calc R . .
C16 C 0.2711(3) 0.1786(7) 0.8215(6) 0.047(2) Uani 1 1 d . . .
C17 C 0.1519(8) 0.3304(17) 0.7319(15) 0.175(5) Uani 1 1 d
DU . .
C18 C 0.0736(8) 0.3886(18) 0.7087(18) 0.193(6) Uani 1 1 d
DU . .
H18A H 0.0687 0.3313 0.7421 0.289 Uiso 1 1 calc R . .
H18B H 0.0471 0.4004 0.6574 0.289 Uiso 1 1 calc R . .
H18C H 0.0770 0.4391 0.7557 0.289 Uiso 1 1 calc R . .
C19 C 0.1488(8) 0.4199(17) 0.6060(17) 0.181(6) Uani 1 1 d
DU . .
H19A H 0.1711 0.3729 0.5953 0.271 Uiso 1 1 calc R . .
H19B H 0.1650 0.4718 0.6409 0.271 Uiso 1 1 calc R . .
H19C H 0.1321 0.4408 0.5431 0.271 Uiso 1 1 calc R . .
C20 C 0.1330(9) 0.0830(15) 0.7627(10) 0.170(4) Uani 1 1 d
DU . .
C21 C 0.1010(9) 0.0245(17) 0.5791(12) 0.178(5) Uani 1 1 d
DU . .
H21A H 0.0916 -0.0354 0.5509 0.267 Uiso 1 1 calc R . .
H21B H 0.1266 0.0480 0.5498 0.267 Uiso 1 1 calc R . .
H21C H 0.0750 0.0671 0.5660 0.267 Uiso 1 1 calc R . .
C22 C 0.1279(9) -0.0653(15) 0.7511(17) 0.192(5) Uani 1 1 d
DU . .
H22A H 0.1394 -0.0440 0.8175 0.287 Uiso 1 1 calc R . .
H22B H 0.1518 -0.1013 0.7274 0.287 Uiso 1 1 calc R . .
H22C H 0.1005 -0.1034 0.7513 0.287 Uiso 1 1 calc R . .

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O2 0.046(4) 0.053(4) 0.127(7) 0.001(4) 0.052(4) -0.003(3)
O3 0.034(3) 0.046(3) 0.059(4) 0.007(3) 0.023(3) 0.007(2)
O4 0.036(3) 0.042(3) 0.089(5) 0.011(3) 0.029(3) 0.006(3)
O5 0.034(3) 0.105(5) 0.056(4) -0.030(4) 0.021(3) -0.003(4)
O6 0.048(4) 0.072(4) 0.051(4) -0.019(3) 0.028(3) -0.013(3)
O7 0.112(5) 0.122(5) 0.119(5) -0.030(3) 0.013(4) 0.007(4)
O8 0.085(4) 0.117(5) 0.141(4) 0.008(4) 0.033(4) -0.011(4)
N1 0.043(4) 0.066(5) 0.061(5) 0.014(4) 0.030(4) 0.017(4)
N2 0.186(6) 0.174(6) 0.172(6) 0.018(4) 0.026(4) 0.003(4)
N3 0.169(7) 0.171(5) 0.159(4) -0.010(3) 0.020(5) 0.001(5)
C1 0.032(5) 0.068(6) 0.059(6) -0.001(5) 0.020(4) 0.002(5)
C2 0.034(5) 0.074(7) 0.063(6) -0.004(5) 0.023(5) 0.004(4)
C3 0.072(9) 0.056(7) 0.164(15) -0.001(7) 0.078(10) -0.001(5)
C4 0.083(10) 0.060(7) 0.171(16) 0.015(8) 0.077(11) 0.005(6)
C5 0.065(7) 0.064(6) 0.069(7) 0.020(5) 0.033(5) 0.011(5)
C6 0.070(7) 0.073(7) 0.090(8) 0.026(6) 0.041(6) 0.019(6)
C7 0.044(5) 0.067(7) 0.104(8) 0.024(6) 0.041(6) 0.008(5)
C8 0.057(6) 0.074(8) 0.074(7) 0.019(6) 0.033(5) 0.006(6)
C9 0.039(4) 0.031(4) 0.052(5) 0.001(4) 0.024(4) 0.002(3)
C10 0.030(4) 0.042(5) 0.057(5) 0.005(4) 0.020(4) 0.003(3)
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C12 0.039(4) 0.053(5) 0.034(4) 0.001(4) 0.018(3) 0.006(4)
C13 0.036(4) 0.046(5) 0.042(4) 0.009(4) 0.023(3) 0.007(4)
C14 0.037(4) 0.060(6) 0.059(5) 0.015(5) 0.029(4) 0.011(4)
C15 0.035(4) 0.042(5) 0.066(5) 0.015(4) 0.029(4) 0.008(4)
C16 0.044(5) 0.065(6) 0.037(4) -0.014(4) 0.021(4) -0.011(4)
C17 0.180(6) 0.175(7) 0.169(6) 0.012(4) 0.027(4) -0.005(4)
C18 0.184(6) 0.196(8) 0.198(8) 0.001(5) 0.033(5) -0.001(5)
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C20 0.174(7) 0.183(6) 0.154(4) -0.009(4) 0.028(5) -0.003(5)
C21 0.185(7) 0.183(7) 0.164(5) -0.010(4) 0.022(5) -0.002(5)
C22 0.198(8) 0.184(5) 0.192(6) 0.014(4) 0.031(5) -0.004(5)

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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Pr1 O8 2.503(11) . ?
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Pr1 O1 2.563(6) . ?
Pr1 O3 2.695(5) . ?
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Pr1 C9 2.971(8) . ?
Pr1 Pr1 4.0645(8) 7_557 ?
O1 C1 1.253(12) . ?
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O3 C9 1.271(9) . ?
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O6 C16 1.278(11) 7_557 ?
O7 C17 1.246(5) . ?
O8 C20 1.255(5) . ?
N1 C8 1.227(13) . ?
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C2 C3 1.391(14) . ?
C3 C4 1.368(16) . ?
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C4 C5 1.385(16) . ?
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C5 C6 1.373(15) . ?
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C6 H6 0.9300 . ?
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C8 H16 0.96(2) . ?
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C11 C12 1.392(11) . ?
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C12 C13 1.396(10) . ?
C12 C16 1.468(11) 6_556 ?
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C14 N1 1.433(10) 3_545 ?
C15 H15 0.9300 . ?
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O3 Pr1 O8 147.6(3) 7_557 . ?
O6 Pr1 O8 139.3(3) . . ?
O5 Pr1 O8 72.1(3) . . ?
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O5 Pr1 O1 143.2(3) . . ?
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O7 C17 N2 121.3(19) . . ?
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N2 C18 H18B 109.5 . . ?
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H18B C18 H18C 109.5 . . ?
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H19B C19 H19C 109.5 . . ?
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_reflns_number_total              4841
_reflns_number_gt                 3851
_reflns_threshold_expression      >2sigma(I)

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1997)'
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1997)'
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;
 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

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G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;
```

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_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0733P)^2^+59.1320P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4841
_refine_ls_number_parameters      310
_refine_ls_number_restraints      79
_refine_ls_R_factor_all           0.0613
_refine_ls_R_factor_gt            0.0491
_refine_ls_wR_factor_ref          0.1509
_refine_ls_wR_factor_gt           0.1433
_refine_ls_goodness_of_fit_ref    1.097
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d . . .
O1 O 0.87970(19) 0.8277(4) 0.0069(5) 0.0587(17) Uani 1 1
d . . .
O2 O 0.8911(2) 0.6792(5) -0.0180(6) 0.0660(19) Uani 1 1 d . . .
O3 O 0.76859(17) 0.8474(4) 0.0406(4) 0.0419(13) Uani 1 1
d . . .
O4 O 0.79399(18) 0.5686(4) -0.0528(5) 0.0486(14) Uani 1 1
d . . .
O5 O 0.79901(19) 0.7621(4) -0.1290(4) 0.0462(13) Uani 1 1
d . . .
O6 O 0.77134(19) 0.6669(5) 0.1663(4) 0.0561(16) Uani 1 1
d . . .
O7 O 0.8580(3) 0.5811(7) 0.1403(9) 0.120(3) Uani 1 1 d DU . .
O8 O 0.8571(4) 0.7805(7) 0.1949(8) 0.110(3) Uani 1 1 d DU . .
N1 N 1.0982(2) 0.9187(5) -0.1491(5) 0.0530(19) Uani 1 1 d . . .
N2 N 0.8834(7) 0.5129(13) 0.3084(13) 0.186(5) Uani 1 1 d DU . .
N3 N 0.8801(6) 0.8764(12) 0.3292(12) 0.158(3) Uani 1 1 d DU . .
```

```
C1 C 0.9035(3) 0.7623(7) -0.0208(6) 0.048(2) Uani 1 1 d . . .
C2 C 0.9488(3) 0.7842(6) -0.0570(7) 0.054(2) Uani 1 1 d . . .
C3 C 0.9628(3) 0.8742(7) -0.0660(8) 0.064(3) Uani 1 1 d . . .
H3 H 0.9435 0.9229 -0.0519 0.077 Uiso 1 1 calc R . .
C4 C 1.0061(3) 0.8943(7) -0.0962(8) 0.065(3) Uani 1 1 d . . .
H4 H 1.0158 0.9558 -0.1010 0.079 Uiso 1 1 calc R . .
C5 C 1.0342(3) 0.8204(7) -0.1191(8) 0.062(3) Uani 1 1 d . . .
C6 C 1.0201(4) 0.7311(8) -0.1117(12) 0.095(5) Uani 1 1 d . . .
H6 H 1.0391 0.6822 -0.1264 0.114 Uiso 1 1 calc R . .
C7 C 0.9771(4) 0.7125(8) -0.0821(12) 0.095(5) Uani 1 1 d . . .
H7 H 0.9671 0.6509 -0.0791 0.114 Uiso 1 1 calc R . .
C8 C 1.0811(3) 0.8388(8) -0.1456(8) 0.068(3) Uani 1 1 d D . .
H16 H 1.098(3) 0.782(4) -0.151(8) 0.081 Uiso 1 1 d D . .
C9 C 0.7504(3) 0.5801(5) -0.0717(6) 0.0382(17) Uani 1 1 d . . .
C10 C 0.7198(3) 0.5067(5) -0.1289(6) 0.0391(17) Uani 1 1
d . . .
C11 C 0.7388(2) 0.4476(5) -0.1933(5) 0.0364(16) Uani 1 1
d . . .
H11 H 0.7703 0.4527 -0.1997 0.044 Uiso 1 1 calc R . .
C12 C 0.7101(3) 0.3809(5) -0.2481(6) 0.0403(18) Uani 1 1
d . . .
C13 C 0.6636(3) 0.3698(6) -0.2360(6) 0.0414(18) Uani 1 1
d . . .
H13 H 0.6447 0.3246 -0.2722 0.050 Uiso 1 1 calc R . .
C14 C 0.6452(3) 0.4283(6) -0.1678(6) 0.045(2) Uani 1 1 d . . .
C15 C 0.6725(3) 0.4978(6) -0.1180(6) 0.0428(18) Uani 1 1
d . . .
H15 H 0.6596 0.5391 -0.0770 0.051 Uiso 1 1 calc R . .
C16 C 0.7715(3) 0.8207(6) -0.1765(6) 0.0434(19) Uani 1 1
d . . .
C17 C 0.8675(10) 0.5845(16) 0.2341(10) 0.190(5) Uani 1 1 d
DU . .
C18 C 0.8721(9) 0.4304(15) 0.2455(16) 0.198(5) Uani 1 1 d
DU . .
H18A H 0.8819 0.3753 0.2838 0.297 Uiso 1 1 calc R . .
H18B H 0.8883 0.4338 0.1892 0.297 Uiso 1 1 calc R . .
H18C H 0.8388 0.4279 0.2222 0.297 Uiso 1 1 calc R . .
C19 C 0.8999(8) 0.5283(17) 0.4146(13) 0.191(5) Uani 1 1 d
DU . .
H19A H 0.9095 0.4699 0.4465 0.287 Uiso 1 1 calc R . .
H19B H 0.8749 0.5547 0.4444 0.287 Uiso 1 1 calc R . .
H19C H 0.9262 0.5706 0.4232 0.287 Uiso 1 1 calc R . .
C20 C 0.8436(6) 0.8237(14) 0.2646(13) 0.154(4) Uani 1 1 d
DU . .
C21 C 0.8535(7) 0.9249(14) 0.3949(14) 0.163(4) Uani 1 1 d
DU . .
H21A H 0.8246 0.8920 0.3969 0.245 Uiso 1 1 calc R . .
H21B H 0.8464 0.9871 0.3702 0.245 Uiso 1 1 calc R . .
H21C H 0.8717 0.9279 0.4610 0.245 Uiso 1 1 calc R . .
C22 C 0.9267(6) 0.8935(15) 0.3059(16) 0.168(4) Uani 1 1 d
DU . .
H22A H 0.9346 0.8447 0.2631 0.251 Uiso 1 1 calc R . .
H22B H 0.9493 0.8944 0.3668 0.251 Uiso 1 1 calc R . .
H22C H 0.9270 0.9526 0.2726 0.251 Uiso 1 1 calc R . .

loop_
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0.00141(14)
O1 0.035(3) 0.064(4) 0.086(5) -0.026(3) 0.036(3) -0.017(3)
O2 0.046(4) 0.052(4) 0.112(6) 0.010(4) 0.047(4) 0.006(3)
O3 0.034(3) 0.038(3) 0.060(3) -0.008(2) 0.026(2) -0.005(2)
O4 0.031(3) 0.039(3) 0.081(4) -0.008(3) 0.023(3) -0.004(2)
O5 0.035(3) 0.064(4) 0.045(3) 0.013(3) 0.022(2) 0.010(3)
O6 0.033(3) 0.084(4) 0.057(3) 0.025(3) 0.023(3) 0.008(3)
O7 0.040(4) 0.144(8) 0.177(6) -0.006(5) 0.027(5) 0.038(5)
O8 0.106(4) 0.112(4) 0.109(3) 0.020(2) 0.013(3) -0.007(3)
N1 0.033(4) 0.069(5) 0.064(4) -0.015(4) 0.029(3) -0.019(3)
N2 0.187(6) 0.187(5) 0.182(5) 0.005(2) 0.028(3) 0.000(3)
N3 0.163(4) 0.155(4) 0.153(4) -0.010(3) 0.023(2) -0.003(3)
C1 0.026(4) 0.073(6) 0.049(5) 0.000(4) 0.016(3) 0.002(4)
C2 0.033(4) 0.067(6) 0.066(6) -0.001(5) 0.025(4) -0.011(4)
C3 0.041(5) 0.073(6) 0.084(7) -0.019(6) 0.028(5) -0.006(5)
C4 0.053(5) 0.067(6) 0.086(7) -0.020(5) 0.038(5) -0.013(5)
C5 0.056(6) 0.060(6) 0.081(7) -0.018(5) 0.037(5) -0.016(5)
C6 0.068(7) 0.070(7) 0.164(13) -0.023(8) 0.072(8) -0.006(6)
C7 0.060(7) 0.064(7) 0.180(14) -0.015(7) 0.077(9) -0.009(5)
C8 0.050(6) 0.080(8) 0.083(7) -0.021(6) 0.041(5) -0.012(5)
C9 0.035(4) 0.038(4) 0.048(4) -0.005(3) 0.023(3) -0.005(3)
C10 0.033(4) 0.039(4) 0.051(4) -0.002(4) 0.023(3) -0.006(3)
C11 0.027(3) 0.043(4) 0.045(4) 0.001(3) 0.020(3) -0.001(3)
C12 0.036(4) 0.046(4) 0.044(4) 0.001(4) 0.024(3) -0.005(3)
C13 0.035(4) 0.050(5) 0.044(4) -0.011(4) 0.020(3) -0.009(3)
C14 0.027(4) 0.059(5) 0.056(5) -0.015(4) 0.027(3) -0.012(4)
C15 0.033(4) 0.046(4) 0.057(5) -0.011(4) 0.028(4) -0.004(3)
C16 0.036(4) 0.061(5) 0.039(4) 0.008(4) 0.021(3) 0.004(4)
C17 0.192(6) 0.193(5) 0.186(5) 0.004(3) 0.030(3) 0.001(3)
C18 0.200(6) 0.195(5) 0.199(6) -0.006(3) 0.034(3) 0.001(3)
C19 0.193(6) 0.193(6) 0.187(5) 0.002(3) 0.031(3) 0.000(3)
C20 0.156(4) 0.156(5) 0.152(4) -0.006(3) 0.028(3) 0.004(3)
C21 0.168(5) 0.162(5) 0.159(5) -0.007(3) 0.027(3) 0.002(3)
C22 0.164(4) 0.169(5) 0.170(5) -0.001(3) 0.028(3) -0.002(3)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
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 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Sm1 O8 2.395(11) . ?
Sm1 O5 2.397(5) . ?
Sm1 O6 2.406(5) . ?
Sm1 O2 2.446(6) . ?
Sm1 O4 2.462(5) . ?
Sm1 O7 2.479(10) . ?
Sm1 O1 2.539(5) . ?
Sm1 O3 2.683(5) 7_665 ?
Sm1 C1 2.845(8) . ?
Sm1 C9 2.948(7) . ?
Sm1 Sm1 4.0065(7) 7_665 ?
O1 C1 1.255(11) . ?
O2 C1 1.244(11) . ?
O3 C9 1.277(9) 7_665 ?
O3 Sm1 2.682(5) 7_665 ?
O4 C9 1.249(9) . ?
O5 C16 1.255(10) . ?
O6 C16 1.277(9) 7_665 ?
O7 C17 1.255(5) . ?
O8 C20 1.246(5) . ?
N1 C8 1.248(12) . ?
N1 C14 1.426(9) 3 ?
N2 C19 1.454(5) . ?
N2 C17 1.455(5) . ?
N2 C18 1.460(5) . ?
N3 C21 1.446(5) . ?
N3 C22 1.451(5) . ?
N3 C20 1.458(5) . ?
C1 C2 1.502(11) . ?
C2 C3 1.362(13) . ?
C2 C7 1.389(13) . ?
C3 C4 1.407(12) . ?
C3 H3 0.9300 . ?
C4 C5 1.399(13) . ?
C4 H4 0.9300 . ?
C5 C6 1.350(15) . ?
C5 C8 1.480(12) . ?
C6 C7 1.392(14) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.96(2) . ?
C9 O3 1.277(9) 7_665 ?
C9 C10 1.501(10) . ?
C10 C11 1.393(10) . ?
C10 C15 1.400(10) . ?
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C11 C12 1.392(11) . ?
C11 H11 0.9300 . ?
C12 C13 1.388(10) . ?
C12 C16 1.499(10) 4_644 ?
C13 C14 1.415(10) . ?
C13 H13 0.9300 . ?
C14 C15 1.373(11) . ?
C14 N1 1.426(9) 3_445 ?
C15 H15 0.9300 . ?
C16 O6 1.276(9) 7_665 ?
C16 C12 1.500(10) 4_654 ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
C21 H21A 0.9600 . ?
C21 H21B 0.9600 . ?
C21 H21C 0.9600 . ?
C22 H22A 0.9600 . ?
C22 H22B 0.9600 . ?
C22 H22C 0.9600 . ?

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O3 Sm1 O5 73.68(19) . . ?
O8 Sm1 O5 135.3(3) . . ?
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O8 Sm1 O6 75.2(3) . . ?
O5 Sm1 O6 134.39(19) . . ?
O3 Sm1 O2 134.32(19) . . ?
O8 Sm1 O2 93.1(3) . . ?
O5 Sm1 O2 78.3(2) . . ?
O6 Sm1 O2 142.5(2) . . ?
O3 Sm1 O4 124.27(18) . . ?
O8 Sm1 O4 147.1(3) . . ?
O5 Sm1 O4 75.3(2) . . ?
O6 Sm1 O4 90.2(2) . . ?
O2 Sm1 O4 80.8(2) . . ?
O3 Sm1 O7 147.3(3) . . ?
O8 Sm1 O7 74.5(3) . . ?
O5 Sm1 O7 138.7(3) . . ?
O6 Sm1 O7 71.5(3) . . ?
O2 Sm1 O7 71.0(3) . . ?
O4 Sm1 O7 73.0(3) . . ?
O3 Sm1 O1 84.71(18) . . ?
O8 Sm1 O1 69.5(3) . . ?
O5 Sm1 O1 71.0(2) . . ?
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O6 Sm1 O1 143.1(2) . . ?
O2 Sm1 O1 52.0(2) . . ?
O4 Sm1 O1 125.80(18) . . ?
O7 Sm1 O1 108.1(3) . . ?
O3 Sm1 O3 75.74(18) . 7_665 ?
O8 Sm1 O3 139.7(3) . 7_665 ?
O5 Sm1 O3 69.71(18) . 7_665 ?
O6 Sm1 O3 67.93(18) . 7_665 ?
O2 Sm1 O3 126.2(2) . 7_665 ?
O4 Sm1 O3 50.32(16) . 7_665 ?
O7 Sm1 O3 107.4(3) . 7_665 ?
O1 Sm1 O3 139.6(2) . 7_665 ?
O3 Sm1 C1 109.7(2) . . ?
O8 Sm1 C1 81.1(3) . . ?
O5 Sm1 C1 72.4(2) . . ?
O6 Sm1 C1 152.9(2) . . ?
O2 Sm1 C1 25.8(2) . . ?
O4 Sm1 C1 103.2(2) . . ?
O7 Sm1 C1 89.8(3) . . ?
O1 Sm1 C1 26.2(2) . . ?
O3 Sm1 C1 138.2(2) 7_665 . ?
O3 Sm1 C9 100.52(19) . . ?
O8 Sm1 C9 152.5(3) . . ?
O5 Sm1 C9 70.5(2) . . ?
O6 Sm1 C9 78.5(2) . . ?
O2 Sm1 C9 103.2(2) . . ?
O4 Sm1 C9 24.65(18) . . ?
O7 Sm1 C9 90.0(3) . . ?
O1 Sm1 C9 137.7(2) . . ?
O3 Sm1 C9 25.66(17) 7_665 . ?
C1 Sm1 C9 122.1(2) . . ?
O3 Sm1 Sm1 40.46(12) . 7_665 ?
O8 Sm1 Sm1 115.8(3) . 7_665 ?
O5 Sm1 Sm1 66.44(12) . 7_665 ?
O6 Sm1 Sm1 69.37(13) . 7_665 ?
O2 Sm1 Sm1 144.30(18) . 7_665 ?
O4 Sm1 Sm1 84.73(12) . 7_665 ?
O7 Sm1 Sm1 134.5(2) . 7_665 ?
O1 Sm1 Sm1 117.05(16) . 7_665 ?
O3 Sm1 Sm1 35.28(11) 7_665 7_665 ?
C1 Sm1 Sm1 134.45(18) . 7_665 ?
C9 Sm1 Sm1 60.35(14) . 7_665 ?
C1 O1 Sm1 90.7(5) . . ?
C1 O2 Sm1 95.3(5) . . ?
C9 O3 Sm1 159.9(5) 7_665 . ?
C9 O3 Sm1 88.8(4) 7_665 7_665 ?
Sm1 O3 Sm1 104.26(18) . 7_665 ?
C9 O4 Sm1 100.0(4) . . ?
C16 O5 Sm1 135.3(5) . . ?
C16 O6 Sm1 134.1(5) 7_665 . ?
C17 O7 Sm1 121.1(12) . . ?
C20 O8 Sm1 133.8(11) . . ?
C8 N1 C14 119.1(8) . 3 ?
C19 N2 C17 126.2(17) . . ?
C19 N2 C18 135(2) . . ?
C17 N2 C18 98.8(17) . . ?
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C21 N3 C22 131.2(18) . . ?
C21 N3 C20 102.4(13) . . ?
C22 N3 C20 123.7(16) . . ?
O2 C1 O1 122.0(7) . . ?
O2 C1 C2 118.6(8) . . ?
O1 C1 C2 119.4(9) . . ?
O2 C1 Sm1 58.9(4) . . ?
O1 C1 Sm1 63.2(4) . . ?
C2 C1 Sm1 177.1(7) . . ?
C3 C2 C7 118.8(8) . . ?
C3 C2 C1 120.9(8) . . ?
C7 C2 C1 120.3(8) . . ?
C2 C3 C4 120.7(9) . . ?
C2 C3 H3 119.7 . . ?
C4 C3 H3 119.7 . . ?
C5 C4 C3 119.0(9) . . ?
C5 C4 H4 120.5 . . ?
C3 C4 H4 120.5 . . ?
C6 C5 C4 120.4(9) . . ?
C6 C5 C8 119.0(10) . . ?
C4 C5 C8 120.5(9) . . ?
C5 C6 C7 119.8(10) . . ?
C5 C6 H6 120.1 . . ?
C7 C6 H6 120.1 . . ?
C2 C7 C6 121.1(10) . . ?
C2 C7 H7 119.4 . . ?
C6 C7 H7 119.4 . . ?
N1 C8 C5 123.6(9) . . ?
N1 C8 H16 124(7) . . ?
C5 C8 H16 112(7) . . ?
O4 C9 O3 120.8(7) . 7_665 ?
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O3 C9 C10 119.4(6) 7_665 . ?
O4 C9 Sm1 55.3(4) . . ?
O3 C9 Sm1 65.5(4) 7_665 . ?
C10 C9 Sm1 175.0(5) . . ?
C11 C10 C15 120.3(7) . . ?
C11 C10 C9 119.3(6) . . ?
C15 C10 C9 120.4(7) . . ?
C12 C11 C10 119.4(6) . . ?
C12 C11 H11 120.3 . . ?
C10 C11 H11 120.3 . . ?
C13 C12 C11 120.8(7) . . ?
C13 C12 C16 118.4(7) . 4_644 ?
C11 C12 C16 120.8(6) . 4_644 ?
C12 C13 C14 119.1(7) . . ?
C12 C13 H13 120.4 . . ?
C14 C13 H13 120.4 . . ?
C15 C14 C13 120.2(6) . . ?
C15 C14 N1 117.8(7) . 3_445 ?
C13 C14 N1 122.0(7) . 3_445 ?
C14 C15 C10 120.0(7) . . ?
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C10 C15 H15 120.0 . . ?
O5 C16 O6 125.2(7) . 7_665 ?
O5 C16 C12 117.9(7) . 4_654 ?
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O6 C16 C12 117.0(7) 7_665 4_654 ?
O7 C17 N2 132(2) . . ?
N2 C18 H18A 109.5 . . ?
N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
O8 C20 N3 115.2(15) . . ?
N3 C21 H21A 109.5 . . ?
N3 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
N3 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
N3 C22 H22A 109.5 . . ?
N3 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
N3 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?

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   4  0.750  0.250  0.000       190        31 ' '
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 '-x, -y, -z'
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Atlas'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.8767(3) 0.3181(6) 0.4996(6) 0.066(2) Uani 1 1 d . . .
O3 O 0.7298(2) 0.1440(5) 0.4710(5) 0.0591(17) Uani 1 1 d . . .
O4 O 0.7880(2) 0.0413(6) 0.4551(5) 0.0618(17) Uani 1 1 d . . .
O5 O 0.7664(3) 0.1775(7) 0.6621(5) 0.072(2) Uani 1 1 d U . .
O6 O 0.8014(2) 0.2427(8) 0.3769(5) 0.066(2) Uani 1 1 d . . .
O7 O 0.8464(3) 0.0471(8) 0.6307(7) 0.092(3) Uani 1 1 d U . .
O8 O 0.8588(3) 0.2704(8) 0.6826(7) 0.089(3) Uani 1 1 d U . .
N1 N 1.0953(3) 0.3990(8) 0.3499(5) 0.056(2) Uani 1 1 d . . .
N2 N 0.8863(7) 0.3558(17) 0.8183(14) 0.149(5) Uani 1 1 d U . .
C1 C 0.8999(3) 0.2442(10) 0.4761(7) 0.058(3) Uani 1 1 d . . .
C2 C 0.9445(3) 0.2615(10) 0.4352(8) 0.061(3) Uani 1 1 d . . .
C3 C 0.9697(4) 0.1776(12) 0.4061(11) 0.084(4) Uani 1 1 d . . .
H3 H 0.9582 0.1095 0.4067 0.101 Uiso 1 1 calc R . .
C4 C 1.0119(5) 0.1960(10) 0.3765(12) 0.091(5) Uani 1 1 d . . .
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C5 C 1.0296(4) 0.2953(10) 0.3739(8) 0.064(3) Uani 1 1 d . . .
C6 C 1.0036(4) 0.3785(11) 0.4034(8) 0.072(3) Uani 1 1 d . . .
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H6 H 1.0147 0.4470 0.4015 0.086 Uiso 1 1 calc R . .
C7 C 0.9619(4) 0.3601(11) 0.4353(9) 0.073(3) Uani 1 1 d . . .
H7 H 0.9456 0.4159 0.4571 0.088 Uiso 1 1 calc R . .
C8 C 1.0764(4) 0.3126(11) 0.3460(8) 0.067(3) Uani 1 1 d D . .
H16 H 1.088(4) 0.245(4) 0.336(9) 0.081 Uiso 1 1 d D . .
C9 C 0.7461(3) 0.0620(8) 0.4351(7) 0.053(2) Uani 1 1 d . . .
C10 C 0.7158(3) -0.0098(8) 0.3749(6) 0.049(2) Uani 1 1 d . . .
C11 C 0.6694(3) -0.0184(9) 0.3845(6) 0.053(2) Uani 1 1 d . . .
H11 H 0.6569 0.0246 0.4274 0.063 Uiso 1 1 calc R . .
C12 C 0.6414(3) -0.0901(8) 0.3311(6) 0.051(2) Uani 1 1 d . . .
C13 C 0.6593(3) -0.1497(9) 0.2617(6) 0.053(2) Uani 1 1 d . . .
H13 H 0.6410 -0.1981 0.2252 0.064 Uiso 1 1 calc R . .
C14 C 0.7058(3) -0.1348(9) 0.2485(6) 0.054(2) Uani 1 1 d . . .
C15 C 0.7342(3) -0.0699(8) 0.3068(6) 0.050(2) Uani 1 1 d . . .
H15 H 0.7654 -0.0659 0.3011 0.060 Uiso 1 1 calc R . .
C16 C 0.7256(3) 0.1945(9) 0.6721(7) 0.057(3) Uani 1 1 d . . .
C17 C 0.8481(10) 0.3107(19) 0.758(2) 0.144(6) Uani 1 1 d U . .
C18 C 0.8656(9) 0.411(2) 0.8927(18) 0.174(7) Uani 1 1 d U . .
H18A H 0.8894 0.4440 0.9357 0.261 Uiso 1 1 calc R . .
H18B H 0.8490 0.3620 0.9266 0.261 Uiso 1 1 calc R . .
H18C H 0.8447 0.4643 0.8645 0.261 Uiso 1 1 calc R . .
C19 C 0.9340(8) 0.372(2) 0.8023(18) 0.170(6) Uani 1 1 d U . .
H19A H 0.9510 0.4038 0.8573 0.254 Uiso 1 1 calc R . .
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0.0011(2)
O1 0.046(4) 0.084(6) 0.105(6) 0.015(5) 0.031(4) -0.006(4)
O2 0.052(4) 0.075(5) 0.077(5) -0.017(4) 0.028(4) -0.018(3)
O3 0.053(4) 0.046(3) 0.084(5) -0.003(3) 0.029(3) -0.001(3)
O4 0.041(3) 0.065(4) 0.081(5) -0.008(4) 0.011(3) -0.005(3)
O5 0.053(3) 0.106(4) 0.060(3) 0.017(3) 0.021(3) 0.006(3)
O6 0.040(4) 0.117(6) 0.043(3) 0.008(4) 0.012(3) 0.003(4)
O7 0.090(4) 0.099(5) 0.085(4) 0.018(4) 0.004(4) 0.010(4)
O8 0.084(4) 0.102(4) 0.077(4) -0.001(4) -0.003(3) 0.000(4)
N1 0.039(4) 0.080(6) 0.051(4) -0.002(4) 0.011(3) -0.009(4)
N2 0.157(6) 0.150(7) 0.138(6) -0.012(5) 0.009(4) -0.010(5)
C1 0.039(5) 0.091(8) 0.048(5) 0.000(5) 0.016(4) -0.011(5)
C2 0.045(5) 0.081(7) 0.058(6) 0.002(6) 0.007(4) -0.013(5)
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C4 0.076(9) 0.078(9) 0.130(13) -0.029(8) 0.062(9) -0.028(6)
C5 0.047(6) 0.094(9) 0.056(6) -0.012(5) 0.018(5) -0.003(5)
C6 0.051(6) 0.084(8) 0.082(8) -0.003(6) 0.015(5) -0.009(5)
C7 0.051(6) 0.093(9) 0.079(7) -0.009(7) 0.020(5) 0.000(6)
C8 0.056(7) 0.089(9) 0.060(6) -0.008(6) 0.021(5) -0.004(6)
C9 0.032(4) 0.069(6) 0.061(5) 0.000(5) 0.015(4) -0.006(4)
C10 0.041(4) 0.053(5) 0.054(5) -0.003(4) 0.014(4) 0.008(4)
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C13 0.043(5) 0.073(6) 0.046(5) -0.006(5) 0.014(4) -0.007(4)
C14 0.041(5) 0.078(7) 0.043(5) -0.008(5) 0.005(4) 0.000(4)
C15 0.036(4) 0.071(6) 0.045(4) 0.008(4) 0.014(3) -0.004(4)
C16 0.038(5) 0.098(8) 0.037(5) 0.019(5) 0.007(4) 0.000(4)
C17 0.148(7) 0.149(7) 0.137(7) -0.004(5) 0.023(5) -0.001(5)
C18 0.179(8) 0.176(8) 0.169(7) -0.009(5) 0.027(5) 0.000(5)
C19 0.165(7) 0.170(8) 0.173(8) -0.002(5) 0.023(5) -0.001(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 C9 2.930(10) . ?
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O6 C16 1.266(13) 7_656 ?
O8 C17 1.27(3) . ?
N1 C8 1.228(15) . ?
N1 C12 1.415(11) 3 ?
N2 C17 1.44(3) . ?
N2 C19 1.46(3) . ?
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C2 C7 1.352(18) . ?
C2 C3 1.390(18) . ?
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C4 C5 1.365(16) . ?
C4 H4 0.9300 . ?
C5 C6 1.397(16) . ?
C5 C8 1.492(15) . ?
C6 C7 1.377(14) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
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C10 C11 1.387(12) . ?
C10 C15 1.396(12) . ?
C11 C12 1.385(14) . ?
C11 H11 0.9300 . ?
C12 C13 1.401(13) . ?
C12 N1 1.415(11) 3_445 ?
C13 C14 1.409(12) . ?
C13 H13 0.9300 . ?
C14 C15 1.372(14) . ?
C14 C16 1.504(13) 6 ?
C15 H15 0.9300 . ?
C16 O6 1.266(13) 7_656 ?
C16 C14 1.504(13) 6_556 ?
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C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9600 . ?
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C19 H19C 0.9600 . ?

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O5 Eu1 O8 75.6(3) . . ?
O3 Eu1 O8 89.0(3) 7_656 . ?
O6 Eu1 O8 136.7(3) . . ?
O5 Eu1 O7 75.9(3) . . ?
O3 Eu1 O7 151.7(3) 7_656 . ?
O6 Eu1 O7 133.9(3) . . ?
O8 Eu1 O7 74.9(3) . . ?
O5 Eu1 O4 95.3(3) . . ?
O3 Eu1 O4 121.1(2) 7_656 . ?
O6 Eu1 O4 71.8(3) . . ?
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O8 Eu1 O4 146.4(3) . . ?
O7 Eu1 O4 71.5(3) . . ?
O5 Eu1 O1 147.5(3) . . ?
O3 Eu1 O1 132.2(2) 7_656 . ?
O6 Eu1 O1 74.8(3) . . ?
O8 Eu1 O1 90.5(3) . . ?
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C17 N2 C19 130(2) . . ?
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O6 C16 C14 116.4(8) 7_656 6_556 ?
O8 C17 N2 114(2) . . ?
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N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
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N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
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 '-x, -y, -z'
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 'x+1/2, -y+1/2, z-1/2'

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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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d . . .
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O2 O 0.1225(3) 0.8316(5) 0.4971(7) 0.060(2) Uani 1 1 d . . .
O3 O 0.2061(2) 0.5716(4) 0.5532(5) 0.0433(15) Uani 1 1 d . . .
O4 O 0.2312(2) 0.8459(4) 0.4589(5) 0.0406(15) Uani 1 1 d . . .
O5 O 0.2014(2) 0.7601(5) 0.6298(5) 0.0389(14) Uani 1 1 d . . .
O6 O 0.2279(2) 0.6698(5) 0.3310(5) 0.0462(17) Uani 1 1 d . . .
O7 O 0.1430(4) 0.5894(8) 0.3601(8) 0.057(2) Uani 0.75 1 d
PDU . .
O7A O 0.1494(14) 0.537(3) 0.359(3) 0.071(4) Uani 0.25 1 d
PU . .
O8 O 0.1400(5) 0.7797(12) 0.3066(14) 0.066(3) Uani 0.75 1 d
PDU . .
O8A O 0.153(2) 0.788(4) 0.302(5) 0.074(5) Uani 0.25 1 d PU . .
N1 N -0.0983(3) 0.9190(6) 0.6476(7) 0.050(2) Uani 1 1 d . . .
N2 N 0.1187(5) 0.5138(10) 0.1938(11) 0.071(3) Uani 0.75 1 d
PDU . .
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N3 N 0.1205(7) 0.8789(13) 0.1748(14) 0.095(4) Uani 0.75 1 d
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C1 C 0.0972(3) 0.7667(8) 0.5217(8) 0.045(2) Uani 1 1 d . . .
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H4 H -0.0397 0.6862 0.6221 0.116 Uiso 1 1 calc R . .
C5 C -0.0342(4) 0.8221(9) 0.6183(10) 0.059(3) Uani 1 1 d . . .
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H6 H -0.0145 0.9561 0.6058 0.072 Uiso 1 1 calc R . .
C7 C 0.0368(4) 0.8766(8) 0.5652(10) 0.057(3) Uani 1 1 d . . .
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C8 C -0.0812(4) 0.8387(10) 0.6470(9) 0.060(3) Uani 1 1 d D . .
H16 H -0.098(4) 0.788(6) 0.670(11) 0.072 Uiso 1 1 d D . .
C9 C 0.2503(3) 0.5819(6) 0.5731(7) 0.0335(18) Uani 1 1 d . . .
C10 C 0.2803(3) 0.5081(6) 0.6276(7) 0.0368(19) Uani 1 1 d . . .
C11 C 0.3273(3) 0.4983(6) 0.6153(8) 0.040(2) Uani 1 1 d . . .
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C12 C 0.3546(3) 0.4257(7) 0.6655(8) 0.042(2) Uani 1 1 d . . .
C13 C 0.3364(3) 0.3698(6) 0.7341(7) 0.038(2) Uani 1 1 d . . .
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C14 C 0.2894(3) 0.3800(6) 0.7476(7) 0.0353(19) Uani 1 1 d . . .
C15 C 0.2610(3) 0.4473(6) 0.6923(7) 0.037(2) Uani 1 1 d . . .
H15 H 0.2293 0.4520 0.6983 0.044 Uiso 1 1 calc R . .
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PDU . .
C18 C 0.1210(9) 0.4262(15) 0.2502(18) 0.100(5) Uani 0.75 1 d
PDU . .
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H18B H 0.1010 0.4297 0.3009 0.150 Uiso 0.75 1 calc PR . .
H18C H 0.1530 0.4150 0.2826 0.150 Uiso 0.75 1 calc PR . .
C19 C 0.1017(8) 0.5248(15) 0.0886(14) 0.084(4) Uani 0.75 1 d
PDU . .
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H19B H 0.1259 0.5515 0.0564 0.126 Uiso 0.75 1 calc PR . .
H19C H 0.0746 0.5649 0.0792 0.126 Uiso 0.75 1 calc PR . .
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PDU . .
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PDU . .
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H21B H 0.0520 0.8779 0.1358 0.150 Uiso 0.75 1 calc PR . .
H21C H 0.0707 0.9528 0.2179 0.150 Uiso 0.75 1 calc PR . .
C22 C 0.1413(9) 0.9243(17) 0.1064(18) 0.102(5) Uani 0.75 1 d
PDU . .
H22A H 0.1729 0.9015 0.1092 0.153 Uiso 0.75 1 calc PR . .
H22B H 0.1423 0.9892 0.1218 0.153 Uiso 0.75 1 calc PR . .
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O8 0.065(5) 0.068(5) 0.061(4) -0.006(3) 0.005(4) 0.009(4)
O8A 0.074(6) 0.073(7) 0.076(6) -0.003(5) 0.011(5) -0.001(5)
N1 0.033(4) 0.062(6) 0.058(5) 0.009(4) 0.018(4) 0.013(4)
N2 0.069(5) 0.073(4) 0.072(4) -0.009(3) 0.014(4) 0.002(4)
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C4 0.059(9) 0.071(9) 0.174(18) 0.039(10) 0.059(10) 0.005(7)
C5 0.049(6) 0.065(7) 0.068(7) 0.018(6) 0.023(5) 0.011(5)
C6 0.054(6) 0.060(7) 0.074(8) 0.017(6) 0.031(6) 0.007(5)
C7 0.037(5) 0.059(7) 0.079(8) -0.001(6) 0.018(5) 0.001(5)
C8 0.047(6) 0.079(9) 0.059(7) 0.017(6) 0.021(5) 0.006(6)
C9 0.028(4) 0.030(4) 0.046(5) 0.000(4) 0.017(3) 0.003(3)
C10 0.029(4) 0.034(5) 0.049(5) -0.002(4) 0.013(4) -0.002(3)
C11 0.033(4) 0.034(5) 0.060(6) 0.010(4) 0.025(4) 0.006(4)
C12 0.025(4) 0.053(6) 0.052(5) 0.009(5) 0.017(4) 0.004(4)
C13 0.033(4) 0.042(5) 0.044(5) 0.013(4) 0.018(4) 0.002(4)
C14 0.029(4) 0.043(5) 0.036(4) 0.001(4) 0.011(3) 0.000(3)
C15 0.028(4) 0.040(5) 0.048(5) -0.003(4) 0.019(4) 0.002(4)
C16 0.043(5) 0.039(5) 0.053(6) -0.009(4) 0.023(4) -0.004(4)
C17 0.075(6) 0.080(5) 0.070(3) -0.004(3) 0.013(4) 0.002(4)
C18 0.108(7) 0.091(5) 0.101(6) 0.010(4) 0.019(5) -0.004(5)
C19 0.086(6) 0.085(6) 0.080(4) -0.005(4) 0.011(4) -0.002(5)
C20 0.090(5) 0.090(6) 0.083(5) 0.002(4) 0.014(4) -0.005(4)
C21 0.100(5) 0.100(7) 0.099(7) 0.000(5) 0.013(4) 0.000(4)
C22 0.107(6) 0.101(7) 0.098(6) 0.008(4) 0.016(4) 0.002(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Gd1 O8 2.389(17) . ?
Gd1 O6 2.392(6) . ?
Gd1 O7 2.395(11) . ?
Gd1 O1 2.404(7) . ?
Gd1 O3 2.435(7) . ?
Gd1 O2 2.548(7) . ?
Gd1 O4 2.669(6) 7_566 ?
Gd1 C1 2.838(9) . ?
Gd1 C9 2.945(9) . ?
O1 C1 1.261(14) . ?
O2 C1 1.263(13) . ?
O3 C9 1.263(10) . ?
O4 C9 1.277(10) 7_566 ?
O4 Gd1 2.669(6) 7_566 ?
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O6 C16 1.263(11) 7_566 ?
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O7A C17 1.49(4) . ?
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N1 C12 1.415(11) 3_455 ?
N2 C17 1.40(2) . ?
N2 C19 1.41(2) . ?
N2 C18 1.47(2) . ?
N3 C22 1.34(2) . ?
N3 C21 1.41(3) . ?
N3 C20 1.45(3) . ?
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C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
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C10 C11 1.395(12) . ?
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C14 C15 1.396(13) . ?
C14 C16 1.472(12) 4_546 ?
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C16 C14 1.472(12) 4_556 ?
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C21 H21B 0.9600 . ?
C21 H21C 0.9600 . ?
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O4 Gd1 O8 83.8(4) . . ?
O8A Gd1 O8 10.0(15) . . ?
O5 Gd1 O6 134.8(2) . . ?
O4 Gd1 O6 79.9(2) . . ?
O8A Gd1 O6 69.4(16) . . ?
O8 Gd1 O6 76.4(4) . . ?
O5 Gd1 O7 139.2(3) . . ?
O4 Gd1 O7 146.2(3) . . ?
O8A Gd1 O7 77.8(15) . . ?
O8 Gd1 O7 72.8(5) . . ?
O6 Gd1 O7 71.3(3) . . ?
O5 Gd1 O1 79.5(3) . . ?
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O8A Gd1 O1 98.8(14) . . ?
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O6 Gd1 O1 141.9(3) . . ?
O7 Gd1 O1 70.8(3) . . ?
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O4 Gd1 O3 124.8(2) . . ?
O8A Gd1 O3 149.3(15) . . ?
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O5 Gd1 O2 70.3(3) . . ?
O4 Gd1 O2 82.9(2) . . ?
O8A Gd1 O2 73.6(16) . . ?
O8 Gd1 O2 68.2(5) . . ?
O6 Gd1 O2 142.0(3) . . ?
O7 Gd1 O2 109.4(3) . . ?
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O4 Gd1 O4 75.9(2) . 7_566 ?
O8A Gd1 O4 132.3(15) . 7_566 ?
O8 Gd1 O4 141.8(4) . 7_566 ?
O6 Gd1 O4 68.4(2) . 7_566 ?
O7 Gd1 O4 108.0(3) . 7_566 ?
O1 Gd1 O4 128.3(3) . 7_566 ?
O3 Gd1 O4 50.60(19) . 7_566 ?
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O6 Gd1 C1 152.0(3) . . ?
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C2 C3 H3 120.2 . . ?
C5 C4 C3 121.1(13) . . ?
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C3 C4 H4 119.5 . . ?
C4 C5 C6 119.9(11) . . ?
C4 C5 C8 118.5(12) . . ?
C6 C5 C8 121.6(12) . . ?
C7 C6 C5 119.7(12) . . ?
C7 C6 H6 120.2 . . ?
C5 C6 H6 120.2 . . ?
C2 C7 C6 121.6(11) . . ?
C2 C7 H7 119.2 . . ?
C6 C7 H7 119.2 . . ?
N1 C8 C5 121.6(11) . . ?
N1 C8 H16 119(8) . . ?
C5 C8 H16 119(8) . . ?
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O3 C9 C10 119.9(8) . . ?
O4 C9 C10 120.7(7) 7_566 . ?
O3 C9 Gd1 54.3(5) . . ?
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C11 C10 C9 120.6(8) . . ?
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C12 C13 C14 120.1(8) . . ?
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C14 C13 H13 119.9 . . ?
C15 C14 C13 119.8(8) . . ?
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C13 C14 C16 119.6(8) . 4_546 ?
C14 C15 C10 120.1(8) . . ?
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O5 C16 C14 117.7(8) . 4_556 ?
O7 C17 N2 131.0(18) . . ?
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N2 C17 O7A 102(2) . . ?
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N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
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H19B C19 H19C 109.5 . . ?
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O8 C20 N3 121(2) . . ?
N3 C21 H21A 109.5 . . ?
N3 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
N3 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
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N3 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
N3 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?

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  _platon_squeeze_void_count_electrons
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   2  0.251  0.750 -0.001       192        52 ' '
   3  0.500  0.001 -0.001       300        80 ' '
   4  0.750  0.250  0.000       190        51 ' '
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loop_
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 MERCURY (Bruno et al. 2002)
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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O1 O 0.87609(17) 0.1807(4) 0.5001(4) 0.0498(14) Uani 1 1
d . . .
O2 O 0.88509(17) 0.3453(5) 0.4757(4) 0.0574(15) Uani 1 1
d . . .
O3 O 0.72912(15) 0.3515(4) 0.4675(3) 0.0400(12) Uani 1 1
d . . .
O4 O 0.78871(15) 0.4508(4) 0.4544(4) 0.0440(12) Uani 1 1
d . . .
O5 O 0.79997(15) 0.2535(4) 0.3745(3) 0.0412(12) Uani 1 1
d . . .
O6 O 0.76715(16) 0.3287(5) 0.6611(4) 0.0564(15) Uani 1 1
d . . .
O7 O 0.8558(2) 0.2286(6) 0.6836(5) 0.086(2) Uani 1 1 d DU . .
O8 O 0.8500(2) 0.4417(5) 0.6337(4) 0.079(2) Uani 1 1 d . . .
N1 N 1.09554(18) 0.0939(5) 0.3527(4) 0.0433(15) Uani 1 1
d . . .
N2 N 0.8823(4) 0.1393(9) 0.8178(8) 0.137(3) Uani 1 1 d DU . .
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C1 C 0.8988(2) 0.2537(7) 0.4732(5) 0.0439(18) Uani 1 1 d . . .
C2 C 0.9444(2) 0.2344(6) 0.4356(5) 0.0419(18) Uani 1 1 d . . .
C3 C 0.9617(2) 0.1380(7) 0.4362(5) 0.050(2) Uani 1 1 d . . .
H3 H 0.9450 0.0841 0.4576 0.060 Uiso 1 1 calc R . .
C4 C 1.0040(2) 0.1197(7) 0.4053(5) 0.050(2) Uani 1 1 d . . .
H4 H 1.0153 0.0532 0.4052 0.061 Uiso 1 1 calc R . .
C5 C 1.0291(3) 0.1968(7) 0.3751(6) 0.049(2) Uani 1 1 d . . .
C6 C 1.0120(3) 0.2943(7) 0.3723(8) 0.075(3) Uani 1 1 d . . .
H6 H 1.0290 0.3482 0.3515 0.090 Uiso 1 1 calc R . .
C7 C 0.9682(3) 0.3116(7) 0.4014(7) 0.071(3) Uani 1 1 d . . .
H7 H 0.9555 0.3769 0.3970 0.085 Uiso 1 1 calc R . .
C8 C 1.0766(3) 0.1828(8) 0.3474(6) 0.055(2) Uani 1 1 d D . .
C9 C 0.7463(2) 0.4325(6) 0.4350(5) 0.0379(17) Uani 1 1 d . . .
C10 C 0.7157(2) 0.5051(6) 0.3749(4) 0.0357(16) Uani 1 1 d . . .
C11 C 0.6689(2) 0.5150(5) 0.3852(5) 0.0357(16) Uani 1 1 d . . .
H11 H 0.6562 0.4732 0.4287 0.043 Uiso 1 1 calc R . .
C12 C 0.6416(2) 0.5848(6) 0.3326(5) 0.0398(18) Uani 1 1 d . . .
C13 C 0.6599(2) 0.6431(6) 0.2632(5) 0.0382(17) Uani 1 1 d . . .
H13 H 0.6411 0.6892 0.2255 0.046 Uiso 1 1 calc R . .
C14 C 0.7064(2) 0.6322(6) 0.2502(4) 0.0384(18) Uani 1 1 d . . .
C15 C 0.7345(2) 0.5658(6) 0.3082(4) 0.0374(17) Uani 1 1 d . . .
H15 H 0.7659 0.5616 0.3027 0.045 Uiso 1 1 calc R . .
C16 C 0.7743(2) 0.1910(6) 0.3276(5) 0.0401(19) Uani 1 1 d . . .
C17 C 0.8450(5) 0.1931(11) 0.7601(8) 0.141(4) Uani 1 1 d DU . .
C18 C 0.9297(4) 0.1319(12) 0.7981(11) 0.151(4) Uani 1 1 d
DU . .
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H18B H 0.9424 0.1993 0.7944 0.227 Uiso 1 1 calc R . .
H18C H 0.9305 0.0972 0.7378 0.227 Uiso 1 1 calc R . .
C19 C 0.8649(5) 0.0825(11) 0.8944(9) 0.149(4) Uani 1 1 d DU . .
H19A H 0.8901 0.0492 0.9333 0.223 Uiso 1 1 calc R . .
H19B H 0.8431 0.0322 0.8667 0.223 Uiso 1 1 calc R . .
H19C H 0.8499 0.1286 0.9339 0.223 Uiso 1 1 calc R . .
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0.00241(16)
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O2 0.032(3) 0.055(4) 0.092(4) -0.016(3) 0.033(3) -0.002(3)
O3 0.030(3) 0.042(3) 0.052(3) 0.005(2) 0.020(2) 0.008(2)
O4 0.025(2) 0.039(3) 0.069(3) 0.006(3) 0.011(2) 0.002(2)
O5 0.027(2) 0.069(3) 0.028(2) -0.010(3) 0.010(2) -0.003(3)
O6 0.026(3) 0.098(4) 0.049(3) -0.032(3) 0.020(2) -0.009(3)
O7 0.064(4) 0.112(6) 0.079(4) -0.026(4) 0.000(3) 0.019(4)
O8 0.063(4) 0.099(5) 0.076(4) -0.041(4) 0.011(3) -0.038(4)
N1 0.024(3) 0.065(4) 0.045(3) 0.012(3) 0.017(2) 0.009(3)
N2 0.144(4) 0.140(5) 0.123(4) 0.007(3) 0.009(3) 0.008(3)
C1 0.024(4) 0.067(5) 0.041(4) 0.000(4) 0.004(3) 0.005(4)
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C2 0.029(4) 0.057(5) 0.042(4) 0.006(4) 0.017(3) 0.010(4)
C3 0.030(4) 0.065(6) 0.060(5) -0.001(4) 0.021(3) -0.004(4)
C4 0.031(4) 0.058(5) 0.064(5) 0.006(4) 0.014(3) 0.008(4)
C5 0.033(4) 0.065(6) 0.054(5) 0.008(4) 0.018(3) 0.007(4)
C6 0.047(5) 0.069(6) 0.121(8) 0.028(6) 0.056(5) 0.019(5)
C7 0.043(5) 0.067(6) 0.112(8) 0.003(6) 0.042(5) 0.003(5)
C8 0.032(4) 0.087(7) 0.048(5) 0.010(5) 0.012(3) 0.001(5)
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C17 0.145(5) 0.146(5) 0.133(5) 0.009(4) 0.019(3) 0.003(4)
C18 0.150(4) 0.152(6) 0.152(5) 0.003(4) 0.023(4) 0.001(4)
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l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Tb1 O8 2.438(5) . ?
Tb1 O2 2.440(5) . ?
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Tb1 O3 2.658(4) . ?
Tb1 C1 2.808(7) . ?
Tb1 C9 2.911(7) . ?
Tb1 Tb1 3.9833(6) 7_656 ?
O1 C1 1.247(10) . ?
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O5 C16 1.237(8) . ?
O6 C16 1.266(8) 7_656 ?
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
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_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1355P)^2^+138.6045P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4727
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_refine_ls_R_factor_all           0.0990
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U . .
O1 O 0.3878(4) 0.1744(12) 0.4794(12) 0.099(4) Uani 1 1 d U . .
O2 O 0.3775(4) 0.3252(11) 0.5067(10) 0.087(4) Uani 1 1 d U . .
O3 O 0.2921(3) 0.0660(8) 0.4480(9) 0.070(3) Uani 1 1 d U . .
O4 O 0.2701(3) 0.3454(8) 0.5405(7) 0.060(3) Uani 1 1 d U . .
O5 O 0.2697(4) 0.1658(9) 0.6616(8) 0.072(3) Uani 1 1 d U . .
O6 O 0.3003(3) 0.2571(9) 0.3754(7) 0.060(3) Uani 1 1 d U . .
O7 O 0.3559(5) 0.0798(14) 0.6379(11) 0.120(6) Uani 1 1 d U . .
O8 O 0.3547(7) 0.2777(13) 0.6886(16) 0.126(5) Uani 1 1 d DU . .
N1 N 0.5978(4) 0.4128(12) 0.3508(10) 0.073(4) Uani 1 1 d U . .
N2 N 0.3805(12) 0.373(2) 0.828(2) 0.176(7) Uani 1 1 d DU . .
C1 C 0.4035(7) 0.2529(19) 0.4765(14) 0.091(7) Uani 1 1 d U . .
C2 C 0.4471(7) 0.2781(14) 0.4405(15) 0.079(5) Uani 1 1 d U . .
C3 C 0.4629(6) 0.3701(17) 0.4400(15) 0.092(6) Uani 1 1 d U . .
H3 H 0.4461 0.4194 0.4646 0.110 Uiso 1 1 calc R . .
C4 C 0.5057(6) 0.3917(16) 0.4015(16) 0.089(6) Uani 1 1 d U . .
H4 H 0.5152 0.4549 0.3941 0.107 Uiso 1 1 calc R . .
C5 C 0.5317(7) 0.3158(18) 0.3761(15) 0.087(5) Uani 1 1 d U . .
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C6 C 0.5171(10) 0.2262(19) 0.373(2) 0.116(7) Uani 1 1 d U . .
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H7 H 0.4582 0.1437 0.3959 0.133 Uiso 1 1 calc R . .
C8 C 0.5789(7) 0.331(2) 0.3498(16) 0.093(6) Uani 1 1 d U . .
C9 C 0.2484(5) 0.0784(11) 0.4322(11) 0.056(4) Uani 1 1 d U . .
C10 C 0.2192(5) 0.0051(12) 0.3725(11) 0.059(4) Uani 1 1 d U . .
C11 C 0.2375(4) -0.0544(10) 0.3050(10) 0.051(3) Uani 1 1 d
U . .
H11 H 0.2689 -0.0488 0.2973 0.061 Uiso 1 1 calc R . .
C12 C 0.2091(5) -0.1213(13) 0.2499(11) 0.064(4) Uani 1 1 d
U . .
C13 C 0.1621(5) -0.1314(13) 0.2634(13) 0.071(5) Uani 1 1 d
U . .
H13 H 0.1431 -0.1762 0.2257 0.085 Uiso 1 1 calc R . .
C14 C 0.1442(5) -0.0777(14) 0.3296(12) 0.068(4) Uani 1 1 d
U . .
C15 C 0.1709(5) -0.0047(12) 0.3835(12) 0.065(4) Uani 1 1 d
U . .
H15 H 0.1575 0.0361 0.4252 0.078 Uiso 1 1 calc R . .
C16 C 0.2280(5) 0.1825(12) 0.6710(11) 0.059(4) Uani 1 1 d U . .
C17 C 0.3445(15) 0.313(3) 0.762(3) 0.179(8) Uani 1 1 d DU . .
C18 C 0.3568(14) 0.419(3) 0.897(3) 0.188(9) Uani 1 1 d DU . .
H18A H 0.3786 0.4568 0.9415 0.282 Uiso 1 1 calc R . .
H18B H 0.3428 0.3713 0.9346 0.282 Uiso 1 1 calc R . .
H18C H 0.3327 0.4594 0.8625 0.282 Uiso 1 1 calc R . .
C19 C 0.4290(14) 0.373(3) 0.807(3) 0.196(9) Uani 1 1 d DU . .
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H19B H 0.4302 0.4081 0.7464 0.295 Uiso 1 1 calc R . .
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0.0023(3)
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O2 0.050(7) 0.119(10) 0.103(10) -0.018(8) 0.045(7) -0.009(7)
O3 0.042(6) 0.067(7) 0.105(8) -0.004(6) 0.023(5) -0.004(5)
O4 0.043(5) 0.085(7) 0.059(6) -0.006(5) 0.027(4) -0.011(5)
O5 0.043(6) 0.106(8) 0.073(7) 0.020(7) 0.025(5) 0.003(6)
O6 0.032(5) 0.098(7) 0.055(5) 0.010(6) 0.022(4) 0.019(5)
O7 0.060(8) 0.200(16) 0.110(10) 0.059(11) 0.046(7) 0.059(10)
O8 0.122(7) 0.127(7) 0.127(6) 0.009(4) 0.015(5) -0.005(5)
N1 0.039(7) 0.111(11) 0.075(8) -0.011(8) 0.027(6) -0.017(7)
N2 0.180(8) 0.175(8) 0.172(8) -0.006(5) 0.023(5) -0.002(5)
C1 0.067(12) 0.130(17) 0.071(11) 0.044(12) -0.006(9) -0.048(13)
C2 0.058(10) 0.096(12) 0.090(13) 0.013(10) 0.033(9) -0.022(8)
C3 0.051(9) 0.125(16) 0.111(14) -0.042(13) 0.048(10) -0.009(10)
C4 0.053(10) 0.096(14) 0.118(16) -0.003(12) 0.012(10) 0.001(9)
C5 0.062(10) 0.127(12) 0.078(11) -0.029(11) 0.032(9) -0.008(10)
```

```
C6 0.109(8) 0.118(9) 0.127(10) -0.007(7) 0.042(7) 0.007(6)
C7 0.102(8) 0.109(9) 0.124(10) 0.002(7) 0.028(7) -0.001(6)
C8 0.061(11) 0.135(18) 0.089(13) 0.005(13) 0.032(10) 0.006(12)
C9 0.039(7) 0.069(9) 0.067(9) -0.006(7) 0.025(6) -0.009(7)
C10 0.032(7) 0.079(10) 0.069(9) -0.002(8) 0.024(6) -0.006(7)
C11 0.031(6) 0.072(9) 0.052(7) 0.001(7) 0.018(5) -0.002(6)
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C13 0.046(8) 0.089(11) 0.088(11) -0.017(9) 0.041(8) -0.021(8)
C14 0.032(7) 0.107(13) 0.067(9) -0.013(9) 0.017(6) -0.008(8)
C15 0.036(7) 0.080(10) 0.086(10) -0.015(9) 0.033(7) -0.009(7)
C16 0.039(8) 0.089(11) 0.055(8) 0.012(8) 0.025(6) 0.002(7)
C17 0.181(9) 0.181(9) 0.177(8) -0.004(5) 0.032(5) 0.001(5)
C18 0.189(10) 0.187(10) 0.187(9) -0.003(5) 0.030(5) 0.001(5)
C19 0.193(9) 0.199(10) 0.198(10) -0.002(5) 0.032(5) -0.002(5)

_geom_special_details
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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Dy1 O5 2.350(10) . ?
Dy1 O1 2.397(11) . ?
Dy1 O3 2.403(11) . ?
Dy1 O7 2.412(14) . ?
Dy1 O2 2.492(13) . ?
Dy1 O4 2.664(10) 7_556 ?
Dy1 C1 2.86(2) . ?
Dy1 C9 2.896(15) . ?
Dy1 Dy1 3.9583(12) 7_556 ?
O1 C1 1.18(3) . ?
O2 C1 1.35(3) . ?
O3 C9 1.253(17) . ?
O4 C9 1.268(18) 7_556 ?
O4 Dy1 2.665(10) 7_556 ?
O5 C16 1.250(17) . ?
O6 C16 1.266(18) 7_556 ?
```

```
O8 C17 1.20(3) . ?
N1 C8 1.27(3) . ?
N1 C14 1.415(18) 3 ?
N2 C18 1.40(3) . ?
N2 C19 1.47(3) . ?
N2 C17 1.51(3) . ?
C1 C2 1.46(3) . ?
C2 C3 1.36(3) . ?
C2 C7 1.37(3) . ?
C3 C4 1.44(2) . ?
C3 H3 0.9300 . ?
C4 C5 1.37(3) . ?
C4 H4 0.9300 . ?
C5 C6 1.31(3) . ?
C5 C8 1.48(3) . ?
C6 C7 1.48(4) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C9 O4 1.268(18) 7_556 ?
C9 C10 1.48(2) . ?
C10 C11 1.40(2) . ?
C10 C15 1.427(18) . ?
C11 C12 1.38(2) . ?
C11 H11 0.9300 . ?
C12 C13 1.400(19) . ?
C12 C16 1.536(19) 6 ?
C13 C14 1.33(2) . ?
C13 H13 0.9300 . ?
C14 C15 1.41(2) . ?
C14 N1 1.415(18) 3_445 ?
C15 H15 0.9300 . ?
C16 O6 1.266(18) 7_556 ?
C16 C12 1.536(19) 6_556 ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
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O4 Dy1 O5 79.9(4) . . ?
O6 Dy1 O5 134.8(3) . . ?
O8 Dy1 O5 75.6(6) . . ?
O4 Dy1 O1 133.5(5) . . ?
O6 Dy1 O1 76.4(4) . . ?
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O8 Dy1 O1 93.7(7) . . ?
O5 Dy1 O1 143.8(5) . . ?
O4 Dy1 O3 124.1(4) . . ?
O6 Dy1 O3 74.4(4) . . ?
O8 Dy1 O3 148.0(5) . . ?
O5 Dy1 O3 90.4(4) . . ?
O1 Dy1 O3 80.8(5) . . ?
O4 Dy1 O7 146.8(4) . . ?
O6 Dy1 O7 138.3(5) . . ?
O8 Dy1 O7 73.4(6) . . ?
O5 Dy1 O7 72.6(4) . . ?
O1 Dy1 O7 71.3(5) . . ?
O3 Dy1 O7 75.0(6) . . ?
O4 Dy1 O2 83.8(4) . . ?
O6 Dy1 O2 70.7(4) . . ?
O8 Dy1 O2 69.0(6) . . ?
O5 Dy1 O2 142.7(4) . . ?
O1 Dy1 O2 52.3(5) . . ?
O3 Dy1 O2 126.2(4) . . ?
O7 Dy1 O2 107.1(5) . . ?
O4 Dy1 O4 74.8(4) . 7_556 ?
O6 Dy1 O4 69.6(3) . 7_556 ?
O8 Dy1 O4 139.4(6) . 7_556 ?
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O2 Dy1 O4 138.5(4) . 7_556 ?
O4 Dy1 C1 110.9(6) . . ?
O6 Dy1 C1 71.8(4) . . ?
O8 Dy1 C1 81.7(7) . . ?
O5 Dy1 C1 153.3(4) . . ?
O1 Dy1 C1 24.1(7) . . ?
O3 Dy1 C1 102.0(6) . . ?
O7 Dy1 C1 87.7(5) . . ?
O2 Dy1 C1 28.3(6) . . ?
O4 Dy1 C1 137.7(4) 7_556 . ?
O4 Dy1 C9 100.1(4) . . ?
O6 Dy1 C9 70.8(4) . . ?
O8 Dy1 C9 152.3(6) . . ?
O5 Dy1 C9 77.6(4) . . ?
O1 Dy1 C9 103.9(5) . . ?
O3 Dy1 C9 25.2(4) . . ?
O7 Dy1 C9 92.0(6) . . ?
O2 Dy1 C9 138.6(4) . . ?
O4 Dy1 C9 25.9(4) 7_556 . ?
C1 Dy1 C9 121.9(6) . . ?
O4 Dy1 Dy1 40.5(2) . 7_556 ?
O6 Dy1 Dy1 67.2(2) . 7_556 ?
O8 Dy1 Dy1 115.6(5) . 7_556 ?
O5 Dy1 Dy1 69.2(3) . 7_556 ?
O1 Dy1 Dy1 143.2(4) . 7_556 ?
O3 Dy1 Dy1 84.6(2) . 7_556 ?
O7 Dy1 Dy1 136.2(3) . 7_556 ?
O2 Dy1 Dy1 116.2(4) . 7_556 ?
O4 Dy1 Dy1 34.3(2) 7_556 7_556 ?
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C1 Dy1 Dy1 134.9(4) . 7_556 ?
C9 Dy1 Dy1 59.8(3) . 7_556 ?
C1 O1 Dy1 100.3(16) . . ?
C1 O2 Dy1 91.1(11) . . ?
C9 O3 Dy1 100.0(9) . . ?
C9 O4 Dy1 162.1(10) 7_556 . ?
C9 O4 Dy1 87.3(8) 7_556 7_556 ?
Dy1 O4 Dy1 105.2(4) . 7_556 ?
C16 O5 Dy1 133.2(10) . . ?
C16 O6 Dy1 133.2(9) 7_556 . ?
C17 O8 Dy1 138(3) . . ?
C8 N1 C14 120.0(16) . 3 ?
C18 N2 C19 135(4) . . ?
C18 N2 C17 107(3) . . ?
C19 N2 C17 118(3) . . ?
O1 C1 O2 116.3(18) . . ?
O1 C1 C2 126(3) . . ?
O2 C1 C2 117.9(19) . . ?
O1 C1 Dy1 55.6(11) . . ?
O2 C1 Dy1 60.7(9) . . ?
C2 C1 Dy1 177.6(15) . . ?
C3 C2 C7 120.5(18) . . ?
C3 C2 C1 122(2) . . ?
C7 C2 C1 117(2) . . ?
C2 C3 C4 120.2(18) . . ?
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C4 C3 H3 119.9 . . ?
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C5 C6 H6 120.9 . . ?
C7 C6 H6 120.9 . . ?
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C2 C7 H7 120.5 . . ?
C6 C7 H7 120.5 . . ?
N1 C8 C5 122(2) . . ?
O3 C9 O4 121.5(14) . 7_556 ?
O3 C9 C10 117.9(13) . . ?
O4 C9 C10 120.4(13) 7_556 . ?
O3 C9 Dy1 54.8(8) . . ?
O4 C9 Dy1 66.8(7) 7_556 . ?
C10 C9 Dy1 172.5(10) . . ?
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C11 C10 C9 121.7(12) . . ?
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C10 C11 H11 119.9 . . ?
C11 C12 C13 119.8(13) . . ?
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C13 C12 C16 119.6(14) . 6 ?
C14 C13 C12 121.2(15) . . ?
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C15 C14 N1 114.6(14) . 3_445 ?
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C14 C15 H15 120.8 . . ?
C10 C15 H15 120.8 . . ?
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O5 C16 C12 114.9(14) . 6_556 ?
O6 C16 C12 116.4(12) 7_556 6_556 ?
O8 C17 N2 119(4) . . ?
N2 C18 H18A 109.5 . . ?
N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
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RESPONSE: The reported formula, molecular weight, F000,
density etc include
the contribution of imine H atoms,
which could not be located.
;
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;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of imine H atoms,
which could not be located.
```

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;
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;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of imine H atoms,
which could not be located.
;
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;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
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which could not be located.
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RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of imine H atoms,
which could not be located.
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data_UCY-12

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
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 'Ho'  'Ho'  -0.2175   4.6783
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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_angle_beta                  99.650(6)
_cell_angle_gamma                 90.00
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Diffraction)'

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Source'
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Atlas'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_coef        ?
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O1 O 0.3892(4) 0.1833(9) 0.9816(12) 0.061(4) Uani 1 1 d . . .
O2 O 0.3772(4) 0.3308(9) 1.0060(11) 0.057(3) Uani 1 1 d . . .
O3 O 0.2937(4) 0.0743(7) 0.9456(9) 0.043(3) Uani 1 1 d . . .
O4 O 0.2700(4) 0.3427(7) 1.0447(8) 0.039(2) Uani 1 1 d . . .
O5 O 0.2993(3) 0.2623(7) 0.8721(9) 0.040(3) Uani 1 1 d . . .
O6 O 0.2288(4) 0.3361(8) 0.8391(9) 0.046(3) Uani 1 1 d . . .
O7 O 0.3589(8) 0.2729(16) 1.1880(17) 0.060(7) Uani 0.75 1 d
PDU . .
O7A O 0.3460(15) 0.288(3) 1.200(3) 0.014(8) Uani 0.25 1 d
PU . .
O8 O 0.3575(5) 0.0891(11) 1.1373(11) 0.043(3) Uani 0.75 1 d
PDU . .
O8A O 0.350(2) 0.025(5) 1.142(5) 0.078(17) Uani 0.25 1 d PU . .
N1 N 0.4023(4) 0.4211(11) 0.6498(12) 0.049(4) Uani 1 1 d . . .
N2 N 0.3771(13) 0.370(3) 1.330(3) 0.119(11) Uani 0.75 1 d
PDU . .
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N3 N 0.3821(11) 0.013(2) 1.304(2) 0.095(9) Uani 0.75 1 d
PDU . .
C1 C 0.4025(6) 0.2636(14) 0.9800(13) 0.047(4) Uani 1 1 d . . .
C2 C 0.4472(6) 0.2873(12) 0.9430(15) 0.048(4) Uani 1 1 d . . .
C3 C 0.4611(7) 0.3762(15) 0.9341(17) 0.063(6) Uani 1 1 d . . .
H3 H 0.4421 0.4247 0.9500 0.076 Uiso 1 1 calc R . .
C4 C 0.5051(6) 0.3967(14) 0.9000(16) 0.057(5) Uani 1 1 d . . .
H4 H 0.5148 0.4580 0.8938 0.069 Uiso 1 1 calc R . .
C5 C 0.4675(7) 0.3232(16) 0.6231(18) 0.068(6) Uani 1 1 d . . .
C6 C 0.5195(10) 0.236(2) 0.888(4) 0.16(2) Uani 1 1 d . . .
H6 H 0.5404 0.1875 0.8808 0.194 Uiso 1 1 calc R . .
C7 C 0.4745(8) 0.2151(17) 0.910(3) 0.107(12) Uani 1 1 d . . .
H7 H 0.4628 0.1546 0.9033 0.128 Uiso 1 1 calc R . .
C8 C 0.4194(6) 0.3415(15) 0.6489(15) 0.058(5) Uani 1 1 d . . .
C9 C 0.2490(5) 0.0855(11) 0.9264(11) 0.035(3) Uani 1 1 d . . .
C10 C 0.2198(5) 0.0107(10) 0.8701(12) 0.035(3) Uani 1 1 d . . .
C11 C 0.2614(5) 0.4509(10) 0.6956(12) 0.035(3) Uani 1 1 d . . .
H11 H 0.2299 0.4564 0.7033 0.041 Uiso 1 1 calc R . .
C12 C 0.2901(5) 0.3831(10) 0.7498(11) 0.034(3) Uani 1 1 d . . .
C13 C 0.3370(5) 0.3732(11) 0.7362(12) 0.040(4) Uani 1 1 d . . .
H13 H 0.3561 0.3285 0.7730 0.048 Uiso 1 1 calc R . .
C14 C 0.3551(5) 0.4296(11) 0.6681(12) 0.040(4) Uani 1 1 d . . .
C15 C 0.3279(5) 0.5015(10) 0.6186(12) 0.038(4) Uani 1 1 d . . .
H15 H 0.3412 0.5433 0.5782 0.046 Uiso 1 1 calc R . .
C16 C 0.2712(5) 0.3222(12) 0.8273(13) 0.041(4) Uani 1 1 d . . .
C17 C 0.3442(16) 0.317(3) 1.253(3) 0.124(16) Uani 0.75 1 d
PDU . .
C18 C 0.3548(16) 0.418(3) 1.393(3) 0.118(14) Uani 0.75 1 d
PDU . .
H18A H 0.3237 0.3930 1.3911 0.177 Uiso 0.75 1 calc PR . .
H18B H 0.3524 0.4823 1.3715 0.177 Uiso 0.75 1 calc PR . .
H18C H 0.3723 0.4144 1.4605 0.177 Uiso 0.75 1 calc PR . .
C19 C 0.4222(14) 0.378(3) 1.305(3) 0.123(15) Uani 0.75 1 d
PDU . .
H19A H 0.4267 0.3311 1.2571 0.184 Uiso 0.75 1 calc PR . .
H19B H 0.4453 0.3710 1.3657 0.184 Uiso 0.75 1 calc PR . .
H19C H 0.4256 0.4387 1.2765 0.184 Uiso 0.75 1 calc PR . .
C20 C 0.3658(13) 0.087(3) 1.233(2) 0.094(11) Uani 0.75 1 d
PDU . .
C21 C 0.372(2) -0.070(4) 1.236(4) 0.18(2) Uani 0.75 1 d PDU . .
H21A H 0.3816 -0.1258 1.2744 0.265 Uiso 0.75 1 calc PR . .
H21B H 0.3901 -0.0654 1.1813 0.265 Uiso 0.75 1 calc PR . .
H21C H 0.3392 -0.0731 1.2089 0.265 Uiso 0.75 1 calc PR . .
C22 C 0.402(2) 0.026(4) 1.411(4) 0.18(2) Uani 0.75 1 d PDU . .
H22A H 0.4100 -0.0331 1.4418 0.263 Uiso 0.75 1 calc PR . .
H22B H 0.3798 0.0576 1.4445 0.263 Uiso 0.75 1 calc PR . .
H22C H 0.4305 0.0634 1.4155 0.263 Uiso 0.75 1 calc PR . .

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0.0014(3)
O1 0.036(6) 0.054(8) 0.103(11) 0.009(7) 0.037(7) 0.005(6)
O2 0.045(7) 0.051(7) 0.084(9) -0.022(7) 0.036(7) -0.015(6)
O3 0.035(6) 0.029(5) 0.069(8) -0.005(5) 0.019(5) -0.003(4)
O4 0.033(5) 0.034(6) 0.054(7) -0.009(5) 0.021(5) -0.004(4)
O5 0.028(5) 0.042(6) 0.055(7) 0.011(5) 0.022(5) 0.016(5)
O6 0.031(6) 0.056(7) 0.057(7) 0.022(6) 0.025(5) 0.005(5)
O7 0.058(8) 0.062(8) 0.058(8) -0.003(5) 0.009(5) 0.001(5)
O7A 0.015(9) 0.014(9) 0.014(9) -0.002(5) 0.001(5) 0.000(5)
O8 0.039(5) 0.046(5) 0.044(5) 0.005(4) 0.010(4) 0.006(4)
O8A 0.077(18) 0.079(18) 0.078(18) -0.001(5) 0.015(6) 0.000(5)
N1 0.025(7) 0.061(10) 0.068(10) 0.015(8) 0.026(7) 0.008(6)
N2 0.120(12) 0.119(12) 0.118(12) -0.001(5) 0.018(5) -0.001(5)
N3 0.095(10) 0.093(10) 0.095(10) 0.002(5) 0.014(5) 0.000(5)
C1 0.031(8) 0.065(12) 0.047(10) 0.003(9) 0.010(7) -0.008(8)
C2 0.034(8) 0.045(10) 0.070(12) -0.003(9) 0.018(8) -0.009(7)
C3 0.047(10) 0.063(12) 0.090(15) -0.016(11) 0.040(11) -0.004(9)
C4 0.044(10) 0.050(11) 0.078(13) -0.014(10) 0.010(9) -0.004(8)
C5 0.050(11) 0.068(13) 0.096(16) 0.026(12) 0.039(11) 0.012(10)
C6 0.073(17) 0.09(2) 0.34(6) -0.13(3) 0.12(3) -0.042(16)
C7 0.043(12) 0.061(14) 0.23(4) 0.029(18) 0.053(17) -0.005(10)
C8 0.042(10) 0.079(14) 0.059(11) 0.008(10) 0.026(9) 0.009(10)
C9 0.028(7) 0.038(8) 0.043(8) 0.001(7) 0.020(6) 0.000(6)
C10 0.027(7) 0.029(7) 0.053(9) 0.005(7) 0.018(7) 0.000(6)
C11 0.024(7) 0.035(8) 0.047(9) 0.002(7) 0.013(6) 0.003(6)
C12 0.030(7) 0.038(8) 0.039(8) 0.005(7) 0.017(6) 0.002(6)
C13 0.034(8) 0.039(8) 0.052(9) 0.017(7) 0.023(7) 0.011(7)
C14 0.029(8) 0.044(9) 0.050(9) 0.001(7) 0.019(7) 0.006(7)
C15 0.038(8) 0.030(8) 0.055(10) 0.013(7) 0.030(7) 0.005(6)
C16 0.026(8) 0.048(9) 0.048(9) 0.015(8) 0.007(7) 0.003(7)
C17 0.124(16) 0.124(16) 0.123(16) 0.001(5) 0.021(6) 0.000(5)
C18 0.119(15) 0.118(15) 0.117(15) 0.001(5) 0.019(5) 0.000(5)
C19 0.123(15) 0.122(15) 0.122(15) 0.000(5) 0.020(6) 0.001(5)
C20 0.093(11) 0.094(11) 0.095(11) 0.000(5) 0.014(5) 0.000(5)
C21 0.18(2) 0.18(2) 0.18(2) -0.002(5) 0.031(6) 0.000(5)
C22 0.18(2) 0.18(2) 0.18(2) -0.001(5) 0.030(6) 0.000(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Ho1 O7 2.31(2) . ?
Ho1 O5 2.322(11) . ?
Ho1 O6 2.345(10) 7_557 ?
Ho1 O1 2.377(11) . ?
Ho1 O3 2.380(11) . ?
Ho1 O8 2.387(15) . ?
Ho1 O7A 2.42(4) . ?
Ho1 O2 2.523(11) . ?
Ho1 O4 2.670(10) 7_557 ?
Ho1 C1 2.812(16) . ?
Ho1 C9 2.895(15) . ?
O1 C1 1.22(2) . ?
O2 C1 1.29(2) . ?
O3 C9 1.275(17) . ?
O4 C9 1.257(17) 7_557 ?
O4 Ho1 2.670(10) 7_557 ?
O5 C16 1.259(18) . ?
O6 C16 1.268(18) . ?
O6 Ho1 2.345(10) 7_557 ?
O7 C17 1.20(4) . ?
O7A C17 0.83(5) . ?
O8 O8A 0.95(7) . ?
O8 C20 1.26(3) . ?
O8A C20 1.51(7) . ?
O8A C21 1.90(9) . ?
N1 C8 1.24(2) . ?
N1 C14 1.422(18) . ?
N2 C18 1.33(4) . ?
N2 C19 1.39(4) . ?
N2 C17 1.49(4) . ?
N3 C20 1.44(3) . ?
N3 C22 1.46(4) . ?
N3 C21 1.50(4) . ?
C1 C2 1.49(2) . ?
C2 C3 1.35(3) . ?
C2 C7 1.41(3) . ?
C3 C4 1.44(2) . ?
C3 H3 0.9300 . ?
C4 C5 1.38(3) 2_656 ?
C4 H4 0.9300 . ?
C5 C6 1.33(4) 2_656 ?
C5 C4 1.38(3) 2_656 ?
C5 C8 1.50(2) . ?
C6 C5 1.33(4) 2_656 ?
C6 C7 1.40(3) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C9 O4 1.257(17) 7_557 ?
C9 C10 1.49(2) . ?
C10 C11 1.40(2) 4_546 ?
C10 C15 1.409(19) 4_546 ?
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C11 C12 1.39(2) . ?
C11 C10 1.40(2) 4_556 ?
C11 H11 0.9300 . ?
C12 C13 1.39(2) . ?
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C13 C14 1.38(2) . ?
C13 H13 0.9300 . ?
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C15 C10 1.409(19) 4_556 ?
C15 H15 0.9300 . ?
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C18 H18C 0.9600 . ?
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C19 H19C 0.9600 . ?
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C21 H21B 0.9600 . ?
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O4 Ho1 O5 75.4(4) . . ?
O7 Ho1 O5 135.0(6) . . ?
O4 Ho1 O6 80.2(4) . 7_557 ?
O7 Ho1 O6 78.1(7) . 7_557 ?
O5 Ho1 O6 134.7(4) . 7_557 ?
O4 Ho1 O1 134.1(4) . . ?
O7 Ho1 O1 89.0(7) . . ?
O5 Ho1 O1 78.3(4) . . ?
O6 Ho1 O1 142.1(4) 7_557 . ?
O4 Ho1 O3 125.6(4) . . ?
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which could not be located.
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;
RESPONSE:The reported formula, molecular weight, F000, density
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the contribution of imine H atoms,
which could not be located.
;
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which could not be located.
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O4 O 0.798(8) 0.238(17) 0.369(16) 0.05(5) Uani 1 1 d . . .
O5 O 0.795(7) 0.433(15) 0.446(19) 0.05(5) Uani 1 1 d . . .
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O7 O 0.859(10) 0.42(2) 0.65(3) 0.09(9) Uani 1 1 d . . .
O8 O 0.860(15) 0.21(2) 0.70(3) 0.08(9) Uani 1 1 d U . .
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N2 N 0.89(3) 0.49(6) 0.81(6) 0.18(17) Uani 1 1 d DU . .
N3 N 0.88(4) 0.12(7) 0.84(8) 0.2(2) Uani 1 1 d DU . .
C1 C 0.951(12) 0.21(2) 0.44(3) 0.06(8) Uani 1 1 d . . .
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C12 C 0.721(9) 0.494(19) 0.37(2) 0.04(6) Uani 1 1 d . . .
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H18C H 0.8708 0.4438 0.9385 0.266 Uiso 1 1 calc R . .
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H19B H 0.8431 0.5840 0.7339 0.268 Uiso 1 1 calc R . .
H19C H 0.8933 0.5773 0.7004 0.268 Uiso 1 1 calc R . .
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H21B H 0.8710 0.0709 0.9625 0.312 Uiso 1 1 calc R . .
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N3 0.2(2) 0.2(2) 0.2(2) 0.00(4) 0.04(5) 0.00(4)
C1 0.04(16) 0.1(2) 0.1(2) 0.01(15) 0.03(16) 0.01(13)
C2 0.1(2) 0.1(2) 0.1(3) 0.0(2) 0.0(2) 0.01(16)
C3 0.1(2) 0.1(2) 0.1(3) 0.0(2) 0.0(2) 0.01(18)
C4 0.1(2) 0.1(2) 0.1(2) 0.02(18) 0.04(19) 0.01(18)
C5 0.1(3) 0.1(2) 0.1(5) 0.0(3) 0.1(3) 0.0(2)
C6 0.1(2) 0.0(2) 0.2(5) 0.0(2) 0.1(3) 0.01(15)
C7 0.1(2) 0.1(3) 0.1(3) 0.0(2) 0.0(2) 0.0(2)
C8 0.03(13) 0.05(16) 0.06(17) 0.01(14) 0.02(13) 0.01(12)
C9 0.04(14) 0.05(16) 0.05(15) -0.01(13) 0.03(12) -0.01(12)
C10 0.04(13) 0.05(15) 0.05(14) 0.00(12) 0.03(12) 0.00(11)
C11 0.03(12) 0.05(15) 0.05(15) 0.00(12) 0.03(11) 0.00(11)
C12 0.03(12) 0.04(13) 0.06(15) 0.00(12) 0.02(12) 0.00(10)
C13 0.04(14) 0.04(14) 0.07(17) 0.00(13) 0.04(13) 0.00(12)
C14 0.03(13) 0.06(17) 0.1(2) 0.01(16) 0.03(14) 0.01(13)
C15 0.04(15) 0.06(18) 0.06(17) 0.00(14) 0.03(14) 0.00(14)
C16 0.04(13) 0.04(13) 0.06(15) 0.00(11) 0.02(12) 0.00(11)
C17 0.18(18) 0.18(17) 0.18(18) 0.00(4) 0.03(5) 0.00(4)
C18 0.18(18) 0.18(18) 0.18(17) 0.00(4) 0.03(5) 0.00(4)
C19 0.18(18) 0.18(17) 0.18(18) 0.00(4) 0.03(5) 0.00(4)
C20 0.2(2) 0.2(2) 0.2(2) 0.00(4) 0.04(5) 0.00(4)
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C22 0.2(2) 0.2(2) 0.2(2) 0.00(4) 0.04(6) 0.00(4)

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;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
```

```
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Ce1 O7 2.5(3) . ?
Ce1 O5 2.5(2) . ?
Ce1 O1 2.6(2) . ?
Ce1 O6 2.72(19) 7_656 ?
Ce1 C14 2.9(3) . ?
Ce1 C16 3.0(3) . ?
Ce1 Ce1 4.09(3) 7_656 ?
O1 C14 1.2(4) . ?
O2 C14 1.3(4) . ?
O3 C15 1.3(4) . ?
O4 C15 1.3(4) 7_656 ?
O5 C16 1.2(3) . ?
O6 C16 1.3(3) 7_656 ?
O6 Ce1 2.72(19) 7_656 ?
O7 C17 1.5(10) . ?
O8 C20 1.1(14) . ?
N1 C7 1.4(5) 3_455 ?
N1 C8 1.4(4) . ?
N2 C18 1.4(10) . ?
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N3 C21 1.4(12) . ?
N3 C22 1.47(19) . ?
N3 C20 1.6(15) . ?
C1 C2 1.4(5) . ?
C1 C6 1.4(5) . ?
C1 C14 1.5(4) . ?
C2 C3 1.4(5) . ?
C2 H2 0.9500 . ?
C3 C4 1.4(6) . ?
C3 H3 0.9500 . ?
C4 C5 1.4(6) . ?
C4 C7 1.4(5) . ?
C5 C6 1.4(6) . ?
C5 H5 0.9500 . ?
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C7 H7B 0.9900 . ?
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C9 C8 1.4(4) 6_566 ?
C9 H9 0.9500 . ?
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C12 C11 1.4(4) 6_565 ?
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C15 O4 1.3(4) 7_656 ?
C16 O6 1.3(3) 7_656 ?
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C19 H19C 0.9800 . ?
C21 H21A 0.9800 . ?
C21 H21B 0.9800 . ?
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O3 Ce1 O8 75(10) . . ?
O4 Ce1 O2 80(9) . . ?
O6 Ce1 O2 134(7) . . ?
O3 Ce1 O2 142(9) . . ?
O8 Ce1 O2 92(10) . . ?
O4 Ce1 O7 140(10) . . ?
O6 Ce1 O7 147(9) . . ?
O3 Ce1 O7 71(9) . . ?
O8 Ce1 O7 74(10) . . ?
O2 Ce1 O7 72(10) . . ?
O4 Ce1 O5 74(8) . . ?
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O6 Ce1 O5 123(7) . . ?
O3 Ce1 O5 91(9) . . ?
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O2 Ce1 O5 82(8) . . ?
O7 Ce1 O5 74(10) . . ?
O4 Ce1 O1 71(8) . . ?
O6 Ce1 O1 85(7) . . ?
O3 Ce1 O1 143(9) . . ?
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O2 Ce1 O1 51(8) . . ?
O7 Ce1 O1 109(10) . . ?
O5 Ce1 O1 125(7) . . ?
O4 Ce1 O6 70(7) . 7_656 ?
O6 Ce1 O6 76(7) . 7_656 ?
O3 Ce1 O6 68(7) . 7_656 ?
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O2 Ce1 O6 127(8) . 7_656 ?
O7 Ce1 O6 106(9) . 7_656 ?
O5 Ce1 O6 49(6) . 7_656 ?
O1 Ce1 O6 140(8) . 7_656 ?
O4 Ce1 C14 74(9) . . ?
O6 Ce1 C14 109(8) . . ?
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O7 Ce1 C14 91(10) . . ?
O5 Ce1 C14 104(8) . . ?
O1 Ce1 C14 25(9) . . ?
O6 Ce1 C14 139(8) 7_656 . ?
O4 Ce1 C16 70(8) . . ?
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O1 Ce1 C16 137(8) . . ?
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C14 Ce1 C16 123(8) . . ?
O4 Ce1 Ce1 66(5) . 7_656 ?
O6 Ce1 Ce1 40(4) . 7_656 ?
O3 Ce1 Ce1 69(5) . 7_656 ?
O8 Ce1 Ce1 116(10) . 7_656 ?
O2 Ce1 Ce1 145(7) . 7_656 ?
O7 Ce1 Ce1 133(7) . 7_656 ?
O5 Ce1 Ce1 84(5) . 7_656 ?
O1 Ce1 Ce1 117(6) . 7_656 ?
O6 Ce1 Ce1 36(4) 7_656 7_656 ?
C14 Ce1 Ce1 135(8) . 7_656 ?
C16 Ce1 Ce1 60(5) . 7_656 ?
C14 O1 Ce1 91(10) . . ?
C14 O2 Ce1 95(10) . . ?
C15 O3 Ce1 134(10) . . ?
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C16 O5 Ce1 100(10) . . ?
C16 O6 Ce1 158(10) 7_656 . ?
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Ce1 O6 Ce1 104(7) . 7_656 ?
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C18 N2 C19 132(10) . . ?
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C19 N2 C17 116(10) . . ?
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C2 C1 C14 121(10) . . ?
C6 C1 C14 120(10) . . ?
C1 C2 C3 122(10) . . ?
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C3 C2 H2 118.9 . . ?
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N1 C7 H7A 106.6 3_545 . ?
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N1 C7 H7B 106.6 3_545 . ?
C4 C7 H7B 106.6 . . ?
H7A C7 H7B 106.6 . . ?
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N1 C8 C13 116(10) . . ?
C9 C8 C13 120(10) 6_565 . ?
C10 C9 C8 120(10) . 6_566 ?
C10 C9 H9 120.2 . . ?
C8 C9 H9 120.2 6_566 . ?
C11 C10 C9 121(10) . . ?
C11 C10 C15 120(10) . . ?
C9 C10 C15 119(10) . . ?
C10 C11 C12 120(10) . 6_566 ?
C10 C11 H11 120.2 . . ?
C12 C11 H11 120.2 6_566 . ?
C13 C12 C11 120(10) . 6_565 ?
C13 C12 C16 121(10) . . ?
C11 C12 C16 119(10) 6_565 . ?
C12 C13 C8 120(10) . . ?
C12 C13 H13 120.2 . . ?
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O1 C14 O2 123(10) . . ?
O1 C14 C1 120(10) . . ?
O2 C14 C1 117(10) . . ?
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C1 C14 Ce1 176(10) . . ?
O3 C15 O4 125(10) . 7_656 ?
O3 C15 C10 118(10) . . ?
O4 C15 C10 117(10) 7_656 . ?
O5 C16 O6 121(10) . 7_656 ?
O5 C16 C12 120(10) . . ?
O6 C16 C12 119(10) 7_656 . ?
O5 C16 Ce1 56(10) . . ?
O6 C16 Ce1 65(10) 7_656 . ?
C12 C16 Ce1 176(10) . . ?
N2 C17 O7 114(10) . . ?
N2 C18 H18A 109.5 . . ?
N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
O8 C20 N3 117(10) . . ?
N3 C21 H21A 109.5 . . ?
N3 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
N3 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
N3 C22 H22A 109.5 . . ?
N3 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
N3 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?

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  _platon_squeeze_void_count_electrons
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   2  0.250  0.750  0.000       156        44 ' '
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   3  0.500  0.000 -0.002       270        95 ' '
   4  0.750  0.250  0.000       156        44 ' '
   5  0.250  0.250  0.500       156        44 ' '
   6  0.750  0.750  0.500       156        44 ' '
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loop_
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 'x+1/2, y+1/2, z'
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 '-x, -y, -z'
 'x, -y, z-1/2'
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 'x+1/2, -y+1/2, z-1/2'

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Diffraction)'

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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material    'WINGX (Farrugia, 1999)'
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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N1 N 0.4002(4) 0.0864(8) 0.6548(10) 0.098(4) Uani 1 1 d D . .
N2 N 0.3704(13) 0.5817(18) 1.227(3) 0.377(10) Uani 1 1 d DU . .
O1 O 0.3796(3) 0.1639(8) 1.0156(8) 0.091(3) Uani 1 1 d . . .
O2 O 0.3943(3) 0.3133(7) 0.9890(7) 0.075(3) Uani 1 1 d . . .
O3 O 0.2293(2) 0.1588(6) 0.8444(5) 0.060(2) Uani 1 1 d . . .
O4 O 0.2996(3) 0.2321(6) 0.8803(5) 0.058(2) Uani 1 1 d . . .
O5 O 0.3553(5) 0.2209(7) 1.1969(10) 0.104(4) Uani 1 1 d U . .
O6 O 0.2667(2) 0.1528(4) 1.0431(5) 0.0471(16) Uani 1 1 d . . .
O7 O 0.2963(3) 0.4316(5) 0.9443(6) 0.0563(18) Uani 1 1 d . . .
O8 O 0.3592(3) 0.4200(8) 1.1307(9) 0.107(4) Uani 1 1 d . . .
C1 C 0.4487(3) 0.2000(11) 0.9453(5) 0.106(6) Uani 1 1 d D . .
C2 C 0.4630(8) 0.1063(12) 0.9293(12) 0.209(8) Uani 1 1 d DU . .
H2 H 0.4444 0.0532 0.9439 0.251 Uiso 1 1 calc R . .
C3 C 0.5043(7) 0.0898(18) 0.8921(14) 0.209(8) Uani 1 1 d DU . .
H3 H 0.5161 0.0278 0.8795 0.251 Uiso 1 1 calc R . .
C4 C 0.5259(6) 0.1768(14) 0.8760(13) 0.168(10) Uani 1 1 d
DU . .
C5 C 0.5200(5) 0.2758(14) 0.8846(14) 0.160(11) Uani 1 1 d D . .
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H5 H 0.5387 0.3286 0.8697 0.192 Uiso 1 1 calc R . .
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H7B H 0.4071 0.2320 0.6525 0.256 Uiso 1 1 calc R . .
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H9 H 0.3565 0.1712 0.7850 0.070 Uiso 1 1 calc R . .
C10 C 0.2903(4) 0.1145(7) 0.7572(7) 0.053(3) Uani 1 1 d . . .
C11 C 0.2599(3) 0.0501(6) 0.7003(7) 0.046(2) Uani 1 1 d . . .
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C15 C 0.2718(4) 0.1744(8) 0.8333(7) 0.051(2) Uani 1 1 d . . .
C16 C 0.2528(3) 0.4190(7) 0.9266(7) 0.045(2) Uani 1 1 d . . .
C17 C 0.359(2) 0.484(3) 1.190(4) 0.376(10) Uani 1 1 d DU . .
C18 C 0.3839(16) 0.631(4) 1.320(3) 0.377(10) Uani 1 1 d DU . .
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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_diffrn_standards_decay_%         ?
_diffrn_reflns_number             14699
_diffrn_reflns_av_R_equivalents   0.0416
_diffrn_reflns_av_sigmaI/netI     0.0450
_diffrn_reflns_limit_h_min        -33
_diffrn_reflns_limit_h_max        29
_diffrn_reflns_limit_k_min        -10
_diffrn_reflns_limit_k_max        16
_diffrn_reflns_limit_l_min        -16
_diffrn_reflns_limit_l_max        15
_diffrn_reflns_theta_min          2.91
_diffrn_reflns_theta_max          25.00
_reflns_number_total              4810
_reflns_number_gt                 3766
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        'CrysAlis RED'
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_computing_data_reduction          'CrysAlis RED'
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1997)'
_computing_structure_refinement    'SHELXL-97 (Sheldrick,
1997)'
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;
 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material    'WINGX (Farrugia, 1999)'
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
```

```
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1051P)^2^+4.1456P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4810
_refine_ls_number_parameters      235
_refine_ls_number_restraints      42
_refine_ls_R_factor_all           0.0632
_refine_ls_R_factor_gt            0.0523
_refine_ls_wR_factor_ref          0.1711
_refine_ls_wR_factor_gt           0.1603
_refine_ls_goodness_of_fit_ref    1.131
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d . . .
N1 N 0.4013(3) 0.0854(6) 0.6601(7) 0.087(3) Uani 1 1 d D . .
O1 O 0.3797(3) 0.1652(6) 1.0175(5) 0.089(2) Uani 1 1 d . . .
O2 O 0.3944(2) 0.3138(6) 0.9876(5) 0.0789(18) Uani 1 1 d . . .
O3 O 0.23004(19) 0.1575(4) 0.8458(4) 0.0611(15) Uani 1 1
d . . .
O4 O 0.3007(2) 0.2308(4) 0.8820(4) 0.0542(14) Uani 1 1 d . . .
O5 O 0.26695(18) 0.1534(3) 1.0444(4) 0.0487(12) Uani 1 1
d . . .
O6 O 0.29635(19) 0.4312(4) 0.9451(4) 0.0567(13) Uani 1 1
d . . .
O7 O 0.3587(3) 0.4223(6) 1.1326(5) 0.099(2) Uani 1 1 d . . .
O8 O 0.3542(4) 0.2199(5) 1.1972(6) 0.099(3) Uani 1 1 d U . .
C1 C 0.4476(4) 0.1968(11) 0.9465(8) 0.112(5) Uani 1 1 d D . .
C2 C 0.4634(7) 0.1046(12) 0.9294(10) 0.205(7) Uani 1 1 d DU . .
H2 H 0.4455 0.0503 0.9433 0.247 Uiso 1 1 calc R . .
C3 C 0.5053(6) 0.0908(12) 0.8919(11) 0.189(7) Uani 1 1 d DU . .
H3 H 0.5177 0.0306 0.8760 0.227 Uiso 1 1 calc R . .
C4 C 0.5253(5) 0.1799(10) 0.8822(14) 0.165(7) Uani 1 1 d DU . .
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C5 C 0.5180(5) 0.2772(10) 0.8793(12) 0.164(8) Uani 1 1 d DU . .
H5 H 0.5337 0.3300 0.8558 0.197 Uiso 1 1 calc R . .
C6 C 0.4784(5) 0.2688(14) 0.9244(12) 0.201(10) Uani 1 1 d
DU . .
H6 H 0.4698 0.3298 0.9466 0.242 Uiso 1 1 calc R . .
C7 C 0.4273(7) 0.1762(10) 0.6808(16) 0.191(8) Uani 1 1 d DU . .
H7A H 0.4396 0.1816 0.7510 0.229 Uiso 1 1 calc R . .
H7B H 0.4054 0.2311 0.6612 0.229 Uiso 1 1 calc R . .
C8 C 0.3553(3) 0.0727(6) 0.6758(6) 0.061(2) Uani 1 1 d . . .
C9 C 0.3370(3) 0.1264(5) 0.7457(6) 0.0551(19) Uani 1 1 d . . .
H9 H 0.3571 0.1708 0.7852 0.066 Uiso 1 1 calc R . .
C10 C 0.2901(3) 0.1151(5) 0.7573(5) 0.0475(17) Uani 1 1 d . . .
C11 C 0.2604(2) 0.0489(5) 0.7002(5) 0.0451(16) Uani 1 1 d . . .
H11 H 0.2279 0.0418 0.7065 0.054 Uiso 1 1 calc R . .
C12 C 0.2206(3) 0.4941(5) 0.8656(5) 0.0458(16) Uani 1 1 d . . .
C13 C 0.3258(3) 0.0037(5) 0.6237(6) 0.0536(19) Uani 1 1 d . . .
H13 H 0.3381 -0.0372 0.5801 0.064 Uiso 1 1 calc R . .
C14 C 0.4043(3) 0.2248(9) 0.9865(7) 0.071(3) Uani 1 1 d . . .
C15 C 0.2721(3) 0.1736(7) 0.8345(5) 0.0529(19) Uani 1 1 d . . .
C16 C 0.2524(3) 0.4200(5) 0.9258(5) 0.0463(17) Uani 1 1 d . . .

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 _atom_site_aniso_U_12
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0.00454(13)
N1 0.068(5) 0.075(5) 0.133(7) -0.020(5) 0.054(5) -0.023(4)
O1 0.063(4) 0.097(5) 0.117(6) 0.040(5) 0.045(4) 0.038(4)
O2 0.049(4) 0.100(5) 0.093(5) -0.007(4) 0.027(3) -0.001(4)
O3 0.047(3) 0.082(4) 0.061(3) -0.027(3) 0.028(3) -0.007(3)
O4 0.049(3) 0.069(3) 0.050(3) -0.022(3) 0.024(3) -0.008(3)
O5 0.046(3) 0.046(3) 0.060(3) 0.009(2) 0.022(2) 0.006(2)
O6 0.049(3) 0.045(3) 0.078(4) 0.008(3) 0.016(3) 0.002(2)
O7 0.072(4) 0.121(6) 0.103(5) -0.022(5) 0.009(4) -0.041(5)
O8 0.099(3) 0.099(3) 0.098(3) 0.0000(10) 0.0168(11) 0.0018(10)
C1 0.043(6) 0.213(16) 0.083(8) -0.024(8) 0.023(5) 0.012(7)
C2 0.200(8) 0.214(9) 0.204(9) -0.003(5) 0.041(5) 0.004(5)
C3 0.194(8) 0.189(8) 0.187(8) 0.002(5) 0.038(5) -0.001(5)
C4 0.064(8) 0.121(10) 0.30(2) 0.101(13) 0.006(10) 0.031(7)
C5 0.165(9) 0.164(9) 0.166(9) -0.002(5) 0.036(5) -0.003(5)
C6 0.058(9) 0.39(3) 0.169(16) -0.080(19) 0.067(10) -0.032(12)
C7 0.184(9) 0.197(9) 0.191(9) -0.004(5) 0.034(5) -0.003(5)
C8 0.049(5) 0.063(5) 0.079(5) -0.007(4) 0.034(4) -0.010(4)
C9 0.048(4) 0.056(4) 0.067(5) -0.017(4) 0.028(4) -0.018(4)
C10 0.049(4) 0.056(4) 0.044(4) -0.007(3) 0.027(3) -0.009(3)
C11 0.044(4) 0.048(4) 0.048(4) -0.003(3) 0.021(3) 0.000(3)
C12 0.049(4) 0.042(4) 0.051(4) 0.007(3) 0.022(3) 0.005(3)
C13 0.053(5) 0.042(4) 0.077(5) -0.012(4) 0.042(4) -0.006(3)
C14 0.041(5) 0.109(8) 0.064(6) 0.003(5) 0.017(4) 0.009(5)
C15 0.038(4) 0.079(5) 0.044(4) -0.009(4) 0.015(3) -0.006(4)
C16 0.056(5) 0.039(4) 0.051(4) 0.006(3) 0.028(3) 0.007(3)
```

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Gd1 O5 2.362(5) . ?
Gd1 O3 2.391(5) 7_557 ?
Gd1 O8 2.423(9) . ?
Gd1 O7 2.436(7) . ?
Gd1 O6 2.441(5) . ?
Gd1 O2 2.459(6) . ?
Gd1 O1 2.508(6) . ?
Gd1 O5 2.637(5) 7_557 ?
Gd1 C14 2.843(10) . ?
Gd1 C16 2.912(7) . ?
Gd1 Gd1 3.9767(9) 7_557 ?
N1 C8 1.377(10) . ?
N1 C7 1.463(5) . ?
O1 C14 1.214(12) . ?
O2 C14 1.269(12) . ?
O3 C15 1.255(9) . ?
O3 Gd1 2.391(5) 7_557 ?
O4 C15 1.243(10) . ?
O5 C16 1.266(8) 7_557 ?
O5 Gd1 2.637(5) 7_557 ?
O6 C16 1.239(9) . ?
C1 C2 1.391(5) . ?
C1 C6 1.401(5) . ?
C1 C14 1.496(14) . ?
C2 C3 1.401(5) . ?
C2 H2 0.9500 . ?
C3 C4 1.379(5) . ?
C3 H3 0.9500 . ?
C4 C5 1.367(5) . ?
C4 C7 1.74(3) 2_656 ?
C4 C6 1.99(2) . ?
C5 C6 1.392(5) . ?
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C5 H5 0.9500 . ?
C6 H6 0.9500 . ?
C7 C4 1.74(3) 2_656 ?
C7 H7A 0.9900 . ?
C7 H7B 0.9900 . ?
C8 C13 1.392(11) . ?
C8 C9 1.408(11) . ?
C9 C10 1.380(10) . ?
C9 H9 0.9500 . ?
C10 C11 1.400(9) . ?
C10 C15 1.518(10) . ?
C11 C12 1.383(9) 4_546 ?
C11 H11 0.9500 . ?
C12 C13 1.359(10) 4_556 ?
C12 C11 1.383(9) 4_556 ?
C12 C16 1.524(10) . ?
C13 C12 1.359(10) 4_546 ?
C13 H13 0.9500 . ?
C16 O5 1.266(8) 7_557 ?

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O4 Gd1 O3 133.74(19) . 7_557 ?
O5 Gd1 O3 79.57(18) . 7_557 ?
O4 Gd1 O8 135.7(2) . . ?
O5 Gd1 O8 81.3(2) . . ?
O3 Gd1 O8 74.5(3) 7_557 . ?
O4 Gd1 O7 138.8(2) . . ?
O5 Gd1 O7 146.6(2) . . ?
O3 Gd1 O7 71.6(2) 7_557 . ?
O8 Gd1 O7 75.2(3) . . ?
O4 Gd1 O6 75.25(19) . . ?
O5 Gd1 O6 123.84(18) . . ?
O3 Gd1 O6 89.4(2) 7_557 . ?
O8 Gd1 O6 147.7(2) . . ?
O7 Gd1 O6 73.1(2) . . ?
O4 Gd1 O2 78.0(2) . . ?
O5 Gd1 O2 134.5(2) . . ?
O3 Gd1 O2 143.2(2) 7_557 . ?
O8 Gd1 O2 94.9(3) . . ?
O7 Gd1 O2 71.7(3) . . ?
O6 Gd1 O2 81.2(2) . . ?
O4 Gd1 O1 70.8(2) . . ?
O5 Gd1 O1 85.3(2) . . ?
O3 Gd1 O1 143.8(2) 7_557 . ?
O8 Gd1 O1 70.8(3) . . ?
O7 Gd1 O1 108.4(3) . . ?
O6 Gd1 O1 125.9(2) . . ?
O2 Gd1 O1 51.6(2) . . ?
```

```
O4 Gd1 O5 69.10(18) . 7_557 ?
O5 Gd1 O5 74.74(17) . 7_557 ?
O3 Gd1 O5 67.61(18) 7_557 7_557 ?
O8 Gd1 O5 138.0(3) . 7_557 ?
O7 Gd1 O5 108.0(2) . 7_557 ?
O6 Gd1 O5 50.59(17) . 7_557 ?
O2 Gd1 O5 126.4(2) . 7_557 ?
O1 Gd1 O5 138.7(2) . 7_557 ?
O4 Gd1 C14 71.0(2) . . ?
O5 Gd1 C14 109.1(3) . . ?
O3 Gd1 C14 154.9(2) 7_557 . ?
O8 Gd1 C14 83.4(3) . . ?
O7 Gd1 C14 91.6(3) . . ?
O6 Gd1 C14 103.7(3) . . ?
O2 Gd1 C14 26.4(3) . . ?
O1 Gd1 C14 25.2(3) . . ?
O5 Gd1 C14 136.9(2) 7_557 . ?
O4 Gd1 C16 70.6(2) . . ?
O5 Gd1 C16 99.87(19) . . ?
O3 Gd1 C16 77.5(2) 7_557 . ?
O8 Gd1 C16 151.3(2) . . ?
O7 Gd1 C16 90.1(2) . . ?
O6 Gd1 C16 24.82(18) . . ?
O2 Gd1 C16 103.8(2) . . ?
O1 Gd1 C16 137.8(2) . . ?
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C14 Gd1 C16 122.2(3) . . ?
O4 Gd1 Gd1 66.48(14) . 7_557 ?
O5 Gd1 Gd1 39.77(12) . 7_557 ?
O3 Gd1 Gd1 68.89(13) 7_557 7_557 ?
O8 Gd1 Gd1 113.7(2) . 7_557 ?
O7 Gd1 Gd1 134.54(19) . 7_557 ?
O6 Gd1 Gd1 84.82(13) . 7_557 ?
O2 Gd1 Gd1 144.11(16) . 7_557 ?
O1 Gd1 Gd1 116.7(2) . 7_557 ?
O5 Gd1 Gd1 34.96(11) 7_557 7_557 ?
C14 Gd1 Gd1 132.7(2) . 7_557 ?
C16 Gd1 Gd1 60.31(15) . 7_557 ?
C8 N1 C7 122.6(11) . . ?
C14 O1 Gd1 93.0(6) . . ?
C14 O2 Gd1 93.9(6) . . ?
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C15 O4 Gd1 137.1(5) . . ?
C16 O5 Gd1 160.5(5) 7_557 . ?
C16 O5 Gd1 89.3(4) 7_557 7_557 ?
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C16 O6 Gd1 99.4(4) . . ?
C2 C1 C6 112.6(15) . . ?
C2 C1 C14 128.1(14) . . ?
C6 C1 C14 119.2(12) . . ?
C1 C2 C3 120.9(18) . . ?
C1 C2 H2 119.6 . . ?
C3 C2 H2 119.6 . . ?
C4 C3 C2 108.1(18) . . ?
C4 C3 H3 126.0 . . ?
C2 C3 H3 126.0 . . ?
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C5 C4 C3 145.6(15) . . ?
C5 C4 C7 98.2(11) . 2_656 ?
C3 C4 C7 113.4(15) . 2_656 ?
C5 C4 C6 44.4(7) . . ?
C3 C4 C6 102.4(13) . . ?
C7 C4 C6 142.5(10) 2_656 . ?
C4 C5 C6 92.1(14) . . ?
C4 C5 H5 133.9 . . ?
C6 C5 H5 133.9 . . ?
C5 C6 C1 138.6(16) . . ?
C5 C6 C4 43.4(7) . . ?
C1 C6 C4 95.9(11) . . ?
C5 C6 H6 110.7 . . ?
C1 C6 H6 110.7 . . ?
C4 C6 H6 151.6 . . ?
N1 C7 C4 109.4(13) . 2_656 ?
N1 C7 H7A 109.8 . . ?
C4 C7 H7A 109.8 2_656 . ?
N1 C7 H7B 109.8 . . ?
C4 C7 H7B 109.8 2_656 . ?
H7A C7 H7B 108.2 . . ?
N1 C8 C13 120.3(7) . . ?
N1 C8 C9 121.7(7) . . ?
C13 C8 C9 118.0(7) . . ?
C10 C9 C8 120.7(7) . . ?
C10 C9 H9 119.7 . . ?
C8 C9 H9 119.7 . . ?
C9 C10 C11 120.1(6) . . ?
C9 C10 C15 118.9(6) . . ?
C11 C10 C15 121.0(6) . . ?
C12 C11 C10 118.5(6) 4_546 . ?
C12 C11 H11 120.7 4_546 . ?
C10 C11 H11 120.7 . . ?
C13 C12 C11 121.7(7) 4_556 4_556 ?
C13 C12 C16 119.7(6) 4_556 . ?
C11 C12 C16 118.6(6) 4_556 . ?
C12 C13 C8 120.9(7) 4_546 . ?
C12 C13 H13 119.6 4_546 . ?
C8 C13 H13 119.6 . . ?
O1 C14 O2 121.0(9) . . ?
O1 C14 C1 121.7(11) . . ?
O2 C14 C1 117.3(11) . . ?
O1 C14 Gd1 61.7(5) . . ?
O2 C14 Gd1 59.6(5) . . ?
C1 C14 Gd1 173.8(8) . . ?
O4 C15 O3 126.2(7) . . ?
O4 C15 C10 117.0(6) . . ?
O3 C15 C10 116.7(7) . . ?
O6 C16 O5 120.7(6) . 7_557 ?
O6 C16 C12 120.8(6) . . ?
O5 C16 C12 118.5(7) 7_557 . ?
O6 C16 Gd1 55.8(4) . . ?
O5 C16 Gd1 64.9(4) 7_557 . ?
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RESPONSE:This is due to the disorder of the ligand.
We have applied several restraints but we were unable to
resolve this problem.
;
_vrf_PLAT232_shelxl
;
RESPONSE:This is due to the disorder of the ligand.
We have applied several restraints but we were unable to
resolve this problem.
;
_vrf_PLAT234_shelxl
;
RESPONSE:This is due to the disorder of the ligand.
We have applied several restraints but we were unable to
resolve this problem.
;
_vrf_PLAT241_shelxl
;
RESPONSE:This is due to the disorder of the ligand.
We have applied several restraints but we were unable to
resolve this problem.
;
_vrf_PLAT363_shelxl
;
RESPONSE:This is due to the disorder of the ligand.
We have applied several restraints but we were unable to
resolve this problem.
;
# end Validation Reply Form


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  _platon_squeeze_void_average_z
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NdCAP
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 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
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_chemical_formula_sum
 'C16 H9 N Nd O8'
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 _atom_type_scat_dispersion_imag
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 'C'  'C'   0.0033   0.0016
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Nd'  'Nd'  -0.1943   3.0179
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'C 2/c'
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loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    28.5025(10)
_cell_length_b                    13.9738(7)
_cell_length_c                    14.0972(8)
_cell_angle_alpha                 90.00
_cell_angle_beta                  100.478(4)
_cell_angle_gamma                 90.00
_cell_volume                      5521.1(5)
_cell_formula_units_Z             8
_cell_measurement_temperature     100(2)
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_cell_measurement_reflns_used     4023
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_exptl_crystal_size_mid           0.04
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_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.173
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_exptl_crystal_F_000              1888
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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_diffrn_ambient_temperature       100(2)
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_diffrn_radiation_source          'SuperNova (Mo) X-ray
Source'
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Atlas'
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_diffrn_reflns_limit_k_max        16
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1674P)^2^+68.7513P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
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_refine_ls_number_reflns          4861
_refine_ls_number_parameters      235
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_refine_ls_R_factor_all           0.0999
_refine_ls_R_factor_gt            0.0777
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d . . .
O1 O 0.2663(2) 0.6510(5) 1.0411(6) 0.0408(17) Uani 1 1 d . . .
O2 O 0.2705(3) 0.8387(8) 1.1591(6) 0.065(3) Uani 1 1 d . . .
O3 O 0.3556(6) 0.7212(10) 1.2007(9) 0.108(5) Uani 1 1 d . . .
O4 O 0.3607(4) 0.9216(9) 1.1355(9) 0.092(4) Uani 1 1 d . . .
O5 O 0.3803(4) 0.6603(8) 1.0150(9) 0.084(4) Uani 1 1 d . . .
O6 O 0.3966(3) 0.8121(8) 0.9894(8) 0.064(3) Uani 1 1 d . . .
O7 O 0.2963(3) 0.9322(6) 0.9426(6) 0.0481(19) Uani 1 1 d . . .
O8 O 0.3003(3) 0.7298(7) 0.8803(6) 0.052(2) Uani 1 1 d . . .
N1 N 0.5993(4) 0.5841(9) 0.8420(9) 0.070(3) Uani 1 1 d DU . .
C1 C 0.4067(4) 0.7269(15) 0.9881(10) 0.066(5) Uani 1 1 d . . .
C2 C 0.4497(7) 0.7049(12) 0.9457(14) 0.088(5) Uani 1 1 d DU . .
C3 C 0.4779(7) 0.7866(15) 0.9188(13) 0.106(7) Uani 1 1 d DU . .
H3 H 0.4670 0.8497 0.9275 0.127 Uiso 1 1 calc R . .
C4 C 0.5195(8) 0.7758(18) 0.8814(15) 0.132(7) Uani 1 1 d DU . .
H4 H 0.5385 0.8259 0.8630 0.158 Uiso 1 1 calc R . .
C5 C 0.5281(8) 0.6805(19) 0.8761(16) 0.119(6) Uani 1 1 d DU . .
C6 C 0.5074(7) 0.595(2) 0.8962(17) 0.142(6) Uani 1 1 d DU . .
H6 H 0.5210 0.5337 0.8929 0.170 Uiso 1 1 calc R . .
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C7 C 0.4635(9) 0.6138(15) 0.922(2) 0.151(7) Uani 1 1 d DU . .
H7 H 0.4420 0.5621 0.9238 0.181 Uiso 1 1 calc R . .
C8 C 0.5666(13) 0.665(3) 0.814(3) 0.28(2) Uani 1 1 d DU . .
H8A H 0.5504 0.6547 0.7462 0.334 Uiso 1 1 calc R . .
H8B H 0.5858 0.7239 0.8155 0.334 Uiso 1 1 calc R . .
C9 C 0.6447(4) 0.5722(8) 0.8235(9) 0.047(3) Uani 1 1 d . . .
C10 C 0.6633(4) 0.6244(9) 0.7554(8) 0.044(3) Uani 1 1 d . . .
H10 H 0.6432 0.6678 0.7148 0.052 Uiso 1 1 calc R . .
C11 C 0.7100(4) 0.6147(9) 0.7456(8) 0.041(3) Uani 1 1 d . . .
C12 C 0.7403(3) 0.5499(8) 0.8008(8) 0.040(3) Uani 1 1 d . . .
H12 H 0.7727 0.5441 0.7942 0.048 Uiso 1 1 calc R . .
C13 C 0.7214(4) 0.4935(8) 0.8664(8) 0.036(2) Uani 1 1 d . . .
C14 C 0.6748(4) 0.5026(8) 0.8767(9) 0.045(3) Uani 1 1 d . . .
H14 H 0.6624 0.4618 0.9201 0.054 Uiso 1 1 calc R . .
C15 C 0.2523(4) 0.9204(8) 0.9263(8) 0.038(2) Uani 1 1 d . . .
C16 C 0.2284(4) 0.8258(11) 1.1691(9) 0.051(3) Uani 1 1 d . . .

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0.00228(19)
O1 0.037(4) 0.036(4) 0.053(5) 0.008(4) 0.019(3) 0.001(3)
O2 0.032(4) 0.112(8) 0.060(5) -0.050(6) 0.026(4) -0.023(5)
O3 0.128(13) 0.131(13) 0.052(7) 0.019(7) -0.015(8) 0.040(9)
O4 0.076(7) 0.104(9) 0.095(9) -0.021(8) 0.016(6) -0.049(7)
O5 0.077(7) 0.086(8) 0.108(9) 0.039(7) 0.064(6) 0.052(6)
O6 0.044(5) 0.078(7) 0.076(7) 0.008(6) 0.025(5) -0.005(5)
O7 0.039(4) 0.045(4) 0.062(5) 0.010(4) 0.016(4) 0.001(4)
O8 0.041(5) 0.080(6) 0.040(5) -0.026(4) 0.024(4) -0.018(4)
N1 0.063(5) 0.071(5) 0.081(5) 0.005(4) 0.031(4) 0.007(4)
C1 0.027(6) 0.134(16) 0.042(7) 0.020(8) 0.016(5) 0.015(7)
C2 0.084(7) 0.096(7) 0.084(7) -0.005(5) 0.020(5) 0.009(4)
C3 0.102(8) 0.111(8) 0.108(8) -0.001(5) 0.027(5) -0.003(5)
C4 0.133(8) 0.131(7) 0.133(8) -0.002(5) 0.027(5) 0.002(5)
C5 0.116(7) 0.119(6) 0.119(7) -0.002(5) 0.013(5) 0.009(4)
C6 0.144(7) 0.143(7) 0.141(8) 0.006(5) 0.030(5) -0.005(5)
C7 0.148(8) 0.156(9) 0.151(9) 0.002(5) 0.032(5) -0.001(5)
C8 0.28(2) 0.28(2) 0.28(2) 0.0000(10) 0.051(4) 0.0000(10)
C9 0.037(5) 0.042(6) 0.070(8) 0.012(6) 0.029(5) 0.014(5)
C10 0.035(5) 0.058(7) 0.043(6) 0.006(5) 0.019(5) 0.016(5)
C11 0.035(5) 0.060(7) 0.034(6) 0.012(5) 0.021(4) 0.006(5)
C12 0.026(5) 0.051(7) 0.046(6) 0.012(5) 0.017(4) 0.006(5)
C13 0.040(5) 0.034(5) 0.040(6) 0.002(5) 0.022(4) 0.001(4)
C14 0.044(6) 0.035(6) 0.066(8) 0.008(6) 0.037(6) 0.002(5)
C15 0.040(6) 0.038(6) 0.041(6) -0.001(5) 0.019(5) 0.000(5)
C16 0.033(6) 0.085(9) 0.041(6) -0.030(7) 0.025(5) -0.015(6)

_geom_special_details
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```
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 O2 2.440(7) . ?
Nd1 O3 2.448(11) . ?
Nd1 O4 2.471(11) . ?
Nd1 O6 2.488(9) . ?
Nd1 O7 2.502(8) . ?
Nd1 O5 2.558(9) . ?
Nd1 O1 2.657(7) 7_567 ?
Nd1 C1 2.869(13) . ?
Nd1 C15 2.952(11) . ?
Nd1 Nd1 4.0385(9) 7_567 ?
O1 C15 1.256(13) 7_567 ?
O1 Nd1 2.657(7) 7_567 ?
O2 C16 1.246(13) . ?
O5 C1 1.30(2) . ?
O6 C1 1.23(2) . ?
O7 C15 1.243(13) . ?
O8 C16 1.244(14) 7_567 ?
N1 C9 1.375(15) . ?
N1 C8 1.4700(10) . ?
C1 C2 1.49(2) . ?
C2 C7 1.3900(10) . ?
C2 C3 1.49(2) . ?
C3 C4 1.391(5) . ?
C3 H3 0.9500 . ?
C4 C5 1.36(3) . ?
C4 H4 0.9500 . ?
C5 C6 1.38(3) . ?
C5 C8 1.5400(11) . ?
C6 C7 1.3902(10) . ?
C6 H6 0.9500 . ?
C7 H7 0.9500 . ?
C8 H8A 0.9900 . ?
C8 H8B 0.9900 . ?
C9 C10 1.384(16) . ?
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C9 C14 1.418(16) . ?
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C10 H10 0.9500 . ?
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C11 C16 1.528(14) 8_565 ?
C12 C13 1.394(14) . ?
C12 H12 0.9500 . ?
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C13 C15 1.505(15) 3_545 ?
C14 H14 0.9500 . ?
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C16 C11 1.528(14) 8_466 ?

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O8 Nd1 O2 133.2(3) . . ?
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O1 Nd1 O3 83.2(4) . . ?
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O3 Nd1 O6 94.4(5) . . ?
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O8 Nd1 O7 74.6(3) . . ?
O1 Nd1 O7 122.2(3) . . ?
O2 Nd1 O7 90.8(3) . . ?
O3 Nd1 O7 147.2(4) . . ?
O4 Nd1 O7 74.1(4) . . ?
O6 Nd1 O7 82.1(3) . . ?
O8 Nd1 O5 70.4(4) . . ?
O1 Nd1 O5 84.3(3) . . ?
O2 Nd1 O5 142.9(4) . . ?
O3 Nd1 O5 72.3(5) . . ?
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O7 Nd1 O5 125.9(3) . . ?
O8 Nd1 O1 69.6(3) . 7_567 ?
O1 Nd1 O1 74.6(3) . 7_567 ?
O2 Nd1 O1 67.3(3) . 7_567 ?
O3 Nd1 O1 137.0(4) . 7_567 ?
O4 Nd1 O1 107.2(4) . 7_567 ?
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O1 Nd1 C1 110.0(5) . . ?
O2 Nd1 C1 153.8(4) . . ?
O3 Nd1 C1 83.8(5) . . ?
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O6 Nd1 C1 25.2(4) . . ?
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O1 Nd1 C1 138.2(3) 7_567 . ?
O8 Nd1 C15 70.4(3) . . ?
O1 Nd1 C15 98.8(3) . . ?
O2 Nd1 C15 78.2(3) . . ?
O3 Nd1 C15 150.1(4) . . ?
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O6 Nd1 C15 104.8(3) . . ?
O7 Nd1 C15 24.6(3) . . ?
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O1 Nd1 C15 25.2(3) 7_567 . ?
C1 Nd1 C15 122.5(4) . . ?
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O1 Nd1 Nd1 39.36(17) . 7_567 ?
O2 Nd1 Nd1 68.57(18) . 7_567 ?
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O1 Nd1 Nd1 35.19(16) 7_567 7_567 ?
C1 Nd1 Nd1 134.0(4) . 7_567 ?
C15 Nd1 Nd1 59.7(2) . 7_567 ?
C15 O1 Nd1 157.2(7) 7_567 . ?
C15 O1 Nd1 90.6(6) 7_567 7_567 ?
Nd1 O1 Nd1 105.4(3) . 7_567 ?
C16 O2 Nd1 135.1(7) . . ?
C1 O5 Nd1 90.0(9) . . ?
C1 O6 Nd1 95.1(8) . . ?
C15 O7 Nd1 98.4(7) . . ?
C16 O8 Nd1 138.8(7) 7_567 . ?
C9 N1 C8 127.8(16) . . ?
O6 C1 O5 122.8(12) . . ?
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C2 C3 H3 118.3 . . ?
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C5 C4 H4 126.2 . . ?
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C5 C8 H8A 108.3 . . ?
N1 C8 H8B 108.3 . . ?
C5 C8 H8B 108.3 . . ?
H8A C8 H8B 107.4 . . ?
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N1 C9 C14 118.8(11) . . ?
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C10 C11 C12 121.6(10) . . ?
C10 C11 C16 118.8(10) . 8_565 ?
C12 C11 C16 119.5(9) . 8_565 ?
C11 C12 C13 117.7(9) . . ?
C11 C12 H12 121.1 . . ?
C13 C12 H12 121.1 . . ?
C14 C13 C12 121.1(10) . . ?
C14 C13 C15 119.0(9) . 3_545 ?
C12 C13 C15 119.9(9) . 3_545 ?
C13 C14 C9 120.9(10) . . ?
C13 C14 H14 119.6 . . ?
C9 C14 H14 119.6 . . ?
O7 C15 O1 121.1(10) . 7_567 ?
O7 C15 C13 118.8(10) . 3_455 ?
O1 C15 C13 120.0(9) 7_567 3_455 ?
O7 C15 Nd1 57.0(6) . . ?
O1 C15 Nd1 64.2(6) 7_567 . ?
C13 C15 Nd1 175.8(7) 3_455 . ?
O8 C16 O2 125.1(10) 7_567 . ?
O8 C16 C11 117.4(9) 7_567 8_466 ?
O2 C16 C11 117.5(10) . 8_466 ?

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 '-x, y, -z+1/2'
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 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
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 '-x+1/2, -y+1/2, -z'
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_cell_angle_gamma                 90.000(5)
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Diffraction)'

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_computing_cell_refinement        ?
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.1315P)^2^+2.3108P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
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C2 C 0.4481(6) 0.8316(14) 0.9524(12) 0.158(4) Uani 1 1 d DU . .
C3 C 0.4859(7) 0.7703(15) 0.9362(15) 0.179(4) Uani 1 1 d DU . .
H3 H 0.4862 0.7038 0.9519 0.215 Uiso 1 1 calc R . .
C7 C 0.4476(7) 0.9271(14) 0.9257(14) 0.186(4) Uani 1 1 d DU . .
H7 H 0.4183 0.9595 0.9179 0.223 Uiso 1 1 calc R . .
C8 C 0.4358(5) 0.9797(10) 0.6427(12) 0.156(4) Uani 1 1 d DU . .
H8A H 0.4483 1.0205 0.6972 0.188 Uiso 1 1 calc R . .
H8B H 0.4206 1.0217 0.5911 0.188 Uiso 1 1 calc R . .
C9 C 0.3545(4) 0.9242(7) 0.6793(7) 0.095(2) Uani 1 1 d U . .
C10 C 0.3360(3) 0.8698(6) 0.7446(7) 0.088(3) Uani 1 1 d . . .
H10 H 0.3557 0.8247 0.7822 0.106 Uiso 1 1 calc R . .
C11 C 0.2897(3) 0.8797(6) 0.7558(5) 0.070(2) Uani 1 1 d . . .
C12 C 0.2596(3) 0.9433(5) 0.6973(5) 0.0632(18) Uani 1 1 d . . .
H12 H 0.2275 0.9486 0.7021 0.076 Uiso 1 1 calc R . .
C13 C 0.2224(3) 0.4991(5) 0.8686(5) 0.0589(16) Uani 1 1 d . . .
C14 C 0.3247(3) 0.9890(6) 0.6222(6) 0.081(2) Uani 1 1 d . . .
H14 H 0.3365 1.0262 0.5773 0.097 Uiso 1 1 calc R . .
C15 C 0.2545(3) 0.5724(5) 0.9305(5) 0.0615(18) Uani 1 1 d . . .
C16 C 0.2716(3) 0.8225(7) 0.8314(6) 0.077(2) Uani 1 1 d . . .
N1 N 0.4018(3) 0.9073(7) 0.6660(7) 0.118(3) Uani 1 1 d DU . .
O1 O 0.3999(2) 0.6938(6) 0.9938(6) 0.102(2) Uani 1 1 d . . .
O2 O 0.3806(3) 0.8414(6) 1.0121(6) 0.121(2) Uani 1 1 d U . .
O3 O 0.3000(2) 0.7633(5) 0.8805(4) 0.0790(16) Uani 1 1 d . . .
O4 O 0.22875(19) 0.8359(5) 0.8389(4) 0.0850(17) Uani 1 1
d . . .
O5 O 0.26609(17) 0.8537(3) 1.0396(3) 0.0620(12) Uani 1 1
d . . .
O6 O 0.29797(19) 0.5594(4) 0.9486(4) 0.0741(14) Uani 1 1
d . . .
O7 O 0.3622(3) 0.5748(7) 1.1393(7) 0.134(3) Uani 1 1 d . . .
O8 O 0.3590(5) 0.7830(6) 1.2016(7) 0.151(5) Uani 1 1 d . . .
Pr1 Pr 0.319912(12) 0.71331(3) 1.04637(2) 0.0540(2) Uani 1 1
d . . .
C4 C 0.5232(7) 0.8100(12) 0.8961(13) 0.169(4) Uani 1 1 d DU . .
H4 H 0.5470 0.7728 0.8765 0.203 Uiso 1 1 calc R . .
C6 C 0.4868(6) 0.9827(12) 0.9084(13) 0.182(4) Uani 1 1 d DU . .
H6 H 0.4901 1.0509 0.9094 0.219 Uiso 1 1 calc R . .
C5 C 0.5198(7) 0.9125(12) 0.8895(14) 0.181(4) Uani 1 1 d DU . .
H1 H 0.4182(17) 0.8418(19) 0.685(3) 0.031(13) Uiso 1 1 d D . .

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C3 0.167(5) 0.197(5) 0.182(7) -0.005(5) 0.057(5) -0.001(4)
C7 0.183(5) 0.184(5) 0.195(7) 0.015(5) 0.049(5) -0.018(4)
C8 0.142(6) 0.167(6) 0.167(7) 0.011(5) 0.047(5) -0.010(4)
C9 0.096(4) 0.098(4) 0.097(4) 0.013(4) 0.037(4) 0.029(4)
C10 0.073(5) 0.106(6) 0.104(6) 0.050(5) 0.060(5) 0.036(5)
C11 0.058(4) 0.096(5) 0.064(4) 0.013(4) 0.030(3) 0.015(4)
C12 0.064(4) 0.071(4) 0.064(4) 0.006(3) 0.037(3) 0.016(3)
C13 0.064(4) 0.064(4) 0.060(4) -0.007(3) 0.040(3) -0.016(3)
C14 0.092(6) 0.072(5) 0.098(6) 0.027(4) 0.067(5) 0.029(4)
C15 0.090(6) 0.051(4) 0.054(4) -0.008(3) 0.039(4) -0.003(4)
C16 0.061(5) 0.113(6) 0.069(5) 0.027(5) 0.043(4) 0.010(5)
N1 0.106(4) 0.124(4) 0.136(5) 0.019(4) 0.052(4) 0.031(3)
O1 0.050(4) 0.147(6) 0.117(6) -0.014(5) 0.035(4) 0.023(4)
O2 0.115(4) 0.115(4) 0.139(5) -0.017(4) 0.037(3) -0.036(3)
O3 0.065(4) 0.117(4) 0.065(3) 0.026(3) 0.037(3) 0.007(3)
O4 0.057(3) 0.134(5) 0.072(3) 0.035(3) 0.031(3) 0.012(3)
O5 0.055(3) 0.067(3) 0.068(3) -0.012(2) 0.023(2) -0.011(2)
O6 0.054(3) 0.072(3) 0.104(4) -0.013(3) 0.033(3) -0.004(2)
O7 0.087(5) 0.179(7) 0.137(7) 0.042(6) 0.023(5) 0.050(6)
O8 0.161(10) 0.169(9) 0.096(6) 0.005(5) -0.044(7) -0.054(6)
Pr1 0.0348(3) 0.0702(4) 0.0608(3) 0.00460(15) 0.0187(2) -
0.00720(13)
C4 0.157(5) 0.179(5) 0.176(7) 0.001(5) 0.040(5) -0.007(4)
C6 0.178(6) 0.178(5) 0.197(7) 0.001(5) 0.053(5) -0.008(4)
C5 0.182(6) 0.181(5) 0.180(7) -0.002(5) 0.039(5) 0.005(4)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C1 Pr1 2.914(15) . ?
C2 C7 1.35(2) . ?
C2 C3 1.42(2) . ?
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C3 H3 0.9300 . ?
C7 C6 1.407(10) . ?
C7 H7 0.9300 . ?
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C8 C5 1.69(2) 2_656 ?
C8 H8A 0.9700 . ?
C8 H8B 0.9700 . ?
C9 C10 1.377(12) . ?
C9 C14 1.378(12) . ?
C9 N1 1.412(13) . ?
C10 C11 1.361(11) . ?
C10 H10 0.9300 . ?
C11 C12 1.383(10) . ?
C11 C16 1.505(10) . ?
C12 C13 1.387(9) 4_556 ?
C12 H12 0.9300 . ?
C13 C14 1.376(11) 4_546 ?
C13 C12 1.387(9) 4_546 ?
C13 C15 1.519(10) . ?
C14 C13 1.376(11) 4_556 ?
C14 H14 0.9300 . ?
C15 O6 1.227(9) . ?
C15 O5 1.275(8) 7_567 ?
C15 Pr1 2.950(7) . ?
C16 O4 1.256(9) . ?
C16 O3 1.256(10) . ?
N1 H1 1.015(5) . ?
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O2 Pr1 2.563(8) . ?
O3 Pr1 2.440(6) . ?
O4 Pr1 2.441(5) 7_567 ?
O5 C15 1.275(8) 7_567 ?
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O5 Pr1 2.678(5) 7_567 ?
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O8 Pr1 2.484(8) . ?
Pr1 O4 2.441(5) 7_567 ?
Pr1 O5 2.678(5) 7_567 ?
Pr1 Pr1 4.0660(9) 7_567 ?
C4 C5 1.397(10) . ?
C4 H4 0.9300 . ?
C6 C5 1.400(10) . ?
C6 H6 0.9300 . ?
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C2 C3 H3 120.1 . . ?
C2 C7 C6 126.9(18) . . ?
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N1 C8 H8A 110.7 . . ?
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C5 C8 H8B 110.7 2_656 . ?
H8A C8 H8B 108.8 . . ?
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C10 C9 N1 120.2(8) . . ?
C14 C9 N1 121.0(9) . . ?
C11 C10 C9 122.2(8) . . ?
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C13 C12 H12 120.4 4_556 . ?
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C14 C13 C15 119.6(6) 4_546 . ?
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C13 C14 C9 120.2(7) 4_556 . ?
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O6 C15 O5 123.4(7) . 7_567 ?
O6 C15 C13 119.9(6) . . ?
O5 C15 C13 116.8(7) 7_567 . ?
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O5 C15 Pr1 65.2(3) 7_567 . ?
C13 C15 Pr1 177.7(5) . . ?
O4 C16 O3 125.0(7) . . ?
O4 C16 C11 117.3(7) . . ?
O3 C16 C11 117.6(7) . . ?
C9 N1 C8 127.6(10) . . ?
C9 N1 H1 121(3) . . ?
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C1 O2 Pr1 94.3(8) . . ?
C16 O3 Pr1 137.0(5) . . ?
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C15 O5 Pr1 157.9(5) 7_567 . ?
C15 O5 Pr1 89.2(4) 7_567 7_567 ?
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C15 O6 Pr1 97.5(4) . . ?
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O4 Pr1 O7 73.0(3) 7_567 . ?
O5 Pr1 O8 84.7(3) . . ?
O3 Pr1 O8 138.9(3) . . ?
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O5 Pr1 O1 131.3(2) . . ?
O3 Pr1 O1 78.0(2) . . ?
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O8 Pr1 O1 92.0(4) . . ?
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O3 Pr1 O2 70.2(3) . . ?
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O7 Pr1 O2 110.1(3) . . ?
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O6 Pr1 O2 123.8(2) . . ?
O1 Pr1 O2 48.7(3) . . ?
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O3 Pr1 O5 67.83(19) . 7_567 ?
O4 Pr1 O5 68.54(18) 7_567 7_567 ?
O7 Pr1 O5 107.3(3) . 7_567 ?
O8 Pr1 O5 139.1(4) . 7_567 ?
O6 Pr1 O5 49.95(16) . 7_567 ?
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O2 Pr1 O5 136.9(2) . 7_567 ?
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O5 Pr1 C15 25.61(18) 7_567 . ?
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C5 C6 C7 104.6(16) . . ?
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

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Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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 goodness of fit S are based on F^2^, conventional R-factors R
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.8602(12) 0.2737(2) 0.03990(13) 0.0308(10) Uani 1 1
d . . .
O3 O 0.3091(12) 0.9272(2) 0.19413(13) 0.0311(11) Uani 1 1
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O4 O 0.0737(12) 0.9452(2) 0.25971(14) 0.0298(10) Uani 1 1
d . . .
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d . . .
O6 O -0.2547(12) 0.7083(2) 0.34421(13) 0.0257(10) Uani 1 1
d . . .
H6 H -0.365(19) 0.679(4) 0.366(3) 0.039 Uiso 1 1 d . . .
O7 O 0.1424(12) -0.2339(2) 0.45812(13) 0.0277(10) Uani 1 1
d . . .
O8 O 0.0746(11) -0.1254(2) 0.50192(13) 0.0258(10) Uani 1 1
d . . .
H8A H 0.0100 -0.1602 0.5190 0.039 Uiso 1 1 calc R . .
O9 O 1.3249(14) 0.0887(2) 0.18852(15) 0.0374(12) Uani 1 1
d . . .
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O10 O 1.2833(14) 0.2084(3) 0.15838(14) 0.0372(12) Uani 1 1
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O11 O 0.9598(12) 0.4431(2) 0.24299(13) 0.0297(10) Uani 1 1
d . . .
O12 O 0.7308(12) 0.4249(2) 0.30907(13) 0.0290(10) Uani 1 1
d . . .
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d . . .
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d . . .
H14 H 0.31(2) 0.676(5) 0.422(2) 0.039 Uiso 1 1 d . . .
O15 O 0.5815(18) 0.1521(3) 0.08994(16) 0.0594(18) Uani 1 1
d . . .
H15 H 0.6580 0.1918 0.0769 0.089 Uiso 1 1 calc R . .
O16 O 0.9455(13) 0.2948(3) 0.92069(13) 0.0326(11) Uani 1 1
d . . .
H16 H 0.8665 0.3137 0.8977 0.049 Uiso 1 1 calc R . .
C1 C 0.8199(15) 0.3446(3) 0.03446(18) 0.0212(13) Uani 1 1
d . . .
C2 C 0.7116(15) 0.4016(3) 0.06907(19) 0.0200(12) Uani 1 1
d . . .
C3 C 0.6579(16) 0.4815(3) 0.05930(19) 0.0223(13) Uani 1 1
d . . .
H3A H 0.6965 0.5002 0.0311 0.027 Uiso 1 1 calc R . .
C4 C 0.5464(16) 0.5334(3) 0.09181(19) 0.0230(13) Uani 1 1
d . . .
H4 H 0.5100 0.5867 0.0852 0.028 Uiso 1 1 calc R . .
C5 C 0.4894(14) 0.5065(3) 0.13388(18) 0.0191(12) Uani 1 1
d . . .
C6 C 0.5507(15) 0.4266(3) 0.14363(19) 0.0210(12) Uani 1 1
d . . .
H6A H 0.5168 0.4082 0.1720 0.025 Uiso 1 1 calc R . .
C7 C 0.6613(16) 0.3749(3) 0.11141(19) 0.0224(13) Uani 1 1
d . . .
H7 H 0.7020 0.3219 0.1182 0.027 Uiso 1 1 calc R . .
C8 C 0.3752(15) 0.5595(3) 0.16926(19) 0.0185(12) Uani 1 1
d . . .
H8 H 0.367(16) 0.543(4) 0.198(2) 0.022 Uiso 1 1 d . . .
C9 C 0.1784(15) 0.6779(3) 0.20044(17) 0.0173(12) Uani 1 1
d . . .
C10 C 0.2269(15) 0.7608(3) 0.19832(18) 0.0188(12) Uani 1 1
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
C18 C 0.2801(14) -0.1016(3) 0.43077(18) 0.0183(12) Uani 1 1
d . . .
C19 C 0.3600(15) -0.1324(4) 0.38906(19) 0.0226(13) Uani 1 1
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
H28 H 1.0952 0.3086 0.2093 0.029 Uiso 1 1 calc R . .
C29 C 0.9127(16) 0.3104(3) 0.27098(19) 0.0230(13) Uani 1 1
d . . .
C30 C 0.8226(15) 0.2610(3) 0.30566(18) 0.0191(12) Uani 1 1
d . . .
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d . . .
C32 C 0.8721(16) 0.3994(4) 0.27260(19) 0.0249(14) Uani 1 1
d . . .
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H33B H 0.8042 0.6712 0.5202 0.042 Uiso 1 1 calc R . .
H33C H 0.4622 0.7129 0.5303 0.042 Uiso 1 1 calc R . .
C34 C 0.8090(16) 0.7148(3) 0.5841(2) 0.0249(13) Uani 1 1
d . . .
H34A H 0.6371 0.7215 0.6060 0.030 Uiso 1 1 calc R . .
H34B H 0.9800 0.6796 0.5960 0.030 Uiso 1 1 calc R . .
C35 C 0.1356(17) 0.5418(4) 0.4503(2) 0.0299(14) Uani 1 1
d . . .
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H35C H 0.3345 0.5367 0.4707 0.045 Uiso 1 1 calc R . .
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d . . .
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C37 C 0.295(3) 0.0233(5) 0.0819(3) 0.065(2) Uani 1 1 d . . .
H37A H 0.1936 -0.0158 0.0598 0.098 Uiso 1 1 calc R . .
H37B H 0.1181 0.0386 0.1010 0.098 Uiso 1 1 calc R . .
H37C H 0.4784 0.0001 0.0991 0.098 Uiso 1 1 calc R . .
C38 C 0.441(3) 0.0951(6) 0.0600(4) 0.074(3) Uani 1 1 d D . .
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H38B H 0.2574 0.1173 0.0417 0.089 Uiso 1 1 calc RD . .
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H39A H 1.3234 0.1331 0.9452 0.062 Uiso 1 1 calc R . .
H39B H 1.0488 0.1755 0.9725 0.062 Uiso 1 1 calc R . .
H39C H 1.4150 0.2206 0.9658 0.062 Uiso 1 1 calc R . .
C40 C 1.0849(18) 0.2189(4) 0.9106(2) 0.0327(15) Uani 1 1
d . . .
H40A H 1.2681 0.2270 0.8899 0.039 Uiso 1 1 calc R . .
H40B H 0.9013 0.1816 0.8966 0.039 Uiso 1 1 calc R . .

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O2 0.053(3) 0.018(2) 0.024(2) -0.0017(17) 0.012(2) 0.0097(19)
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O4 0.045(3) 0.018(2) 0.028(2) -0.0001(18) 0.009(2) 0.0038(19)
O5 0.035(2) 0.014(2) 0.023(2) 0.0014(16) 0.0075(18) 0.0003(17)
O6 0.039(3) 0.022(2) 0.017(2) -0.0006(17) 0.0124(18) 0.0019(18)
O7 0.044(3) 0.019(2) 0.021(2) 0.0024(16) 0.0113(19) 0.0010(18)
O8 0.040(3) 0.018(2) 0.021(2) 0.0049(16) 0.0126(18) 0.0052(18)
O9 0.066(3) 0.017(2) 0.032(2) 0.0002(18) 0.027(2) 0.001(2)
O10 0.068(4) 0.023(2) 0.022(2) 0.0017(18) 0.021(2) 0.001(2)
O11 0.047(3) 0.020(2) 0.023(2) 0.0034(18) 0.010(2) 0.0041(19)
O12 0.050(3) 0.015(2) 0.023(2) 0.0001(16) 0.009(2) 0.0084(19)
O13 0.044(3) 0.021(2) 0.022(2) 0.0012(16) 0.0062(19) -
0.0051(19)
O14 0.033(3) 0.020(2) 0.026(2) 0.0019(17) 0.0130(19) 0.0063(18)
O15 0.121(5) 0.024(3) 0.036(3) -0.003(2) 0.039(3) -0.003(3)
O16 0.054(3) 0.026(2) 0.019(2) 0.0016(17) 0.004(2) 0.012(2)
C1 0.024(3) 0.023(3) 0.017(3) -0.003(2) 0.006(2) 0.003(2)
C2 0.020(3) 0.017(3) 0.023(3) 0.000(2) 0.005(2) 0.006(2)
C3 0.028(3) 0.022(3) 0.019(3) 0.002(2) 0.009(2) 0.005(2)
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C6 0.021(3) 0.022(3) 0.021(3) 0.002(2) 0.006(2) 0.004(2)
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C10 0.022(3) 0.022(3) 0.013(3) 0.003(2) 0.004(2) 0.003(2)
C11 0.023(3) 0.021(3) 0.018(3) -0.001(2) 0.000(2) 0.002(2)
C12 0.021(3) 0.024(3) 0.016(3) -0.001(2) 0.003(2) 0.007(2)
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
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Netherlands.
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
```

```
 'calc w=1/[\s^2^(Fo^2^)+(0.1049P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4869
_refine_ls_number_parameters      315
_refine_ls_number_restraints      309
_refine_ls_R_factor_all           0.0771
_refine_ls_R_factor_gt            0.0594
_refine_ls_wR_factor_ref          0.1768
_refine_ls_wR_factor_gt           0.1640
_refine_ls_goodness_of_fit_ref    1.039
_refine_ls_restrained_S_all       1.027
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
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 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Nd1 Nd 0.182055(11) 0.21246(3) 0.95661(3) 0.0479(2) Uani 1 1 d
U . .
N1 N -0.0985(2) 0.4171(5) 1.1491(5) 0.0648(18) Uani 1 1 d U . .
N2 N 0.1193(8) 0.3816(12) 0.6736(13) 0.230(7) Uani 1 1 d DU . .
N3 N 0.1143(6) 0.0189(10) 0.6850(12) 0.073(5) Uani 0.40 1 d
PDU . .
O1 O 0.1078(2) 0.1774(5) 1.0172(6) 0.089(2) Uani 1 1 d U . .
O2 O 0.11916(19) 0.3276(4) 0.9937(5) 0.0785(17) Uani 1 1 d
U . .
O3 O 0.20582(16) 0.0661(4) 1.0520(4) 0.0640(14) Uani 1 1 d
U . .
O4 O 0.26821(15) 0.1512(3) 1.0392(4) 0.0546(12) Uani 1 1 d
U . .
O5 O 0.22861(18) 0.1685(5) 0.8308(4) 0.0780(17) Uani 1 1 d
U . .
O6 O 0.20113(19) 0.2607(4) 1.1286(4) 0.0640(14) Uani 1 1 d
U . .
O7 O 0.1423(4) 0.2832(5) 0.8022(7) 0.118(3) Uani 1 1 d DU . .
O8 O 0.1380(5) 0.0949(15) 0.8445(13) 0.060(5) Uani 0.40 1 d
PU . .
O8A O 0.1438(7) 0.0673(13) 0.8712(14) 0.106(7) Uani 0.60 1 d
PU . .
```

```
C1 C 0.0953(3) 0.2602(8) 1.0210(7) 0.066(2) Uani 1 1 d U . .
C2 C 0.0507(3) 0.2832(6) 1.0576(7) 0.067(2) Uani 1 1 d U . .
C3 C 0.0223(4) 0.2124(6) 1.0835(11) 0.108(5) Uani 1 1 d U . .
H3 H 0.0324 0.1506 1.0827 0.130 Uiso 1 1 calc R . .
C4 C -0.0205(4) 0.2315(7) 1.1106(11) 0.113(5) Uani 1 1 d U . .
H4 H -0.0401 0.1826 1.1219 0.136 Uiso 1 1 calc R . .
C5 C -0.0337(3) 0.3195(6) 1.1205(7) 0.073(2) Uani 1 1 d U . .
C6 C -0.0065(3) 0.3927(7) 1.0951(7) 0.082(3) Uani 1 1 d U . .
H6 H -0.0166 0.4544 1.0981 0.098 Uiso 1 1 calc R . .
C7 C 0.0362(3) 0.3728(7) 1.0649(8) 0.084(3) Uani 1 1 d U . .
H7 H 0.0550 0.4217 1.0497 0.101 Uiso 1 1 calc R . .
C8 C -0.0815(3) 0.3389(8) 1.1452(8) 0.082(3) Uani 1 1 d DU . .
H16 H -0.099(3) 0.285(4) 1.113(7) 0.098 Uiso 1 1 d D . .
C9 C 0.2499(2) 0.0782(5) 1.0707(6) 0.0535(18) Uani 1 1 d U . .
C10 C 0.2801(2) 0.0049(5) 1.1271(6) 0.0531(18) Uani 1 1 d U . .
C11 C 0.3277(2) -0.0032(5) 1.1188(6) 0.058(2) Uani 1 1 d U . .
H11 H 0.3408 0.0388 1.0793 0.070 Uiso 1 1 calc R . .
C12 C 0.3549(2) -0.0734(5) 1.1692(6) 0.0587(19) Uani 1 1 d
U . .
C13 C 0.3368(2) -0.1286(5) 1.2367(6) 0.0551(18) Uani 1 1 d
U . .
H13 H 0.3563 -0.1713 1.2754 0.066 Uiso 1 1 calc R . .
C14 C 0.2895(2) -0.1213(5) 1.2478(5) 0.0543(18) Uani 1 1 d
U . .
C15 C 0.2618(2) -0.0547(5) 1.1924(5) 0.0527(18) Uani 1 1 d
U . .
H15 H 0.2303 -0.0493 1.1984 0.063 Uiso 1 1 calc R . .
C16 C 0.2716(3) 0.1805(6) 0.8212(6) 0.061(2) Uani 1 1 d U . .
C17 C 0.1559(9) 0.3153(17) 0.7325(17) 0.223(7) Uani 1 1 d
DU . .
C18 C 0.0668(10) 0.3871(18) 0.698(2) 0.272(8) Uani 1 1 d U . .
H18A H 0.0615 0.3343 0.7386 0.408 Uiso 1 1 calc R . .
H18B H 0.0444 0.3863 0.6375 0.408 Uiso 1 1 calc R . .
H18C H 0.0633 0.4440 0.7339 0.408 Uiso 1 1 calc R . .
C19 C 0.1412(6) 0.4253(10) 0.6021(11) 0.228(7) Uani 1 1 d
DU . .
H19A H 0.1687 0.3907 0.5942 0.343 Uiso 1 1 calc R . .
H19B H 0.1499 0.4880 0.6233 0.343 Uiso 1 1 calc R . .
H19C H 0.1198 0.4274 0.5398 0.343 Uiso 1 1 calc R . .
C20 C 0.1304(6) 0.0940(10) 0.7512(11) 0.140(12) Uani 0.40 1 d
PRDU . .
C21 C 0.0969(6) 0.0302(10) 0.5800(11) 0.108(9) Uani 0.40 1 d
PRDU . .
H21A H 0.0895 0.0949 0.5660 0.162 Uiso 0.40 1 calc PR . .
H21B H 0.0691 -0.0070 0.5613 0.162 Uiso 0.40 1 calc PR . .
H21C H 0.1204 0.0103 0.5429 0.162 Uiso 0.40 1 calc PR . .
C22 C 0.1264(15) -0.065(2) 0.750(3) 0.162(15) Uani 0.40 1 d
PDU . .
H22A H 0.1299 -0.0465 0.8185 0.243 Uiso 0.40 1 calc PR . .
H22B H 0.1553 -0.0917 0.7376 0.243 Uiso 0.40 1 calc PR . .
H22C H 0.1017 -0.1105 0.7355 0.243 Uiso 0.40 1 calc PR . .

loop_
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 _atom_site_aniso_U_23
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0.00092(15)
N1 0.041(3) 0.082(5) 0.079(5) 0.020(4) 0.033(3) 0.024(3)
N2 0.284(13) 0.209(14) 0.196(14) 0.053(11) 0.038(12) 0.024(12)
N3 0.071(11) 0.052(9) 0.088(12) -0.002(9) -0.008(10) -0.007(8)
O1 0.049(3) 0.078(4) 0.157(7) -0.004(4) 0.061(4) -0.003(3)
O2 0.043(3) 0.089(4) 0.115(5) 0.022(4) 0.045(3) 0.017(3)
O3 0.038(3) 0.061(3) 0.100(4) 0.010(3) 0.029(3) 0.004(2)
O4 0.037(2) 0.054(3) 0.078(3) 0.004(2) 0.026(2) 0.001(2)
O5 0.038(3) 0.122(5) 0.080(4) -0.035(4) 0.026(3) -0.009(3)
O6 0.045(3) 0.086(4) 0.067(3) -0.020(3) 0.025(3) -0.009(3)
O7 0.117(7) 0.135(7) 0.092(6) -0.009(4) -0.010(5) 0.024(5)
O8 0.029(7) 0.089(13) 0.054(9) 0.018(9) -0.012(6) -0.028(7)
O8A 0.101(8) 0.106(8) 0.109(9) 0.013(5) 0.016(5) -0.012(4)
C1 0.033(4) 0.102(7) 0.069(5) 0.003(5) 0.023(4) 0.001(4)
C2 0.047(5) 0.080(6) 0.081(6) 0.012(4) 0.028(4) 0.012(4)
C3 0.065(6) 0.084(7) 0.198(14) 0.006(7) 0.085(8) -0.005(5)
C4 0.073(7) 0.083(7) 0.202(14) 0.032(7) 0.079(9) 0.012(5)
C5 0.065(5) 0.066(5) 0.098(7) 0.014(5) 0.041(5) 0.013(5)
C6 0.049(5) 0.092(6) 0.112(8) 0.027(6) 0.036(5) 0.015(4)
C7 0.046(5) 0.091(7) 0.125(8) 0.013(6) 0.038(5) 0.010(5)
C8 0.057(5) 0.099(8) 0.098(7) 0.017(6) 0.039(5) 0.003(5)
C9 0.038(4) 0.053(4) 0.075(5) 0.006(4) 0.025(4) 0.008(3)
C10 0.035(3) 0.066(4) 0.065(5) 0.002(4) 0.028(3) 0.006(3)
C11 0.038(4) 0.063(5) 0.084(5) 0.018(4) 0.039(4) 0.010(3)
C12 0.039(4) 0.072(5) 0.072(5) 0.006(4) 0.028(4) 0.008(4)
C13 0.044(4) 0.067(5) 0.061(4) 0.008(4) 0.028(3) 0.009(3)
C14 0.039(4) 0.072(5) 0.058(4) 0.000(4) 0.026(3) 0.006(3)
C15 0.035(3) 0.071(5) 0.057(4) -0.011(4) 0.020(3) -0.007(3)
C16 0.044(4) 0.078(5) 0.069(5) -0.011(4) 0.034(4) 0.000(4)
C17 0.229(8) 0.226(8) 0.216(8) 0.013(5) 0.042(5) -0.002(5)
C18 0.265(8) 0.275(10) 0.277(9) 0.000(5) 0.049(5) 0.003(5)
C19 0.236(8) 0.226(8) 0.222(8) 0.008(5) 0.036(5) -0.002(5)
C20 0.131(15) 0.144(15) 0.148(15) -0.006(9) 0.030(9) 0.002(9)
C21 0.115(12) 0.099(11) 0.114(12) 0.013(9) 0.031(9) 0.009(8)
C22 0.165(17) 0.163(16) 0.161(17) 0.011(9) 0.039(10) -0.005(9)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;
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 _geom_bond_site_symmetry_2
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Nd1 O4 2.414(5) 7_557 ?
Nd1 O6 2.415(6) . ?
Nd1 O7 2.436(8) . ?
Nd1 O5 2.440(5) . ?
Nd1 O8 2.468(17) . ?
Nd1 O1 2.480(5) . ?
Nd1 O3 2.494(5) . ?
Nd1 O8A 2.54(2) . ?
Nd1 O2 2.565(5) . ?
Nd1 O4 2.693(5) . ?
Nd1 C1 2.879(8) . ?
Nd1 C9 2.979(7) . ?
N1 C8 1.224(11) . ?
N1 C12 1.427(8) 3_455 ?
N2 C19 1.398(15) . ?
N2 C17 1.537(17) . ?
N2 C18 1.61(3) . ?
N3 C20 1.426(14) . ?
N3 C21 1.442(15) . ?
N3 C22 1.493(18) . ?
O1 C1 1.240(11) . ?
O2 C1 1.276(11) . ?
O3 C9 1.267(8) . ?
O4 C9 1.277(8) . ?
O4 Nd1 2.414(5) 7_557 ?
O5 C16 1.283(9) . ?
O6 C16 1.268(10) 7_557 ?
O7 C17 1.183(16) . ?
O8 O8A 0.54(3) . ?
O8 C20 1.25(2) . ?
O8A C20 1.66(2) . ?
C1 C2 1.497(11) . ?
C2 C7 1.354(11) . ?
C2 C3 1.386(12) . ?
C3 C4 1.377(13) . ?
C3 H3 0.9300 . ?
C4 C5 1.325(13) . ?
C4 H4 0.9300 . ?
C5 C6 1.387(12) . ?
C5 C8 1.506(12) . ?
C6 C7 1.398(11) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.982(10) . ?
C9 C10 1.488(10) . ?
C10 C15 1.400(10) . ?
C10 C11 1.403(9) . ?
C11 C12 1.381(10) . ?
C11 H11 0.9300 . ?
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C12 C13 1.381(10) . ?
C12 N1 1.427(8) 3_545 ?
C13 C14 1.407(9) . ?
C13 H13 0.9300 . ?
C14 C15 1.381(10) . ?
C14 C16 1.471(10) 6_556 ?
C15 H15 0.9300 . ?
C16 O6 1.268(10) 7_557 ?
C16 C14 1.471(10) 6 ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
C21 H21A 0.9600 . ?
C21 H21B 0.9600 . ?
C21 H21C 0.9600 . ?
C22 H22A 0.9600 . ?
C22 H22B 0.9600 . ?
C22 H22C 0.9600 . ?

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O4 Nd1 O6 73.33(18) 7_557 . ?
O4 Nd1 O7 82.8(3) 7_557 . ?
O6 Nd1 O7 135.7(2) . . ?
O4 Nd1 O5 79.91(19) 7_557 . ?
O6 Nd1 O5 134.14(18) . . ?
O7 Nd1 O5 74.5(3) . . ?
O4 Nd1 O8 143.4(4) 7_557 . ?
O6 Nd1 O8 143.3(4) . . ?
O7 Nd1 O8 68.4(5) . . ?
O5 Nd1 O8 71.2(4) . . ?
O4 Nd1 O1 134.45(19) 7_557 . ?
O6 Nd1 O1 78.3(2) . . ?
O7 Nd1 O1 93.8(3) . . ?
O5 Nd1 O1 142.9(2) . . ?
O8 Nd1 O1 71.8(5) . . ?
O4 Nd1 O3 123.68(16) 7_557 . ?
O6 Nd1 O3 74.7(2) . . ?
O7 Nd1 O3 147.6(2) . . ?
O5 Nd1 O3 90.9(2) . . ?
O8 Nd1 O3 79.6(5) . . ?
O1 Nd1 O3 80.36(19) . . ?
O4 Nd1 O8A 151.7(5) 7_557 . ?
O6 Nd1 O8A 133.4(4) . . ?
O7 Nd1 O8A 80.8(4) . . ?
O5 Nd1 O8A 73.5(5) . . ?
O8 Nd1 O8A 12.4(6) . . ?
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```
O1 Nd1 O8A 69.8(5) . . ?
O3 Nd1 O8A 67.2(4) . . ?
O4 Nd1 O2 85.31(17) 7_557 . ?
O6 Nd1 O2 71.0(2) . . ?
O7 Nd1 O2 70.2(3) . . ?
O5 Nd1 O2 143.1(2) . . ?
O8 Nd1 O2 104.6(5) . . ?
O1 Nd1 O2 51.66(19) . . ?
O3 Nd1 O2 125.01(18) . . ?
O8A Nd1 O2 110.3(5) . . ?
O4 Nd1 O4 75.44(16) 7_557 . ?
O6 Nd1 O4 69.43(17) . . ?
O7 Nd1 O4 139.3(3) . . ?
O5 Nd1 O4 68.16(18) . . ?
O8 Nd1 O4 112.2(5) . . ?
O1 Nd1 O4 125.8(2) . . ?
O3 Nd1 O4 50.17(14) . . ?
O8A Nd1 O4 103.0(4) . . ?
O2 Nd1 O4 139.50(19) . . ?
O4 Nd1 C1 110.4(2) 7_557 . ?
O6 Nd1 C1 72.5(2) . . ?
O7 Nd1 C1 82.0(3) . . ?
O5 Nd1 C1 153.1(2) . . ?
O8 Nd1 C1 88.2(5) . . ?
O1 Nd1 C1 25.4(2) . . ?
O3 Nd1 C1 102.4(2) . . ?
O8A Nd1 C1 90.0(5) . . ?
O2 Nd1 C1 26.3(2) . . ?
O4 Nd1 C1 137.7(2) . . ?
O4 Nd1 C9 99.86(18) 7_557 . ?
O6 Nd1 C9 70.0(2) . . ?
O7 Nd1 C9 152.5(3) . . ?
O5 Nd1 C9 79.0(2) . . ?
O8 Nd1 C9 96.2(5) . . ?
O1 Nd1 C9 103.0(2) . . ?
O3 Nd1 C9 24.80(17) . . ?
O8A Nd1 C9 84.8(4) . . ?
O2 Nd1 C9 137.2(2) . . ?
O4 Nd1 C9 25.38(15) . . ?
C1 Nd1 C9 121.4(2) . . ?
C8 N1 C12 119.6(7) . 3_455 ?
C19 N2 C17 106.6(16) . . ?
C19 N2 C18 132.9(19) . . ?
C17 N2 C18 120.4(17) . . ?
C20 N3 C21 124.3(13) . . ?
C20 N3 C22 102.1(18) . . ?
C21 N3 C22 133.2(18) . . ?
C1 O1 Nd1 95.6(5) . . ?
C1 O2 Nd1 90.7(5) . . ?
C9 O3 Nd1 99.6(4) . . ?
C9 O4 Nd1 158.4(5) . 7_557 ?
C9 O4 Nd1 90.0(4) . . ?
Nd1 O4 Nd1 104.56(16) 7_557 . ?
C16 O5 Nd1 134.4(5) . . ?
C16 O6 Nd1 136.8(5) 7_557 . ?
C17 O7 Nd1 133.1(15) . . ?
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O8A O8 C20 131(5) . . ?
O8A O8 Nd1 91(3) . . ?
C20 O8 Nd1 128.1(13) . . ?
O8 O8A C20 35(3) . . ?
O8 O8A Nd1 77(3) . . ?
C20 O8A Nd1 105.9(10) . . ?
O1 C1 O2 121.9(7) . . ?
O1 C1 C2 119.8(8) . . ?
O2 C1 C2 118.2(9) . . ?
O1 C1 Nd1 59.0(4) . . ?
O2 C1 Nd1 63.0(4) . . ?
C2 C1 Nd1 178.1(7) . . ?
C7 C2 C3 117.7(8) . . ?
C7 C2 C1 121.7(8) . . ?
C3 C2 C1 120.5(8) . . ?
C4 C3 C2 121.5(9) . . ?
C4 C3 H3 119.3 . . ?
C2 C3 H3 119.3 . . ?
C5 C4 C3 120.2(9) . . ?
C5 C4 H4 119.9 . . ?
C3 C4 H4 119.9 . . ?
C4 C5 C6 120.2(8) . . ?
C4 C5 C8 119.3(9) . . ?
C6 C5 C8 119.9(8) . . ?
C5 C6 C7 119.1(9) . . ?
C5 C6 H6 120.4 . . ?
C7 C6 H6 120.4 . . ?
C2 C7 C6 121.0(9) . . ?
C2 C7 H7 119.5 . . ?
C6 C7 H7 119.5 . . ?
N1 C8 C5 124.7(8) . . ?
N1 C8 H16 124(6) . . ?
C5 C8 H16 100(6) . . ?
O3 C9 O4 120.3(6) . . ?
O3 C9 C10 119.1(6) . . ?
O4 C9 C10 120.6(6) . . ?
O3 C9 Nd1 55.6(4) . . ?
O4 C9 Nd1 64.7(3) . . ?
C10 C9 Nd1 174.7(5) . . ?
C15 C10 C11 119.1(7) . . ?
C15 C10 C9 120.2(6) . . ?
C11 C10 C9 120.6(6) . . ?
C12 C11 C10 119.9(6) . . ?
C12 C11 H11 120.0 . . ?
C10 C11 H11 120.0 . . ?
C13 C12 C11 119.9(6) . . ?
C13 C12 N1 123.5(7) . 3_545 ?
C11 C12 N1 116.6(6) . 3_545 ?
C12 C13 C14 121.1(7) . . ?
C12 C13 H13 119.4 . . ?
C14 C13 H13 119.4 . . ?
C15 C14 C13 118.3(7) . . ?
C15 C14 C16 122.0(6) . 6_556 ?
C13 C14 C16 119.7(7) . 6_556 ?
C14 C15 C10 121.3(6) . . ?
C14 C15 H15 119.3 . . ?
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C10 C15 H15 119.3 . . ?
O6 C16 O5 123.7(7) 7_557 . ?
O6 C16 C14 119.2(6) 7_557 6 ?
O5 C16 C14 117.1(7) . 6 ?
O7 C17 N2 111.3(19) . . ?
N2 C18 H18A 109.5 . . ?
N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
O8 C20 N3 129.2(15) . . ?
O8 C20 O8A 14.4(15) . . ?
N3 C20 O8A 116.5(12) . . ?
N3 C21 H21A 109.5 . . ?
N3 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
N3 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
N3 C22 H22A 109.5 . . ?
N3 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
N3 C22 H22C 109.5 . . ?
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H22B C22 H22C 109.5 . . ?

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 '-x, -y, -z'
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_cell_length_c                    13.5868(5)
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C.,
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 Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement. R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.0638P)^2^+11.9629P] where P=(Fo^2^+2Fc^2^)/3'
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O1 O 0.38904(14) 0.1845(3) 0.4450(3) 0.0356(10) Uani 1 1
d . . .
O2 O 0.39102(15) 0.3079(3) 0.5309(4) 0.0490(13) Uani 1 1
d . . .
O3 O 0.29701(12) 0.0902(2) 0.4202(3) 0.0274(9) Uani 1 1 d . . .
O4 O 0.26664(12) 0.3328(3) 0.5620(3) 0.0284(9) Uani 1 1 d . . .
O5 O 0.30156(15) 0.2964(3) 0.3871(3) 0.0374(11) Uani 1 1
d . . .
O6 O 0.27147(13) 0.1393(3) 0.6466(3) 0.0362(10) Uani 1 1
d . . .
O7 O 0.35326(19) 0.2643(4) 0.7115(4) 0.0581(14) Uani 1 1 d
D . .
O8 O 0.37040(16) 0.0922(3) 0.6274(4) 0.0507(12) Uani 1 1 d
D . .
O9 O 0.3839(3) -0.0747(6) 0.7738(6) 0.125(3) Uani 1 1 d U . .
H9 H 0.3798 -0.1012 0.8242 0.187 Uiso 1 1 calc R . .
N1 N 0.59844(17) 0.4404(4) 0.3417(4) 0.0396(14) Uani 1 1
d . . .
N2 N 0.3519(6) 0.3386(12) 0.8674(11) 0.183(6) Uani 1 1 d DU . .
C1 C 0.4081(2) 0.2568(5) 0.4721(5) 0.0365(15) Uani 1 1 d . . .
C2 C 0.4523(2) 0.2856(4) 0.4323(5) 0.0386(16) Uani 1 1 d . . .
C3 C 0.4822(2) 0.2227(5) 0.3995(6) 0.0475(19) Uani 1 1 d . . .
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H4 H 0.5453 0.2067 0.3519 0.069 Uiso 1 1 calc R . .
C5 C 0.5370(2) 0.3396(5) 0.3710(5) 0.0472(19) Uani 1 1 d . . .
C6 C 0.5065(2) 0.4003(5) 0.4008(6) 0.057(2) Uani 1 1 d . . .
H6 H 0.5137 0.4600 0.3989 0.069 Uiso 1 1 calc R . .
C7 C 0.4649(2) 0.3740(5) 0.4337(6) 0.053(2) Uani 1 1 d . . .
H7 H 0.4454 0.4157 0.4568 0.063 Uiso 1 1 calc R . .
C8 C 0.5835(2) 0.3614(5) 0.3435(5) 0.0468(18) Uani 1 1 d D . .
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C9 C 0.25250(19) 0.0997(4) 0.4057(4) 0.0242(12) Uani 1 1
d . . .
C10 C 0.22119(18) 0.0303(4) 0.3502(4) 0.0245(12) Uani 1 1
d . . .
C11 C 0.17379(19) 0.0198(4) 0.3659(4) 0.0298(14) Uani 1 1
d . . .
H11 H 0.1614 0.0574 0.4090 0.036 Uiso 1 1 calc R . .
C12 C 0.14548(19) -0.0467(4) 0.3170(4) 0.0309(14) Uani 1 1
d . . .
C13 C 0.1627(2) -0.0989(4) 0.2474(4) 0.0326(14) Uani 1 1
d . . .
H13 H 0.1427 -0.1408 0.2115 0.039 Uiso 1 1 calc R . .
C14 C 0.20990(19) -0.0889(4) 0.2308(4) 0.0279(13) Uani 1 1
d . . .
C15 C 0.23918(18) -0.0242(4) 0.2831(4) 0.0249(12) Uani 1 1
d . . .
H15 H 0.2707 -0.0175 0.2731 0.030 Uiso 1 1 calc R . .
C16 C 0.2719(2) 0.3527(4) 0.3428(4) 0.0304(14) Uani 1 1 d . . .
C17 C 0.3307(6) 0.2838(11) 0.7846(12) 0.162(6) Uani 1 1 d
DU . .
C18 C 0.3103(10) 0.373(2) 0.918(2) 0.365(16) Uani 1 1 d DU . .
H18A H 0.3231 0.4116 0.9724 0.548 Uiso 1 1 calc R . .
H18B H 0.2945 0.3243 0.9435 0.548 Uiso 1 1 calc R . .
H18C H 0.2876 0.4048 0.8703 0.548 Uiso 1 1 calc R . .
C19 C 0.4015(8) 0.3728(19) 0.870(2) 0.304(13) Uani 1 1 d DU . .
H19A H 0.4101 0.4107 0.9268 0.455 Uiso 1 1 calc R . .
H19B H 0.4027 0.4054 0.8100 0.455 Uiso 1 1 calc R . .
H19C H 0.4236 0.3244 0.8749 0.455 Uiso 1 1 calc R . .
C20 C 0.3867(4) 0.0090(7) 0.5904(8) 0.102(4) Uani 1 1 d U . .
H20A H 0.4185 -0.0043 0.6269 0.122 Uiso 1 1 calc R . .
H20B H 0.3892 0.0161 0.5207 0.122 Uiso 1 1 calc R . .
C21 C 0.3539(4) -0.0681(6) 0.6000(8) 0.081(3) Uani 1 1 d DU . .
C22 C 0.3525(3) -0.1066(6) 0.6929(7) 0.067(2) Uani 1 1 d DU . .
C23 C 0.3229(4) -0.1726(6) 0.7009(8) 0.077(3) Uani 1 1 d DU . .
H23 H 0.3223 -0.1976 0.7631 0.092 Uiso 1 1 calc R . .
C24 C 0.2934(6) -0.2040(8) 0.6196(12) 0.195(9) Uani 1 1 d
DU . .
H24 H 0.2726 -0.2503 0.6251 0.234 Uiso 1 1 calc R . .
C25 C 0.2949(7) -0.1661(12) 0.5285(16) 0.228(10) Uani 1 1 d
DU . .
H25 H 0.2746 -0.1869 0.4720 0.273 Uiso 1 1 calc R . .
C26 C 0.3250(5) -0.0998(10) 0.5201(10) 0.168(7) Uani 1 1 d
DU . .
H26 H 0.3258 -0.0755 0.4576 0.201 Uiso 1 1 calc R . .
H16 H 0.592(5) 0.321(8) 0.290(8) 0.201 Uiso 1 1 d D . .
H17 H 0.373(5) 0.071(9) 0.698(4) 0.201 Uiso 1 1 d D . .

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O2 0.035(2) 0.060(3) 0.058(3) -0.030(3) 0.029(2) -0.028(2)
O3 0.021(2) 0.023(2) 0.039(2) -0.0051(18) 0.0110(17) -
0.0022(16)
O4 0.025(2) 0.024(2) 0.038(2) -0.0120(18) 0.0100(17) -
0.0014(16)
O5 0.038(2) 0.036(3) 0.044(3) 0.024(2) 0.025(2) 0.0199(19)
O6 0.030(2) 0.038(3) 0.047(3) 0.016(2) 0.0226(19) 0.0080(19)
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O8 0.043(3) 0.048(3) 0.061(3) 0.012(3) 0.009(2) 0.019(2)
O9 0.132(6) 0.144(8) 0.104(6) 0.051(6) 0.035(5) -0.045(6)
N1 0.027(3) 0.046(3) 0.052(3) -0.022(3) 0.024(2) -0.015(2)
N2 0.158(11) 0.234(16) 0.144(11) -0.067(12) -0.006(9) -
0.039(11)
C1 0.019(3) 0.050(4) 0.042(4) 0.005(3) 0.008(3) -0.005(3)
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C4 0.051(4) 0.050(5) 0.083(6) -0.021(4) 0.042(4) -0.012(4)
C5 0.036(3) 0.055(5) 0.058(5) -0.025(4) 0.028(3) -0.020(3)
C6 0.043(4) 0.045(4) 0.093(6) -0.022(4) 0.037(4) -0.018(3)
C7 0.040(4) 0.045(4) 0.081(5) -0.021(4) 0.035(4) -0.015(3)
C8 0.042(4) 0.049(4) 0.056(5) -0.019(4) 0.028(3) -0.020(3)
C9 0.027(3) 0.024(3) 0.025(3) -0.005(2) 0.015(2) -0.004(2)
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C13 0.030(3) 0.035(3) 0.037(3) -0.014(3) 0.017(3) -0.012(3)
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C18 0.367(17) 0.366(17) 0.362(17) -0.004(5) 0.064(6) 0.004(5)
C19 0.304(13) 0.306(14) 0.303(14) 0.005(5) 0.057(6) 0.002(5)
C20 0.114(8) 0.094(8) 0.116(9) 0.045(7) 0.070(7) 0.054(7)
C21 0.109(8) 0.059(6) 0.079(7) 0.027(5) 0.029(6) 0.031(6)
C22 0.063(5) 0.072(6) 0.066(6) 0.005(5) 0.015(5) 0.011(5)
C23 0.112(8) 0.052(5) 0.071(6) 0.016(5) 0.030(6) 0.015(6)
C24 0.32(2) 0.118(12) 0.112(12) 0.053(10) -0.063(14) -0.072(13)
C25 0.235(10) 0.221(10) 0.223(11) 0.008(5) 0.031(5) -0.007(5)
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0.057(13)

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l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
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 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 O6 2.439(3) . ?
Nd1 O3 2.478(4) . ?
Nd1 O7 2.500(5) . ?
Nd1 O2 2.498(4) . ?
Nd1 O8 2.510(4) . ?
Nd1 O1 2.560(4) . ?
Nd1 O4 2.670(4) 7_556 ?
Nd1 C1 2.885(5) . ?
Nd1 C9 2.939(6) . ?
Nd1 Nd1 4.0375(4) 7_556 ?
O1 C1 1.249(8) . ?
O2 C1 1.270(8) . ?
O3 C9 1.247(6) . ?
O4 C9 1.272(6) 7_556 ?
O4 Nd1 2.670(4) 7_556 ?
O5 C16 1.272(7) . ?
O6 C16 1.265(6) 7_556 ?
O7 C17 1.306(14) . ?
O8 C20 1.464(11) . ?
O8 H17 1.01(2) . ?
O9 C22 1.375(11) . ?
O9 H9 0.8200 . ?
N1 C8 1.273(8) . ?
N1 C12 1.440(7) 3 ?
N2 C17 1.444(14) . ?
N2 C19 1.489(16) . ?
N2 C18 1.555(17) . ?
C1 C2 1.511(8) . ?
C2 C7 1.388(9) . ?
C2 C3 1.398(9) . ?
C3 C4 1.382(9) . ?
C3 H3 0.9300 . ?
C4 C5 1.424(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.373(9) . ?
C5 C8 1.466(8) . ?
C6 C7 1.385(8) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 1.00(2) . ?
C9 O4 1.272(6) 7_556 ?
C9 C10 1.494(8) . ?
C10 C15 1.392(7) . ?
C10 C11 1.402(7) . ?
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C11 H11 0.9300 . ?
C12 C13 1.387(8) . ?
C12 N1 1.440(7) 3_445 ?
C13 C14 1.399(7) . ?
C13 H13 0.9300 . ?
C14 C15 1.397(8) . ?
C14 C16 1.495(7) 4_545 ?
C15 H15 0.9300 . ?
C16 O6 1.265(6) 7_556 ?
C16 C14 1.494(7) 4 ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9600 . ?
C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
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C20 H20B 0.9700 . ?
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C21 C22 1.398(11) . ?
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C23 C24 1.350(17) . ?
C23 H23 0.9300 . ?
C24 C25 1.372(16) . ?
C24 H24 0.9300 . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
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factors based
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on F, and R-
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H3 H 0.9439 0.0838 0.4579 0.048 Uiso 1 1 calc R . .
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DU . .
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DU . .
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O2 0.035(3) 0.047(3) 0.065(4) 0.010(3) 0.035(3) 0.009(3)
O3 0.022(2) 0.035(3) 0.061(3) -0.002(2) 0.014(2) -0.001(2)
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O7 0.098(6) 0.128(7) 0.041(4) 0.003(4) 0.004(4) 0.075(5)
O8 0.077(5) 0.225(9) 0.093(6) -0.033(6) 0.033(5) -0.092(6)
N1 0.027(3) 0.051(4) 0.058(4) 0.016(3) 0.027(3) 0.012(3)
C1 0.019(4) 0.053(5) 0.053(5) -0.007(4) 0.014(3) 0.000(4)
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C3 0.028(4) 0.042(5) 0.056(5) 0.004(4) 0.021(3) 0.007(3)
C4 0.046(5) 0.048(5) 0.052(5) 0.009(4) 0.027(4) 0.005(4)
C5 0.038(5) 0.054(5) 0.066(6) 0.011(4) 0.031(4) 0.012(4)
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C8 0.035(4) 0.060(6) 0.070(6) 0.009(5) 0.031(4) 0.011(4)
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C13 0.024(3) 0.039(4) 0.039(4) 0.008(3) 0.014(3) 0.012(3)
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C15 0.019(3) 0.032(4) 0.039(4) -0.002(3) 0.015(3) -0.001(3)
C16 0.031(4) 0.039(4) 0.034(4) 0.001(3) 0.016(3) 0.006(3)
C17 0.144(14) 0.166(15) 0.069(9) 0.000(10) -0.017(9) 0.013(13)
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0.067(13)
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C22 0.214(8) 0.212(8) 0.197(7) -0.027(5) 0.041(5) 0.006(5)

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 are estimated using the full covariance matrix.  The cell
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 C9 2.962(7) . ?
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C20 C21 1.505(3) . ?
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O8 Nd1 C1 88.8(3) . . ?
O3 Nd1 C1 102.3(2) . . ?
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C6 C5 C8 117.5(8) . . ?
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N1 C8 H16 126(5) . . ?
C5 C8 H16 112(5) . . ?
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O3 C9 C10 120.4(6) . . ?
O4 C9 C10 118.4(6) 7_656 . ?
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C10 C9 Nd1 176.2(4) . . ?
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C15 C10 C9 120.0(5) . . ?
C11 C10 C9 121.1(6) . . ?
C10 C11 C12 119.0(6) . . ?
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C13 C12 N1 123.7(6) . 3_455 ?
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C10 C15 H15 119.0 . . ?
O6 C16 O5 126.8(7) 7_656 . ?
O6 C16 C14 118.2(6) 7_656 6_566 ?
O5 C16 C14 115.0(6) . 6_566 ?
O7 C17 C18 117.3(12) . . ?
O7 C17 C19 129.0(12) . . ?
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H19B C19 H19C 109.5 . . ?
O8 C20 C22 141(2) . . ?
O8 C20 C21 115(2) . . ?
C22 C20 C21 102.1(15) . . ?
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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P=(Fo^2^+2Fc^2^)/3'
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d . . .
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d . . .
O4 O 0.76934(13) 0.1501(2) 0.0338(3) 0.0405(9) Uani 1 1 d . . .
O5 O 0.76772(14) 0.3185(3) 0.1802(4) 0.0530(12) Uani 1 1
d . . .
O6 O 0.80364(14) 0.2502(3) -0.1229(3) 0.0488(11) Uani 1 1
d . . .
O7 O 0.8563(2) 0.2059(4) 0.2278(5) 0.0809(17) Uani 1 1 d U . .
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d . . .
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d . . .
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N4 N 0.87396(19) 0.5478(4) 0.2983(4) 0.0515(13) Uani 1 1 d
D . .
N5 N 0.8510(2) 0.3986(4) 0.3576(5) 0.0696(17) Uani 1 1 d . . .
C1 C 0.9060(2) 0.2630(4) -0.0066(5) 0.0463(15) Uani 1 1 d . . .
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d . . .
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d . . .
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N4 0.059(3) 0.045(3) 0.060(3) -0.010(3) 0.034(3) -0.014(3)
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C17 0.041(3) 0.043(3) 0.058(4) 0.001(3) 0.026(3) -0.001(3)
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esds are taken
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
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l.s. planes.
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
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Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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Cryst</i>.
<b>30</b>, 565.

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Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0911P)^2^+8.6637P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
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_refine_ls_shift/su_max           0.001
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d U . .
N1 N 0.5975(2) 0.0682(5) -0.1527(5) 0.0587(18) Uani 1 1 d U . .
O1 O 0.38405(17) 0.1793(4) 0.0247(4) 0.0568(14) Uani 1 1 d U
B .
O2 O 0.39105(16) 0.3149(3) -0.0329(4) 0.0530(14) Uani 1 1 d U
B .
O3 O 0.29879(16) 0.2246(3) -0.1278(4) 0.0375(11) Uani 1 1 d U
B .
O4 O 0.27215(14) 0.3441(3) 0.1635(3) 0.0410(11) Uani 1 1 d
U . .
O5 O 0.29537(14) 0.4192(3) -0.0662(4) 0.0455(12) Uani 1 1 d U
B .
O6 O 0.26773(14) 0.1581(3) 0.0496(3) 0.0349(10) Uani 1 1 d
U . .
O8 O 0.3654(2) 0.4112(4) 0.1375(5) 0.0793(19) Uani 1 1 d U B .
C1 C 0.4052(2) 0.2370(6) -0.0194(6) 0.0458(18) Uani 1 1 d U B .
C2 C 0.4495(2) 0.2105(5) -0.0576(7) 0.0498(19) Uani 1 1 d U . .
C3 C 0.4627(3) 0.1233(6) -0.0629(9) 0.087(3) Uani 1 1 d U B .
H3 H 0.4428 0.0787 -0.0462 0.104 Uiso 1 1 calc R . .
C4 C 0.5054(3) 0.1001(7) -0.0929(9) 0.088(3) Uani 1 1 d U . .
H4 H 0.5142 0.0406 -0.0955 0.106 Uiso 1 1 calc R B .
C5 C 0.5349(3) 0.1675(6) -0.1190(7) 0.061(2) Uani 1 1 d U B .
C6 C 0.5211(3) 0.2537(6) -0.1183(10) 0.084(3) Uani 1 1 d U . .
H6 H 0.5405 0.2981 -0.1374 0.101 Uiso 1 1 calc R B .
C7 C 0.4784(3) 0.2769(6) -0.0897(10) 0.087(4) Uani 1 1 d U B .
H7 H 0.4689 0.3362 -0.0916 0.104 Uiso 1 1 calc R . .
C8 C 0.5812(3) 0.1457(6) -0.1469(7) 0.064(2) Uani 1 1 d DU . .
H16 H 0.588(3) 0.190(4) -0.194(5) 0.077 Uiso 1 1 d D . .
C9 C 0.2710(2) 0.1667(4) -0.1723(5) 0.0367(15) Uani 1 1 d U . .
C10 C 0.2899(2) 0.1056(4) -0.2453(5) 0.0331(14) Uani 1 1 d U
B .
C11 C 0.3372(2) 0.1138(4) -0.2591(5) 0.0408(16) Uani 1 1 d
U . .
H11 H 0.3567 0.1568 -0.2227 0.049 Uiso 1 1 calc R B .
C12 C 0.3552(2) 0.0582(5) -0.3268(6) 0.0447(17) Uani 1 1 d
U . .
C13 C 0.3271(2) -0.0100(5) -0.3757(5) 0.0410(16) Uani 1 1 d
U . .
H13 H 0.3398 -0.0507 -0.4162 0.049 Uiso 1 1 calc R B .
C14 C 0.2800(2) -0.0171(4) -0.3637(5) 0.0325(14) Uani 1 1 d
U . .
C15 C 0.2617(2) 0.0405(4) -0.3002(5) 0.0343(14) Uani 1 1 d
U . .
H15 H 0.2299 0.0357 -0.2939 0.041 Uiso 1 1 calc R B .
```

```
C16 C 0.2514(2) 0.4112(4) -0.0800(5) 0.0324(14) Uani 1 1 d
U . .
S1 S 0.3663(5) 0.0913(10) 0.3873(10) 0.266(5) Uani 0.65 1 d
PDU B .
C18 C 0.3720(15) 0.2085(11) 0.416(3) 0.240(8) Uani 0.65 1 d
PDU B .
H18A H 0.3591 0.2267 0.4756 0.288 Uiso 0.65 1 calc PR . .
H18B H 0.4037 0.2325 0.4176 0.288 Uiso 0.65 1 calc PR . .
C17 C 0.3379(14) 0.221(3) 0.314(3) 0.229(9) Uani 0.65 1 d
PDU . .
H17A H 0.3147 0.1731 0.3102 0.275 Uiso 0.65 1 calc PRD A 1
H17B H 0.3208 0.2757 0.3200 0.275 Uiso 0.65 1 calc PRD A 1
O7A O 0.3508(6) 0.2237(17) 0.2191(14) 0.055(4) Uani 0.65 1 d
PU B 1
O7B O 0.3644(11) 0.219(3) 0.203(3) 0.048(7) Uani 0.35 1 d PU B
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0.00015(12)
N1 0.039(3) 0.060(4) 0.088(5) 0.026(4) 0.037(3) 0.016(3)
O1 0.037(3) 0.053(3) 0.089(4) 0.027(3) 0.035(3) 0.020(2)
O2 0.033(3) 0.044(3) 0.090(4) -0.001(3) 0.034(3) -0.004(2)
O3 0.033(2) 0.042(3) 0.042(3) -0.014(2) 0.018(2) -0.006(2)
O4 0.025(2) 0.053(3) 0.050(3) -0.018(2) 0.0201(19) -0.003(2)
O5 0.029(2) 0.032(2) 0.079(3) 0.015(2) 0.019(2) 0.004(2)
O6 0.028(2) 0.032(2) 0.049(3) 0.005(2) 0.0169(19) 0.0024(18)
O8 0.064(3) 0.071(4) 0.106(5) -0.034(4) 0.024(3) -0.030(3)
C1 0.021(3) 0.060(5) 0.059(5) -0.003(4) 0.015(3) -0.003(3)
C2 0.029(4) 0.054(5) 0.072(5) 0.005(4) 0.022(3) 0.006(3)
C3 0.058(5) 0.067(6) 0.153(10) 0.037(6) 0.068(6) 0.022(5)
C4 0.070(6) 0.065(6) 0.148(10) 0.039(6) 0.069(6) 0.024(5)
C5 0.047(4) 0.054(5) 0.087(6) 0.011(5) 0.028(4) 0.008(4)
C6 0.062(6) 0.053(5) 0.158(10) 0.013(6) 0.073(6) 0.003(5)
C7 0.061(6) 0.056(6) 0.164(11) 0.012(6) 0.076(7) -0.001(4)
C8 0.047(4) 0.071(6) 0.084(6) 0.022(5) 0.038(4) 0.015(4)
C9 0.038(3) 0.038(4) 0.039(4) 0.002(3) 0.018(3) -0.001(3)
C10 0.032(3) 0.030(3) 0.043(4) -0.005(3) 0.020(3) -0.011(3)
C11 0.034(3) 0.040(4) 0.053(4) -0.015(3) 0.018(3) -0.011(3)
C12 0.029(3) 0.046(4) 0.067(5) -0.014(4) 0.030(3) -0.009(3)
C13 0.033(3) 0.038(4) 0.059(4) -0.013(3) 0.026(3) -0.005(3)
C14 0.028(3) 0.030(3) 0.045(4) -0.005(3) 0.019(3) -0.004(3)
C15 0.025(3) 0.039(4) 0.042(4) -0.001(3) 0.016(3) 0.004(3)
C16 0.027(3) 0.033(3) 0.042(4) 0.003(3) 0.018(3) 0.000(3)
S1 0.294(7) 0.250(6) 0.249(7) 0.009(4) 0.032(5) -0.016(5)
C18 0.241(10) 0.241(8) 0.237(9) 0.002(5) 0.043(5) 0.002(5)
C17 0.228(10) 0.234(9) 0.227(9) -0.007(5) 0.045(5) 0.005(5)
O7A 0.049(11) 0.078(8) 0.039(8) -0.002(6) 0.014(6) 0.029(8)
O7B 0.034(15) 0.073(13) 0.045(12) -0.019(10) 0.025(9) 0.019(12)
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```
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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 O1 2.500(5) . ?
Nd1 O7B 2.51(4) . ?
Nd1 O8 2.515(5) . ?
Nd1 O7A 2.54(2) . ?
Nd1 O6 2.682(4) 7 ?
Nd1 C1 2.837(7) . ?
Nd1 C16 2.957(6) . ?
N1 C8 1.259(10) . ?
N1 C12 1.434(8) 2_654 ?
O1 C1 1.258(9) . ?
O2 C1 1.239(9) . ?
O3 C9 1.252(8) . ?
O4 C9 1.268(7) 7 ?
O5 C16 1.242(7) . ?
O6 C16 1.273(7) 7 ?
O6 Nd1 2.682(4) 7 ?
C1 C2 1.497(9) . ?
C2 C3 1.366(11) . ?
C2 C7 1.407(11) . ?
C3 C4 1.394(11) . ?
C3 H3 0.9300 . ?
C4 C5 1.398(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.352(12) . ?
C5 C8 1.471(10) . ?
C6 C7 1.384(11) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
```

```
C8 H16 0.95(2) . ?
C9 O4 1.268(7) 7 ?
C9 C10 1.504(9) . ?
C10 C15 1.386(9) . ?
C10 C11 1.398(8) . ?
C11 C12 1.390(9) . ?
C11 H11 0.9300 . ?
C12 C13 1.387(9) . ?
C12 N1 1.434(8) 2_654 ?
C13 C14 1.385(8) . ?
C13 H13 0.9300 . ?
C14 C15 1.375(8) . ?
C14 C16 1.510(8) 4_544 ?
C15 H15 0.9300 . ?
C16 O6 1.273(7) 7 ?
C16 C14 1.510(8) 4_554 ?
S1 C18 1.801(3) . ?
S1 C17 2.26(4) . ?
C18 C17 1.535(5) . ?
C18 H18A 0.9700 . ?
C18 H18B 0.9700 . ?
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C17 O7B 1.77(4) . ?
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C17 H17B 0.9700 . ?

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O3 Nd1 O4 134.07(15) . . ?
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O6 Nd1 O5 124.18(14) . . ?
O4 Nd1 O5 88.45(16) . . ?
O3 Nd1 O2 76.28(17) . . ?
O6 Nd1 O2 134.71(15) . . ?
O4 Nd1 O2 142.60(16) . . ?
O5 Nd1 O2 77.30(16) . . ?
O3 Nd1 O1 73.93(18) . . ?
O6 Nd1 O1 87.87(15) . . ?
O4 Nd1 O1 143.10(17) . . ?
O5 Nd1 O1 125.83(16) . . ?
O2 Nd1 O1 52.14(17) . . ?
O3 Nd1 O7B 130.3(9) . . ?
O6 Nd1 O7B 82.8(10) . . ?
O4 Nd1 O7B 80.9(5) . . ?
O5 Nd1 O7B 149.3(11) . . ?
O2 Nd1 O7B 93.9(6) . . ?
O1 Nd1 O7B 62.6(6) . . ?
O3 Nd1 O8 140.36(19) . . ?
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```
O6 Nd1 O8 147.43(19) . . ?
O4 Nd1 O8 72.58(17) . . ?
O5 Nd1 O8 75.6(2) . . ?
O2 Nd1 O8 70.43(19) . . ?
O1 Nd1 O8 100.7(2) . . ?
O7B Nd1 O8 73.8(11) . . ?
O3 Nd1 O7A 135.5(5) . . ?
O6 Nd1 O7A 78.1(6) . . ?
O4 Nd1 O7A 70.7(3) . . ?
O5 Nd1 O7A 147.7(6) . . ?
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O8 Nd1 O7A 74.8(6) . . ?
O3 Nd1 O6 69.55(14) . 7 ?
O6 Nd1 O6 75.96(15) . 7 ?
O4 Nd1 O6 67.77(14) . 7 ?
O5 Nd1 O6 49.87(13) . 7 ?
O2 Nd1 O6 121.54(16) . 7 ?
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O7B Nd1 O6 144.1(5) . 7 ?
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O7A Nd1 O6 133.4(3) . 7 ?
O3 Nd1 C1 72.60(19) . . ?
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O1 Nd1 C1 26.3(2) . . ?
O7B Nd1 C1 78.2(5) . . ?
O8 Nd1 C1 85.7(2) . . ?
O7A Nd1 C1 89.0(3) . . ?
O6 Nd1 C1 136.59(18) 7 . ?
O3 Nd1 C16 72.95(16) . . ?
O6 Nd1 C16 101.01(15) . . ?
O4 Nd1 C16 75.90(16) . . ?
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O7B Nd1 C16 155.6(7) . . ?
O8 Nd1 C16 91.9(2) . . ?
O7A Nd1 C16 146.4(4) . . ?
O6 Nd1 C16 25.49(14) 7 . ?
C1 Nd1 C16 121.2(2) . . ?
C8 N1 C12 118.6(7) . 2_654 ?
C1 O1 Nd1 92.0(4) . . ?
C1 O2 Nd1 92.8(4) . . ?
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C9 O4 Nd1 132.1(4) 7 . ?
C16 O5 Nd1 99.5(4) . . ?
C16 O6 Nd1 162.7(4) 7 . ?
C16 O6 Nd1 89.5(3) 7 7 ?
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O2 C1 O1 122.9(6) . . ?
O2 C1 C2 118.4(6) . . ?
O1 C1 C2 118.7(7) . . ?
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O1 C1 Nd1 61.7(3) . . ?
C2 C1 Nd1 177.0(6) . . ?
C3 C2 C7 118.6(7) . . ?
C3 C2 C1 121.9(7) . . ?
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C2 C3 C4 121.2(8) . . ?
C2 C3 H3 119.4 . . ?
C4 C3 H3 119.4 . . ?
C3 C4 C5 119.1(8) . . ?
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C7 C6 H6 119.5 . . ?
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C2 C7 H7 120.0 . . ?
N1 C8 C5 125.3(8) . . ?
N1 C8 H16 119(6) . . ?
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O3 C9 O4 126.1(6) . 7 ?
O3 C9 C10 117.2(5) . . ?
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C14 C13 C12 119.6(6) . . ?
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C14 C15 C10 121.0(5) . . ?
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O5 C16 O6 120.8(6) . 7 ?
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S1 C18 H18A 114.5 . . ?
C17 C18 H18B 114.5 . . ?
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O7A C17 S1 107(2) . . ?
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C18 C17 H17A 105.9 . . ?
O7B C17 H17A 109.9 . . ?
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O7A C17 H17B 105.9 . . ?
C18 C17 H17B 105.9 . . ?
O7B C17 H17B 112.5 . . ?
S1 C17 H17B 147.2 . . ?
H17A C17 H17B 106.2 . . ?
C17 O7A Nd1 138.3(18) . . ?
C17 O7B Nd1 117.8(19) . . ?

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'C 2/c'

loop_
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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    28.5336(16)
_cell_length_b                    14.7711(8)
_cell_length_c                    13.6945(9)
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_cell_angle_beta                  98.997(7)
_cell_angle_gamma                 90.00
_cell_volume                      5700.8(6)
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_exptl_absorpt_process_details
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Diffraction)'

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Source'
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Atlas'
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 MERCURY (Bruno et al. 2002)
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_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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```

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Sheldrick, G. M. (1997). SHELXL97. University of G\"ottingen, Germany.

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;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement. R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.1053P)^2^+0.5896P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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O2 O 0.1126(2) 0.3134(4) 0.4701(5) 0.0549(17) Uani 1 1 d U . .
O3 O 0.20499(18) 0.0781(3) 0.5673(4) 0.0457(14) Uani 1 1 d
U . .
O4 O 0.23346(17) 0.3379(3) 0.4455(4) 0.0357(12) Uani 1 1 d
U . .
O5 O 0.1991(2) 0.2879(3) 0.6187(4) 0.0413(14) Uani 1 1 d U . .
O6 O 0.23117(18) 0.1430(4) 0.3511(4) 0.0453(14) Uani 1 1 d
U . .
O7 O 0.1516(3) 0.2737(5) 0.2852(6) 0.074(2) Uani 1 1 d U . .
Cl1 Cl 0.1186(4) 0.0850(12) 0.3655(11) 0.112(4) Uani 0.50 1 d
PU . .
O8 O 0.1396(10) 0.085(3) 0.371(3) 0.134(14) Uani 0.50 1 d
PU . .
N1 N -0.0971(2) 0.4381(5) 0.6538(5) 0.0450(17) Uani 1 1 d U . .
N2 N 0.0372(11) 0.2985(17) 0.2828(19) 0.284(16) Uani 1 1 d
DU . .
C1 C 0.0947(3) 0.2610(6) 0.5276(6) 0.043(2) Uani 1 1 d U . .
C2 C 0.0511(3) 0.2878(5) 0.5663(6) 0.0398(19) Uani 1 1 d U . .
C3 C 0.0230(4) 0.2237(7) 0.6018(9) 0.066(3) Uani 1 1 d U . .
H3 H 0.0327 0.1635 0.6059 0.079 Uiso 1 1 calc R . .
C4 C -0.0194(4) 0.2478(7) 0.6315(9) 0.070(3) Uani 1 1 d U . .
H4 H -0.0384 0.2037 0.6541 0.084 Uiso 1 1 calc R . .
C5 C -0.0336(3) 0.3368(6) 0.6277(6) 0.044(2) Uani 1 1 d U . .
C6 C -0.0051(3) 0.4022(6) 0.5938(6) 0.045(2) Uani 1 1 d U . .
H6 H -0.0142 0.4627 0.5927 0.055 Uiso 1 1 calc R . .
C7 C 0.0365(3) 0.3784(6) 0.5618(6) 0.050(2) Uani 1 1 d U . .
H7 H 0.0549 0.4223 0.5373 0.060 Uiso 1 1 calc R . .
C8 C -0.0801(3) 0.3580(6) 0.6557(6) 0.047(2) Uani 1 1 d DU . .
H16 H -0.094(4) 0.299(4) 0.677(8) 0.09(4) Uiso 1 1 d D . .
C9 C 0.2483(3) 0.0921(5) 0.5852(5) 0.0344(17) Uani 1 1 d U . .
C10 C 0.2803(3) 0.0237(5) 0.6429(5) 0.0352(17) Uani 1 1 d U . .
C11 C 0.3271(3) 0.0150(5) 0.6274(5) 0.0375(18) Uani 1 1 d U . .
H11 H 0.3391 0.0537 0.5838 0.045 Uiso 1 1 calc R . .
C12 C 0.3561(3) -0.0522(5) 0.6778(6) 0.0377(18) Uani 1 1 d
U . .
C13 C 0.3387(3) -0.1062(5) 0.7472(5) 0.0390(19) Uani 1 1 d
U . .
H13 H 0.3583 -0.1488 0.7832 0.047 Uiso 1 1 calc R . .
C14 C 0.2919(3) -0.0967(5) 0.7629(5) 0.0340(17) Uani 1 1 d
U . .
C15 C 0.2625(3) -0.0326(5) 0.7096(5) 0.0342(17) Uani 1 1 d
U . .
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H15 H 0.2310 -0.0274 0.7187 0.041 Uiso 1 1 calc R . .
C16 C 0.2275(3) 0.3438(5) 0.6627(5) 0.0387(18) Uani 1 1 d U . .
C17 C 0.0000 0.241(3) 0.2500 0.26(2) Uani 1 2 d SDU . .
H17 H 0.0000 0.1776 0.2500 0.312 Uiso 1 2 calc SR . .
C18 C 0.0238(7) 0.3854(13) 0.2637(18) 0.161(10) Uani 1 1 d
DU . .
H18 H 0.0437 0.4357 0.2684 0.193 Uiso 1 1 calc R . .

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0.00216(14)
O1 0.038(3) 0.037(3) 0.099(5) 0.014(3) 0.039(3) 0.006(3)
O2 0.039(3) 0.063(4) 0.072(4) 0.033(3) 0.035(3) 0.032(3)
O3 0.030(3) 0.032(3) 0.080(4) 0.019(3) 0.025(3) 0.010(2)
O4 0.034(3) 0.027(3) 0.052(3) 0.012(2) 0.024(3) 0.004(2)
O5 0.046(4) 0.041(3) 0.044(3) -0.017(2) 0.028(3) -0.015(3)
O6 0.032(3) 0.055(4) 0.055(3) -0.029(3) 0.025(3) -0.010(3)
O7 0.040(4) 0.070(5) 0.107(6) 0.031(4) -0.008(4) 0.025(3)
Cl1 0.108(9) 0.119(7) 0.115(6) -0.036(5) 0.039(7) -0.050(8)
O8 0.09(2) 0.13(2) 0.20(3) -0.119(19) 0.08(2) -0.051(18)
N1 0.035(4) 0.053(4) 0.053(4) 0.018(3) 0.025(3) 0.012(3)
N2 0.26(3) 0.37(4) 0.20(2) 0.10(2) -0.04(2) 0.10(2)
C1 0.030(4) 0.042(5) 0.061(5) 0.004(4) 0.016(4) 0.003(4)
C2 0.019(4) 0.048(5) 0.054(5) 0.001(4) 0.009(4) 0.006(3)
C3 0.045(6) 0.057(6) 0.104(8) 0.012(5) 0.038(6) 0.012(5)
C4 0.051(6) 0.053(6) 0.115(9) 0.029(6) 0.042(6) 0.014(5)
C5 0.043(5) 0.048(5) 0.045(4) 0.016(4) 0.017(4) 0.014(4)
C6 0.036(5) 0.043(5) 0.061(5) 0.010(4) 0.020(4) 0.013(4)
C7 0.035(4) 0.046(5) 0.073(6) 0.021(4) 0.029(4) 0.012(4)
C8 0.044(5) 0.047(5) 0.055(5) 0.020(4) 0.022(4) 0.016(4)
C9 0.038(4) 0.031(4) 0.039(4) 0.010(3) 0.020(4) 0.004(3)
C10 0.035(4) 0.029(4) 0.048(4) 0.008(3) 0.025(4) 0.003(3)
C11 0.039(4) 0.036(4) 0.043(4) 0.016(3) 0.027(4) 0.002(3)
C12 0.030(4) 0.038(4) 0.051(4) 0.011(4) 0.025(4) 0.011(3)
C13 0.039(4) 0.036(4) 0.049(4) 0.017(3) 0.027(4) 0.016(3)
C14 0.038(4) 0.030(4) 0.039(4) 0.011(3) 0.022(4) 0.005(3)
C15 0.031(4) 0.032(4) 0.045(4) 0.005(3) 0.024(4) 0.007(3)
C16 0.043(5) 0.033(4) 0.046(4) -0.010(3) 0.023(4) 0.000(4)
C17 0.20(4) 0.19(3) 0.37(5) 0.000 0.00(3) 0.000
C18 0.21(2) 0.117(13) 0.177(18) -0.041(14) 0.09(2) -0.019(12)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
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```
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 O3 2.483(5) . ?
Nd1 O2 2.500(5) . ?
Nd1 O1 2.534(5) . ?
Nd1 O7 2.587(8) . ?
Nd1 O4 2.660(5) 7_556 ?
Nd1 Cl1 2.775(14) . ?
Nd1 C1 2.874(8) . ?
Nd1 C9 2.937(7) . ?
O1 C1 1.254(10) . ?
O2 C1 1.268(10) . ?
O3 C9 1.237(9) . ?
O4 C9 1.260(9) 7_556 ?
O4 Nd1 2.660(5) 7_556 ?
O5 C16 1.243(9) . ?
O6 C16 1.240(9) 7_556 ?
Cl1 O8 0.59(3) . ?
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N1 C12 1.432(9) 3_455 ?
N2 C18 1.353(16) . ?
N2 C17 1.383(18) . ?
C1 C2 1.479(11) . ?
C2 C3 1.378(12) . ?
C2 C7 1.400(10) . ?
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C4 C5 1.375(13) . ?
C4 H4 0.9300 . ?
C5 C6 1.388(11) . ?
C5 C8 1.472(11) . ?
C6 C7 1.373(10) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 1.01(2) . ?
C9 O4 1.260(9) 7_556 ?
C9 C10 1.502(10) . ?
C10 C15 1.388(9) . ?
C10 C11 1.391(9) . ?
C11 C12 1.403(10) . ?
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C13 H13 0.9300 . ?
C14 C15 1.394(9) . ?
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C15 H15 0.9300 . ?
C16 O6 1.240(9) 7_556 ?
C16 C14 1.514(9) 4_556 ?
C17 N2 1.383(18) 2 ?
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O5 Nd1 O8 145.1(10) . . ?
O6 Nd1 O8 70.1(7) . . ?
O4 Nd1 O3 123.65(18) . . ?
O5 Nd1 O3 81.01(19) . . ?
O6 Nd1 O3 84.54(19) . . ?
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O4 Nd1 O2 92.14(19) . . ?
O5 Nd1 O2 74.1(2) . . ?
O6 Nd1 O2 145.2(2) . . ?
O8 Nd1 O2 99.1(8) . . ?
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O5 Nd1 O1 71.8(2) . . ?
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O8 Nd1 O1 77.2(7) . . ?
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O4 Nd1 O7 76.4(2) . . ?
O5 Nd1 O7 131.0(2) . . ?
O6 Nd1 O7 73.6(2) . . ?
O8 Nd1 O7 74.9(12) . . ?
O3 Nd1 O7 148.0(2) . . ?
O2 Nd1 O7 71.7(2) . . ?
O1 Nd1 O7 110.4(2) . . ?
O4 Nd1 O4 74.35(17) . 7_556 ?
O5 Nd1 O4 69.57(18) . 7_556 ?
O6 Nd1 O4 67.20(17) . 7_556 ?
O8 Nd1 O4 111.8(10) . 7_556 ?
O3 Nd1 O4 50.00(16) . 7_556 ?
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O1 Nd1 Cl1 68.6(3) . . ?
O7 Nd1 Cl1 73.0(4) . . ?
O4 Nd1 Cl1 121.1(4) 7_556 . ?
O4 Nd1 C1 113.7(2) . . ?
O5 Nd1 C1 70.2(2) . . ?
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O1 Nd1 C1 25.8(2) . . ?
O7 Nd1 C1 91.6(2) . . ?
O4 Nd1 C1 132.9(2) 7_556 . ?
Cl1 Nd1 C1 77.9(3) . . ?
O4 Nd1 C9 99.55(19) . . ?
O5 Nd1 C9 74.7(2) . . ?
O6 Nd1 C9 73.9(2) . . ?
O8 Nd1 C9 93.1(11) . . ?
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O4 Nd1 C9 25.41(18) 7_556 . ?
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C1 O2 Nd1 93.6(5) . . ?
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C9 O4 Nd1 89.7(4) 7_556 7_556 ?
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C16 O6 Nd1 133.3(5) 7_556 . ?
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Cl1 O8 Nd1 118(5) . . ?
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O1 C1 C2 117.9(7) . . ?
O2 C1 C2 120.1(7) . . ?
O1 C1 Nd1 61.8(4) . . ?
O2 C1 Nd1 60.2(4) . . ?
C2 C1 Nd1 177.5(6) . . ?
C3 C2 C7 119.0(7) . . ?
C3 C2 C1 120.7(7) . . ?
C7 C2 C1 120.1(7) . . ?
C2 C3 C4 120.8(9) . . ?
C2 C3 H3 119.6 . . ?
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O4 C9 C10 118.6(7) 7_556 . ?
O3 C9 Nd1 56.7(4) . . ?
O4 C9 Nd1 64.9(4) 7_556 . ?
C10 C9 Nd1 174.6(5) . . ?
C15 C10 C11 120.3(7) . . ?
C15 C10 C9 119.6(6) . . ?
C11 C10 C9 120.1(6) . . ?
C10 C11 C12 119.8(6) . . ?
C10 C11 H11 120.1 . . ?
C12 C11 H11 120.1 . . ?
C13 C12 C11 119.7(6) . . ?
C13 C12 N1 123.1(6) . 3_545 ?
C11 C12 N1 117.3(6) . 3_545 ?
C14 C13 C12 120.1(6) . . ?
C14 C13 H13 119.9 . . ?
C12 C13 H13 119.9 . . ?
C13 C14 C15 120.1(6) . . ?
C13 C14 C16 120.3(6) . 4_546 ?
C15 C14 C16 119.6(6) . 4_546 ?
C10 C15 C14 120.0(6) . . ?
C10 C15 H15 120.0 . . ?
C14 C15 H15 120.0 . . ?
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O6 C16 C14 117.9(7) 7_556 4_556 ?
O5 C16 C14 115.7(7) . 4_556 ?
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N2 C17 H17 128.2 . . ?
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N2 C18 C18 107.2(17) . 2 ?
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C18 C18 H18 126.4 2 . ?

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 '-x, y, -z+1/2'
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 'x+1/2, -y+1/2, z-1/2'

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Diffraction)'

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 MERCURY (Bruno et al. 2002)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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O1 O 0.38438(16) 0.1795(3) 0.5278(4) 0.0378(12) Uani 1 1
d . . .
O2 O 0.39270(18) 0.3220(4) 0.4850(5) 0.0550(15) Uani 1 1
d . . .
O3 O 0.29546(15) 0.4277(3) 0.4586(4) 0.0416(12) Uani 1 1
d . . .
O4 O 0.26871(14) 0.1538(3) 0.5387(3) 0.0307(10) Uani 1 1
d . . .
O5 O 0.27351(15) 0.3229(4) 0.6875(4) 0.0385(12) Uani 1 1
d . . .
O6 O 0.29869(16) 0.2418(3) 0.3661(4) 0.0341(11) Uani 1 1
d . . .
O7 O 0.3628(3) 0.2091(4) 0.7289(5) 0.071(2) Uani 1 1 d D . .
O8 O 0.3656(2) 0.4067(5) 0.6769(6) 0.082(2) Uani 1 1 d DU . .
N1 N 0.59584(17) 0.0765(4) 0.3477(5) 0.0351(13) Uani 1 1
d . . .
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C1 C 0.4056(2) 0.2405(5) 0.4894(6) 0.0338(16) Uani 1 1 d . . .
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C3 C 0.4781(3) 0.2852(5) 0.4208(8) 0.052(2) Uani 1 1 d . . .
H3 H 0.4688 0.3452 0.4227 0.063 Uiso 1 1 calc R . .
C4 C 0.5203(3) 0.2639(5) 0.3911(7) 0.047(2) Uani 1 1 d . . .
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C5 C 0.5339(2) 0.1746(5) 0.3852(5) 0.0347(16) Uani 1 1 d . . .
C6 C 0.5041(2) 0.1062(5) 0.4076(5) 0.0354(16) Uani 1 1 d . . .
H6 H 0.5123 0.0460 0.4015 0.042 Uiso 1 1 calc R . .
C7 C 0.4620(2) 0.1284(5) 0.4393(5) 0.0325(15) Uani 1 1 d . . .
H7 H 0.4422 0.0830 0.4548 0.039 Uiso 1 1 calc R . .
C8 C 0.5803(2) 0.1552(5) 0.3589(5) 0.0327(15) Uani 1 1 d . . .
C9 C 0.2508(2) 0.4168(4) 0.4356(5) 0.0288(14) Uani 1 1 d . . .
C10 C 0.2191(2) 0.4912(4) 0.3755(5) 0.0278(14) Uani 1 1 d . . .
C11 C 0.1712(2) 0.4990(4) 0.3840(5) 0.0298(14) Uani 1 1 d . . .
H11 H 0.1584 0.4576 0.4249 0.036 Uiso 1 1 calc R . .
C12 C 0.1431(2) 0.5695(5) 0.3306(5) 0.0314(15) Uani 1 1 d . . .
C13 C 0.1620(2) 0.6285(5) 0.2670(5) 0.0305(15) Uani 1 1 d . . .
H13 H 0.1429 0.6744 0.2299 0.037 Uiso 1 1 calc R . .
C14 C 0.2092(2) 0.6206(4) 0.2574(5) 0.0286(14) Uani 1 1 d . . .
C15 C 0.2378(2) 0.5528(4) 0.3144(5) 0.0287(14) Uani 1 1 d . . .
H15 H 0.2699 0.5489 0.3114 0.034 Uiso 1 1 calc R . .
C16 C 0.2292(2) 0.3151(5) 0.6884(5) 0.0310(15) Uani 1 1 d . . .
C17 C 0.3620(5) 0.2157(9) 0.8395(10) 0.101(4) Uani 1 1 d D . .
H17A H 0.3451 0.2699 0.8519 0.121 Uiso 1 1 calc R . .
H17B H 0.3945 0.2189 0.8838 0.121 Uiso 1 1 calc R . .
C18 C 0.3373(6) 0.1350(11) 0.8696(14) 0.153(6) Uani 1 1 d
DU . .
H18A H 0.3352 0.1398 0.9442 0.229 Uiso 1 1 calc R . .
H18B H 0.3551 0.0818 0.8606 0.229 Uiso 1 1 calc R . .
H18C H 0.3057 0.1311 0.8236 0.229 Uiso 1 1 calc R . .
C19 C 0.3595(8) 0.4308(18) 0.7841(11) 0.251(8) Uani 1 1 d
DU . .
H19A H 0.3604 0.3697 0.8119 0.301 Uiso 1 1 calc R . .
H19B H 0.3255 0.4438 0.7618 0.301 Uiso 1 1 calc R . .
C20 C 0.3676(6) 0.4767(12) 0.8928(11) 0.177(6) Uani 1 1 d
DU . .
H20A H 0.3945 0.5169 0.9013 0.265 Uiso 1 1 calc R . .
H20B H 0.3740 0.4322 0.9496 0.265 Uiso 1 1 calc R . .
H20C H 0.3395 0.5104 0.8971 0.265 Uiso 1 1 calc R . .
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0.00060(14)
O1 0.028(2) 0.040(3) 0.055(3) 0.011(2) 0.028(2) 0.010(2)
O2 0.040(3) 0.041(3) 0.099(5) -0.009(3) 0.046(3) -0.007(3)
O3 0.023(2) 0.035(3) 0.070(3) 0.001(3) 0.018(2) -0.004(2)
O4 0.024(2) 0.031(2) 0.042(3) 0.000(2) 0.0174(19) 0.0042(19)
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O5 0.023(2) 0.057(3) 0.041(3) -0.013(2) 0.018(2) 0.002(2)
O6 0.028(3) 0.039(3) 0.040(3) -0.005(2) 0.018(2) -0.002(2)
O7 0.099(5) 0.069(5) 0.039(3) -0.003(3) 0.007(3) 0.015(4)
O8 0.058(4) 0.091(5) 0.097(5) -0.015(4) 0.016(4) -0.039(4)
N1 0.018(3) 0.042(3) 0.051(3) 0.005(3) 0.020(2) 0.003(3)
C1 0.023(3) 0.032(4) 0.050(4) -0.003(3) 0.014(3) 0.000(3)
C2 0.019(3) 0.045(4) 0.039(4) 0.004(3) 0.012(3) -0.001(3)
C3 0.035(4) 0.036(4) 0.096(7) 0.001(4) 0.036(4) 0.006(3)
C4 0.034(4) 0.042(4) 0.074(6) -0.001(4) 0.034(4) -0.001(4)
C5 0.025(3) 0.044(4) 0.039(4) -0.001(3) 0.015(3) 0.002(3)
C6 0.019(3) 0.039(4) 0.050(4) -0.004(3) 0.013(3) 0.004(3)
C7 0.021(3) 0.037(4) 0.044(4) 0.004(3) 0.016(3) 0.002(3)
C8 0.021(3) 0.039(4) 0.042(4) 0.006(3) 0.016(3) 0.001(3)
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C10 0.020(3) 0.033(4) 0.034(3) -0.002(3) 0.014(3) 0.001(3)
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C12 0.022(3) 0.042(4) 0.034(4) -0.006(3) 0.015(3) -0.006(3)
C13 0.023(3) 0.039(4) 0.033(3) 0.005(3) 0.012(3) 0.008(3)
C14 0.022(3) 0.033(4) 0.034(3) -0.006(3) 0.014(3) 0.002(3)
C15 0.018(3) 0.038(4) 0.033(3) -0.003(3) 0.012(2) -0.002(3)
C16 0.025(3) 0.040(4) 0.032(4) 0.001(3) 0.016(3) 0.001(3)
C17 0.101(10) 0.133(13) 0.068(8) 0.003(7) 0.017(7) -0.014(8)
C18 0.161(8) 0.153(8) 0.145(7) 0.000(5) 0.034(5) -0.012(5)
C19 0.265(10) 0.262(10) 0.231(8) -0.024(5) 0.070(5) 0.005(5)
C20 0.182(8) 0.180(8) 0.170(7) -0.011(5) 0.046(5) 0.004(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 C1 2.854(6) . ?
Nd1 C9 2.952(6) . ?
Nd1 Nd1 4.0772(6) 7_556 ?
O1 C1 1.250(8) . ?
O2 C1 1.261(9) . ?
O3 C9 1.255(7) . ?
O4 C9 1.265(7) 7_556 ?
O4 Nd1 2.710(4) 7_556 ?
O5 C16 1.279(7) . ?
O6 C16 1.253(8) 7_556 ?
O7 C17 1.405(13) . ?
O8 C19 1.450(5) . ?
N1 C8 1.269(9) . ?
N1 C12 1.424(7) 3_545 ?
C1 C2 1.512(9) . ?
C2 C7 1.377(9) . ?
C2 C3 1.386(10) . ?
C3 C4 1.385(10) . ?
C3 H3 0.9300 . ?
C4 C5 1.387(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.397(9) . ?
C5 C8 1.473(8) . ?
C6 C7 1.396(8) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.90(8) . ?
C9 O4 1.265(7) 7_556 ?
C9 C10 1.516(9) . ?
C10 C15 1.382(8) . ?
C10 C11 1.406(8) . ?
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C12 N1 1.424(7) 3_455 ?
C13 C14 1.390(8) . ?
C13 H13 0.9300 . ?
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C15 H15 0.9300 . ?
C16 O6 1.253(8) 7_556 ?
C16 C14 1.491(9) 6_566 ?
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C17 H17B 0.9700 . ?
C18 H18A 0.9600 . ?
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C18 H18C 0.9600 . ?
C19 C20 1.502(5) . ?
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C20 H20B 0.9600 . ?
C20 H20C 0.9600 . ?
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O5 Nd1 O6 133.23(15) . . ?
O4 Nd1 O6 71.60(15) . . ?
O5 Nd1 O3 90.29(16) . . ?
O4 Nd1 O3 122.86(14) . . ?
O6 Nd1 O3 75.45(16) . . ?
O5 Nd1 O7 75.6(2) . . ?
O4 Nd1 O7 83.55(19) . . ?
O6 Nd1 O7 134.67(18) . . ?
O3 Nd1 O7 147.95(18) . . ?
O5 Nd1 O1 141.94(16) . . ?
O4 Nd1 O1 86.33(14) . . ?
O6 Nd1 O1 73.43(16) . . ?
O3 Nd1 O1 126.35(15) . . ?
O7 Nd1 O1 67.57(19) . . ?
O5 Nd1 O8 73.42(19) . . ?
O4 Nd1 O8 148.70(18) . . ?
O6 Nd1 O8 139.55(19) . . ?
O3 Nd1 O8 74.7(2) . . ?
O7 Nd1 O8 73.7(2) . . ?
O1 Nd1 O8 103.9(2) . . ?
O5 Nd1 O2 146.08(18) . . ?
O4 Nd1 O2 132.56(16) . . ?
O6 Nd1 O2 74.85(18) . . ?
O3 Nd1 O2 78.18(17) . . ?
O7 Nd1 O2 97.6(2) . . ?
O1 Nd1 O2 52.10(16) . . ?
O8 Nd1 O2 72.8(2) . . ?
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
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factors based
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on F, and R-
 factors based on ALL data will be even larger.
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C18 0.267(18) 0.263(18) 0.263(18) 0.001(5) 0.055(6) 0.006(5)
C19 0.259(16) 0.259(16) 0.254(16) 0.000(5) 0.058(6) -0.001(5)
C20 0.051(4) 0.051(4) 0.046(4) -0.011(3) 0.011(3) -0.011(3)
C21 0.39(3) 0.39(3) 0.38(3) 0.000(5) 0.085(8) -0.005(5)
C22 0.34(2) 0.33(2) 0.33(2) 0.001(5) 0.076(7) -0.005(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 N2 2.551(10) . ?
Nd1 N4 2.588(7) . ?
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Nd1 C1 2.852(7) . ?
Nd1 C16 2.943(7) . ?
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O3 C9 1.256(9) . ?
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O5 C16 1.274(8) 7_556 ?
O5 Nd1 2.684(5) 7_556 ?
O6 C16 1.239(8) . ?
N1 C8 1.229(11) . ?
N1 C12 1.442(8) 2_556 ?
N2 C17 1.352(5) . ?
N2 C18 1.353(5) . ?
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N4 C22 1.349(3) . ?
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N5 C21 1.349(3) . ?
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C2 C3 1.368(12) . ?
C2 C7 1.374(12) . ?
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C4 H4 0.9300 . ?
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C7 H7 0.9300 . ?
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C16 C14 1.503(9) 4_546 ?
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N4 Nd1 O5 108.8(2) . 7_556 ?
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C3 C4 H4 120.4 . . ?
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C2 C7 H7 119.8 . . ?
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N1 C8 H16 122(4) . . ?
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O4 C9 C10 116.5(7) 7_556 . ?
O3 C9 C10 117.0(6) . . ?
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O5 C16 C14 118.0(6) 7_556 4_546 ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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d . . .
O3 O 0.22860(11) -0.1376(3) 0.4809(2) 0.0116(7) Uani 1 1
d . . .
O4 O 0.28518(12) -0.0280(3) 0.4668(2) 0.0162(8) Uani 1 1
d . . .
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O6 O 0.20196(12) 0.2746(3) 0.1347(2) 0.0146(8) Uani 1 1 d . . .
O7 O 0.35998(13) -0.2785(3) 0.6748(3) 0.0192(8) Uani 1 1
d . . .
O8 O 0.06464(17) 0.8981(4) 0.3482(5) 0.0677(18) Uani 1 1
d . . .
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N2 N 0.34562(15) -0.0399(3) 0.6410(3) 0.0169(10) Uani 1 1
d . . .
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N4 N 0.20139(19) 0.7264(4) 0.0332(4) 0.0336(13) Uani 1 1
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d . . .
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C7 C 0.47515(19) -0.1646(5) 0.4267(4) 0.0250(13) Uani 1 1
d . . .
H7 H 0.4666 -0.0960 0.4416 0.030 Uiso 1 1 calc R . .
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C9 C 0.24437(17) -0.0528(4) 0.4485(3) 0.0143(11) Uani 1 1
d . . .
C10 C 0.21477(17) 0.0202(4) 0.3871(3) 0.0127(10) Uani 1 1
d . . .
C11 C 0.16890(17) 0.0257(4) 0.3968(3) 0.0145(11) Uani 1 1
d . . .
H11 H 0.1562 -0.0178 0.4403 0.017 Uiso 1 1 calc R . .
C12 C 0.14192(17) 0.0973(4) 0.3404(3) 0.0146(11) Uani 1 1
d . . .
C13 C 0.16102(17) 0.1548(4) 0.2699(3) 0.0131(11) Uani 1 1
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H13 H 0.1428 0.1985 0.2293 0.016 Uiso 1 1 calc R . .
C14 C 0.20618(17) 0.1481(4) 0.2594(3) 0.0121(11) Uani 1 1
d . . .
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C15 C 0.23381(17) 0.0820(4) 0.3195(3) 0.0128(11) Uani 1 1
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d . . .
C17 C 0.3200(2) 0.0257(4) 0.6850(4) 0.0207(12) Uani 1 1 d . . .
H17 H 0.2894 0.0360 0.6681 0.025 Uiso 1 1 calc R . .
C18 C 0.3873(2) 0.0403(4) 0.7599(4) 0.0256(14) Uani 1 1 d . . .
H18 H 0.4117 0.0603 0.8023 0.031 Uiso 1 1 calc R . .
C19 C 0.38747(19) -0.0306(5) 0.6871(4) 0.0237(13) Uani 1 1
d . . .
H19 H 0.4127 -0.0675 0.6713 0.028 Uiso 1 1 calc R . .
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H20 H 0.2491 0.8463 0.0636 0.027 Uiso 1 1 calc R . .
C21 C 0.1633(2) 0.7077(5) 0.0706(4) 0.0299(16) Uani 1 1 d . . .
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0.0022(16)
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0.0043(15)
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 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 Nd1 4.0902(5) 7_546 ?
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_computing_cell_refinement         'CrysAlis RED'
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_computing_structure_solution      'SHELXL-97 (Sheldrick,
1997)'
_computing_structure_refinement    'SHELXL-97 (Sheldrick,
1997)'
_computing_molecular_graphics
;
 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;
```

```
_computing_publication_material   'WINGX (Farrugia, 1999)'
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0991P)^2^+26.7037P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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_refine_ls_R_factor_gt            0.0578
_refine_ls_wR_factor_ref          0.1664
_refine_ls_wR_factor_gt           0.1548
_refine_ls_goodness_of_fit_ref    1.058
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d . . .
O1 O 0.3945(2) 0.1682(5) 0.0034(6) 0.0537(18) Uani 1 1 d . . .
O2 O 0.3870(2) 0.3174(5) 0.0338(7) 0.059(2) Uani 1 1 d . . .
O3 O 0.2980(2) 0.0651(5) -0.0176(6) 0.0475(15) Uani 1 1 d . . .
O4 O 0.23200(18) 0.1502(4) -0.0301(5) 0.0345(12) Uani 1 1
d . . .
O5 O 0.2756(2) 0.1905(5) 0.2023(5) 0.0430(15) Uani 1 1 d . . .
O6 O 0.2989(2) 0.2459(4) -0.1329(5) 0.0405(14) Uani 1 1 d . . .
O7 O 0.3651(3) 0.3099(6) 0.2406(7) 0.071(2) Uani 1 1 d . . .
O8 O 0.3713(3) 0.1035(6) 0.2066(7) 0.074(2) Uani 1 1 d . . .
O9 O 0.4471(2) 0.4156(6) 0.2348(8) 0.073(2) Uani 1 1 d . . .
N1 N 0.5960(2) 0.4093(6) -0.1490(6) 0.0427(18) Uani 1 1 d . . .
C1 C 0.4078(3) 0.2526(7) -0.0016(8) 0.044(2) Uani 1 1 d . . .
C2 C 0.4508(3) 0.2704(7) -0.0454(9) 0.048(2) Uani 1 1 d . . .
C3 C 0.4641(3) 0.3617(8) -0.0543(8) 0.047(2) Uani 1 1 d . . .
H3 H 0.4452 0.4089 -0.0377 0.057 Uiso 1 1 calc R . .
C4 C 0.5058(3) 0.3828(7) -0.0882(8) 0.049(2) Uani 1 1 d . . .
H4 H 0.5142 0.4438 -0.0964 0.059 Uiso 1 1 calc R . .
C5 C 0.5342(3) 0.3117(7) -0.1091(8) 0.044(2) Uani 1 1 d . . .
C6 C 0.5203(4) 0.2196(8) -0.1027(11) 0.063(3) Uani 1 1 d . . .
H6 H 0.5387 0.1720 -0.1205 0.076 Uiso 1 1 calc R . .
C7 C 0.4787(4) 0.2010(8) -0.0691(11) 0.064(3) Uani 1 1 d . . .
H7 H 0.4696 0.1402 -0.0628 0.077 Uiso 1 1 calc R . .
C8 C 0.5810(3) 0.3282(7) -0.1357(8) 0.044(2) Uani 1 1 d . . .
C9 C 0.2519(3) 0.0765(6) -0.0504(8) 0.040(2) Uani 1 1 d . . .
C10 C 0.2204(3) 0.0002(6) -0.1123(7) 0.0381(19) Uani 1 1
d . . .
C11 C 0.1720(3) -0.0080(6) -0.1091(7) 0.0364(18) Uani 1 1
d . . .
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H11 H 0.1587 0.0356 -0.0711 0.044 Uiso 1 1 calc R . .
C12 C 0.1438(3) -0.0820(7) -0.1632(7) 0.040(2) Uani 1 1 d . . .
C13 C 0.1621(3) -0.1428(7) -0.2282(7) 0.0394(19) Uani 1 1
d . . .
H13 H 0.1423 -0.1897 -0.2683 0.047 Uiso 1 1 calc R . .
C14 C 0.2103(3) -0.1334(6) -0.2331(7) 0.0351(18) Uani 1 1
d . . .
C15 C 0.2393(3) -0.0636(6) -0.1725(7) 0.0361(18) Uani 1 1
d . . .
H15 H 0.2719 -0.0594 -0.1720 0.043 Uiso 1 1 calc R . .
C16 C 0.2303(3) 0.1976(6) 0.1944(7) 0.0353(18) Uani 1 1 d . . .
C17 C 0.3564(11) 0.330(2) 0.3422(18) 0.198(13) Uani 1 1 d U . .
H17A H 0.3823 0.3684 0.3868 0.297 Uiso 1 1 calc R . .
H17B H 0.3550 0.2741 0.3825 0.297 Uiso 1 1 calc R . .
H17C H 0.3257 0.3621 0.3281 0.297 Uiso 1 1 calc R . .
H16 H 0.602(4) 0.278(7) -0.112(9) 0.05(3) Uiso 1 1 d . . .

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Nd1 0.0208(2) 0.0378(3) 0.0472(3) 0.0016(2) 0.02308(18) -
0.00091(18)
O1 0.037(3) 0.052(4) 0.090(5) 0.014(4) 0.047(3) 0.005(3)
O2 0.042(3) 0.066(4) 0.090(5) -0.021(4) 0.053(4) -0.014(3)
O3 0.027(3) 0.045(4) 0.079(4) -0.003(3) 0.028(3) -0.005(3)
O4 0.027(2) 0.035(3) 0.052(3) 0.000(3) 0.029(2) -0.003(2)
O5 0.026(3) 0.069(4) 0.045(3) 0.008(3) 0.029(2) 0.002(3)
O6 0.035(3) 0.046(3) 0.049(3) 0.006(3) 0.026(3) 0.003(3)
O7 0.067(5) 0.080(6) 0.058(4) -0.001(4) 0.008(4) -0.033(4)
O8 0.071(5) 0.084(6) 0.076(5) 0.020(5) 0.036(4) 0.034(5)
O9 0.035(3) 0.061(5) 0.122(7) -0.004(5) 0.023(4) -0.004(3)
N1 0.026(3) 0.057(5) 0.056(4) -0.003(4) 0.028(3) -0.002(3)
C1 0.028(4) 0.061(6) 0.050(5) 0.016(5) 0.023(4) -0.006(4)
C2 0.029(4) 0.061(6) 0.064(6) 0.005(5) 0.029(4) -0.002(4)
C3 0.031(4) 0.067(7) 0.053(5) -0.002(5) 0.027(4) -0.001(4)
C4 0.035(4) 0.055(6) 0.068(6) -0.002(5) 0.033(4) -0.006(4)
C5 0.031(4) 0.052(5) 0.061(5) 0.002(5) 0.032(4) 0.002(4)
C6 0.049(6) 0.060(7) 0.098(9) 0.008(6) 0.048(6) -0.001(5)
C7 0.050(6) 0.060(7) 0.101(9) 0.001(6) 0.050(6) -0.002(5)
C8 0.030(4) 0.057(6) 0.056(5) 0.007(5) 0.029(4) 0.003(4)
C9 0.032(4) 0.043(5) 0.059(5) -0.001(4) 0.035(4) -0.001(4)
C10 0.025(4) 0.040(5) 0.057(5) 0.002(4) 0.025(4) -0.003(4)
C11 0.027(4) 0.035(4) 0.057(5) 0.002(4) 0.028(4) 0.003(3)
C12 0.025(4) 0.050(5) 0.053(5) 0.003(4) 0.027(4) -0.001(4)
C13 0.026(4) 0.051(5) 0.049(5) -0.006(4) 0.023(3) -0.006(4)
C14 0.023(3) 0.044(5) 0.047(4) 0.002(4) 0.023(3) 0.000(3)
C15 0.029(4) 0.037(4) 0.052(5) 0.005(4) 0.026(3) 0.004(3)
C16 0.028(4) 0.048(5) 0.035(4) 0.001(4) 0.017(3) 0.002(4)
C17 0.25(3) 0.26(3) 0.099(14) -0.017(18) 0.065(17) -0.12(2)

_geom_special_details
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;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

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Nd1 O4 2.421(6) 7 ?
Nd1 O6 2.430(6) . ?
Nd1 O3 2.473(7) . ?
Nd1 O8 2.483(8) . ?
Nd1 O7 2.490(8) . ?
Nd1 O2 2.491(6) . ?
Nd1 O1 2.537(6) . ?
Nd1 O4 2.689(5) . ?
Nd1 C1 2.874(8) . ?
Nd1 C9 2.947(9) . ?
Nd1 Nd1 4.0774(9) 7 ?
O1 C1 1.290(12) . ?
O2 C1 1.255(12) . ?
O3 C9 1.271(10) . ?
O4 C9 1.268(10) . ?
O4 Nd1 2.421(6) 7 ?
O5 C16 1.269(10) . ?
O6 C16 1.254(11) 7 ?
O7 C17 1.37(2) . ?
N1 C8 1.278(13) . ?
N1 C12 1.429(9) 3 ?
C1 C2 1.496(11) . ?
C2 C7 1.364(15) . ?
C2 C3 1.392(14) . ?
C3 C4 1.402(11) . ?
C3 H3 0.9300 . ?
C4 C5 1.381(13) . ?
C4 H4 0.9300 . ?
C5 C6 1.403(15) . ?
C5 C8 1.483(10) . ?
C6 C7 1.391(14) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.93(11) . ?
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C9 C10 1.490(12) . ?
C10 C15 1.388(12) . ?
C10 C11 1.396(10) . ?
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C11 H11 0.9300 . ?
C12 C13 1.390(12) . ?
C12 N1 1.429(9) 3_445 ?
C13 C14 1.399(10) . ?
C13 H13 0.9300 . ?
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C14 C16 1.510(11) 6 ?
C15 H15 0.9300 . ?
C16 O6 1.254(11) 7 ?
C16 C14 1.510(11) 6_556 ?
C17 H17A 0.9600 . ?
C17 H17B 0.9600 . ?
C17 H17C 0.9600 . ?

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O5 Nd1 O6 133.1(2) . . ?
O4 Nd1 O6 71.75(19) 7 . ?
O5 Nd1 O3 90.7(2) . . ?
O4 Nd1 O3 122.8(2) 7 . ?
O6 Nd1 O3 75.1(2) . . ?
O5 Nd1 O8 75.4(2) . . ?
O4 Nd1 O8 150.4(2) 7 . ?
O6 Nd1 O8 137.8(2) . . ?
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O3 Nd1 O7 149.0(3) . . ?
O8 Nd1 O7 75.3(3) . . ?
O5 Nd1 O2 143.1(2) . . ?
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O3 Nd1 O2 124.6(2) . . ?
O8 Nd1 O2 101.9(3) . . ?
O7 Nd1 O2 68.1(3) . . ?
O5 Nd1 O1 146.2(2) . . ?
O4 Nd1 O1 133.37(19) 7 . ?
O6 Nd1 O1 73.7(2) . . ?
O3 Nd1 O1 75.7(2) . . ?
O8 Nd1 O1 71.1(2) . . ?
O7 Nd1 O1 100.1(3) . . ?
O2 Nd1 O1 52.4(2) . . ?
O5 Nd1 O4 67.23(19) . . ?
O4 Nd1 O4 74.3(2) 7 . ?
```

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O5 Nd1 C1 156.8(2) . . ?
O4 Nd1 C1 110.1(2) 7 . ?
O6 Nd1 C1 69.9(2) . . ?
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O5 Nd1 C9 78.5(2) . . ?
O4 Nd1 C9 98.6(2) 7 . ?
O6 Nd1 C9 69.9(2) . . ?
O3 Nd1 C9 25.2(2) . . ?
O8 Nd1 C9 92.6(3) . . ?
O7 Nd1 C9 153.6(2) . . ?
O2 Nd1 C9 138.1(2) . . ?
O1 Nd1 C9 97.9(2) . . ?
O4 Nd1 C9 25.5(2) . . ?
C1 Nd1 C9 118.8(3) . . ?
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O4 Nd1 Nd1 39.41(13) 7 7 ?
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O8 Nd1 Nd1 138.1(2) . 7 ?
O7 Nd1 Nd1 115.1(2) . 7 ?
O2 Nd1 Nd1 119.87(19) . 7 ?
O1 Nd1 Nd1 137.82(18) . 7 ?
O4 Nd1 Nd1 34.85(12) . 7 ?
C1 Nd1 Nd1 131.99(18) . 7 ?
C9 Nd1 Nd1 59.55(17) . 7 ?
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C1 O2 Nd1 94.4(6) . . ?
C9 O3 Nd1 98.7(6) . . ?
C9 O4 Nd1 157.2(6) . 7 ?
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Nd1 O4 Nd1 105.7(2) 7 . ?
C16 O5 Nd1 132.8(5) . . ?
C16 O6 Nd1 131.9(5) 7 . ?
C17 O7 Nd1 134.9(12) . . ?
C8 N1 C12 117.5(8) . 3 ?
O2 C1 O1 121.4(7) . . ?
O2 C1 C2 121.0(9) . . ?
O1 C1 C2 117.6(9) . . ?
O2 C1 Nd1 59.8(4) . . ?
O1 C1 Nd1 61.9(4) . . ?
C2 C1 Nd1 177.0(7) . . ?
C7 C2 C3 120.0(8) . . ?
C7 C2 C1 122.5(10) . . ?
C3 C2 C1 117.4(9) . . ?
C2 C3 C4 120.2(9) . . ?
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C2 C3 H3 119.9 . . ?
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C5 C4 C3 118.9(9) . . ?
C5 C4 H4 120.5 . . ?
C3 C4 H4 120.5 . . ?
C4 C5 C6 120.9(8) . . ?
C4 C5 C8 122.2(9) . . ?
C6 C5 C8 116.9(9) . . ?
C7 C6 C5 118.6(10) . . ?
C7 C6 H6 120.7 . . ?
C5 C6 H6 120.7 . . ?
C2 C7 C6 121.2(11) . . ?
C2 C7 H7 119.4 . . ?
C6 C7 H7 119.4 . . ?
N1 C8 C5 122.1(9) . . ?
N1 C8 H16 124(7) . . ?
C5 C8 H16 109(7) . . ?
O4 C9 O3 121.8(8) . . ?
O4 C9 C10 119.4(7) . . ?
O3 C9 C10 118.7(8) . . ?
O4 C9 Nd1 65.8(4) . . ?
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C15 C10 C11 119.7(8) . . ?
C15 C10 C9 120.1(7) . . ?
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C10 C11 H11 120.3 . . ?
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C13 C12 N1 122.8(8) . 3_445 ?
C11 C12 N1 116.7(7) . 3_445 ?
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C14 C13 H13 120.1 . . ?
C15 C14 C13 119.3(7) . . ?
C15 C14 C16 120.2(7) . 6 ?
C13 C14 C16 120.5(8) . 6 ?
C14 C15 C10 121.0(7) . . ?
C14 C15 H15 119.5 . . ?
C10 C15 H15 119.5 . . ?
O6 C16 O5 125.6(8) 7 . ?
O6 C16 C14 117.5(7) 7 6_556 ?
O5 C16 C14 116.9(7) . 6_556 ?
O7 C17 H17A 109.5 . . ?
O7 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
O7 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
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 'Nd'  'Nd'  -0.1943   3.0179
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 'S'  'S'   0.1246   0.1234
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_symmetry_space_group_name_H-M    'C 2/c'

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 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_length_b                    14.4488(6)
_cell_length_c                    13.0926(5)
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_cell_angle_beta                  98.748(4)
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_cell_formula_units_Z              8
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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_diffrn_radiation_source           'SuperNova (Mo) X-ray
Source'
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Atlas'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
```

```
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.0951P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4795
_refine_ls_number_parameters      329
_refine_ls_number_restraints      57
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_refine_ls_wR_factor_ref          0.1531
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d . . .
S1 S 0.29113(17) 0.6627(3) 0.5831(3) 0.1024(13) Uani 1 1 d
U . .
S2 S 0.3996(4) 0.0756(6) 0.8614(7) 0.269(6) Uani 1 1 d U . .
N1 N 0.09556(19) 0.5786(5) 0.3577(4) 0.0268(15) Uani 1 1
d . . .
O1 O 0.38336(18) 0.1918(4) 0.5266(4) 0.0331(14) Uani 1 1
d . . .
O2 O 0.38706(16) 0.3314(4) 0.4604(4) 0.0245(11) Uani 1 1
d . . .
O3 O 0.22942(14) 0.3450(4) 0.4572(3) 0.0180(10) Uani 1 1
d . . .
O4 O 0.28958(14) 0.4351(4) 0.4527(4) 0.0224(11) Uani 1 1
d . . .
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O5 O 0.26758(15) 0.3311(4) 0.6701(3) 0.0203(11) Uani 1 1
d . . .
O6 O 0.30075(15) 0.2391(4) 0.3684(3) 0.0178(10) Uani 1 1
d . . .
O7 O 0.35899(19) 0.4184(5) 0.6478(4) 0.0397(15) Uani 1 1
d . . .
O8 O 0.3547(2) 0.2281(5) 0.7168(4) 0.0389(15) Uani 1 1 d . . .
O9 O 0.3936(4) 0.5589(11) 0.7916(9) 0.158(6) Uani 1 1 d DU . .
H9 H 0.3759 0.5598 0.8348 0.237 Uiso 1 1 calc R . .
O10 O 0.3814(8) 0.3786(13) 0.8537(9) 0.260(11) Uani 1 1 d U . .
H10 H 0.3884 0.3756 0.7955 0.390 Uiso 1 1 calc R . .
C1 C 0.4034(2) 0.2499(6) 0.4775(5) 0.0220(16) Uani 1 1 d . . .
C2 C 0.4473(2) 0.2243(6) 0.4417(5) 0.0240(17) Uani 1 1 d . . .
C3 C 0.4617(3) 0.1341(6) 0.4425(6) 0.0335(19) Uani 1 1 d . . .
H3 H 0.4431 0.0885 0.4649 0.040 Uiso 1 1 calc R . .
C4 C 0.5030(2) 0.1085(6) 0.4113(6) 0.035(2) Uani 1 1 d . . .
H4 H 0.5117 0.0465 0.4112 0.042 Uiso 1 1 calc R . .
C5 C 0.5319(2) 0.1781(6) 0.3796(6) 0.0289(18) Uani 1 1 d . . .
C6 C 0.5175(3) 0.2694(7) 0.3801(8) 0.048(3) Uani 1 1 d . . .
H6 H 0.5364 0.3158 0.3603 0.057 Uiso 1 1 calc R . .
C7 C 0.4753(3) 0.2926(6) 0.4099(7) 0.042(2) Uani 1 1 d . . .
H7 H 0.4658 0.3541 0.4085 0.050 Uiso 1 1 calc R . .
C8 C 0.5781(3) 0.1556(7) 0.3547(6) 0.0291(18) Uani 1 1 d . . .
C9 C 0.2470(2) 0.4194(5) 0.4328(5) 0.0143(13) Uani 1 1 d . . .
C10 C 0.2163(2) 0.4955(5) 0.3784(5) 0.0164(14) Uani 1 1 d . . .
C11 C 0.1697(2) 0.4999(5) 0.3891(5) 0.0181(14) Uani 1 1 d . . .
H11 H 0.1571 0.4566 0.4295 0.022 Uiso 1 1 calc R . .
C12 C 0.1418(2) 0.5699(5) 0.3387(5) 0.0194(15) Uani 1 1 d . . .
C13 C 0.1607(2) 0.3718(5) 0.7693(5) 0.0182(14) Uani 1 1 d . . .
H13 H 0.1420 0.3279 0.7314 0.022 Uiso 1 1 calc R . .
C14 C 0.2068(2) 0.3794(6) 0.7575(5) 0.0170(14) Uani 1 1 d . . .
C15 C 0.2346(2) 0.5547(5) 0.3133(5) 0.0155(14) Uani 1 1 d . . .
H15 H 0.2658 0.5506 0.3068 0.019 Uiso 1 1 calc R . .
C16 C 0.2260(2) 0.3198(5) 0.6809(5) 0.0156(15) Uani 1 1 d . . .
C17 C 0.3761(5) 0.5079(12) 0.6189(12) 0.103(6) Uani 1 1 d . . .
H17A H 0.4089 0.5035 0.6139 0.124 Uiso 1 1 calc R . .
H17B H 0.3597 0.5265 0.5520 0.124 Uiso 1 1 calc R . .
C18 C 0.3691(5) 0.5761(11) 0.6958(10) 0.088(4) Uani 1 1 d
DU . .
H18 H 0.3813 0.6344 0.6728 0.105 Uiso 1 1 calc R . .
C19 C 0.3201(5) 0.5932(10) 0.7007(10) 0.094(5) Uani 1 1 d
DU . .
H19A H 0.3173 0.6271 0.7634 0.113 Uiso 1 1 calc R . .
H19B H 0.3042 0.5345 0.7034 0.113 Uiso 1 1 calc R . .
C20 C 0.3458(5) 0.2323(14) 0.8246(10) 0.098(5) Uani 1 1 d
DU . .
H20 H 0.3151 0.2601 0.8237 0.117 Uiso 1 1 calc R . .
C21 C 0.3789(8) 0.2877(12) 0.8945(11) 0.131(8) Uani 1 1 d
DU . .
H21A H 0.3691 0.2908 0.9620 0.157 Uiso 1 1 calc R . .
H21B H 0.4093 0.2589 0.9025 0.157 Uiso 1 1 calc R . .
C22 C 0.3437(6) 0.1317(13) 0.8678(11) 0.113(6) Uani 1 1 d U . .
H22A H 0.3189 0.0973 0.8269 0.135 Uiso 1 1 calc R . .
H22B H 0.3378 0.1335 0.9387 0.135 Uiso 1 1 calc R . .
H16 H 0.592(3) 0.204(5) 0.340(6) 0.012(19) Uiso 1 1 d . . .
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0.00146(14)
S1 0.139(4) 0.066(3) 0.097(3) -0.025(2) 0.000(2) 0.003(3)
S2 0.377(13) 0.148(8) 0.219(7) -0.043(6) -0.155(8) 0.111(8)
N1 0.014(3) 0.035(4) 0.034(3) 0.010(3) 0.014(2) 0.006(3)
O1 0.023(3) 0.027(3) 0.054(3) 0.020(3) 0.021(3) 0.014(3)
O2 0.018(2) 0.019(3) 0.039(3) -0.001(2) 0.013(2) 0.001(2)
O3 0.015(2) 0.014(3) 0.027(2) 0.003(2) 0.0098(18) 0.004(2)
O4 0.009(2) 0.020(3) 0.038(3) 0.004(2) 0.0049(19) 0.001(2)
O5 0.014(2) 0.029(3) 0.020(2) -0.007(2) 0.0096(18) -0.002(2)
O6 0.013(2) 0.020(3) 0.022(2) -0.002(2) 0.0072(18) -0.003(2)
O7 0.040(3) 0.044(4) 0.036(3) -0.014(3) 0.010(2) -0.022(3)
O8 0.044(3) 0.046(4) 0.026(3) 0.002(3) 0.000(2) 0.006(3)
O9 0.098(8) 0.222(18) 0.148(10) -0.122(11) 0.003(7) -0.011(9)
O10 0.54(3) 0.139(15) 0.078(7) 0.044(9) -0.033(12) -0.109(18)
C1 0.012(3) 0.034(5) 0.020(3) 0.000(3) 0.005(3) 0.008(3)
C2 0.011(3) 0.036(5) 0.027(4) 0.001(4) 0.007(3) 0.002(3)
C3 0.027(4) 0.024(5) 0.056(5) 0.003(4) 0.026(4) 0.004(4)
C4 0.019(3) 0.028(5) 0.059(5) 0.002(4) 0.011(3) 0.006(4)
C5 0.021(4) 0.034(5) 0.033(4) 0.009(4) 0.009(3) 0.000(4)
C6 0.032(5) 0.037(6) 0.082(7) 0.029(5) 0.033(5) 0.012(5)
C7 0.033(5) 0.031(5) 0.068(6) 0.014(5) 0.027(4) 0.014(4)
C8 0.024(4) 0.031(5) 0.036(4) 0.012(4) 0.015(3) 0.009(4)
C9 0.018(3) 0.008(3) 0.018(3) -0.002(3) 0.008(2) 0.005(3)
C10 0.012(3) 0.018(4) 0.019(3) -0.003(3) 0.003(2) 0.001(3)
C11 0.019(3) 0.013(4) 0.024(3) -0.001(3) 0.007(3) 0.001(3)
C12 0.013(3) 0.025(4) 0.022(3) 0.004(3) 0.009(2) 0.001(3)
C13 0.016(3) 0.018(4) 0.021(3) -0.007(3) 0.006(2) -0.006(3)
C14 0.014(3) 0.024(4) 0.015(3) 0.001(3) 0.005(2) 0.001(3)
C15 0.011(3) 0.017(4) 0.020(3) -0.004(3) 0.009(2) 0.000(3)
C16 0.013(3) 0.018(4) 0.016(3) 0.005(3) 0.004(3) 0.002(3)
C17 0.097(10) 0.096(12) 0.130(12) -0.066(11) 0.057(9) -
0.049(10)
C18 0.103(10) 0.063(9) 0.091(9) -0.011(8) -0.004(8) -0.014(9)
C19 0.142(12) 0.065(9) 0.095(9) 0.012(8) 0.079(9) 0.011(9)
C20 0.092(10) 0.134(16) 0.064(8) 0.030(9) 0.000(7) 0.033(11)
C21 0.24(2) 0.065(11) 0.061(8) -0.012(8) -0.044(11) -0.026(12)
C22 0.158(15) 0.095(13) 0.071(8) 0.032(9) -0.026(9) -0.038(12)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
```

```
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 O5 2.396(4) . ?
Nd1 O6 2.404(4) . ?
Nd1 O4 2.447(5) . ?
Nd1 O1 2.482(5) . ?
Nd1 O7 2.488(6) . ?
Nd1 O8 2.544(5) . ?
Nd1 O2 2.548(4) . ?
Nd1 O3 2.717(4) . ?
Nd1 C1 2.881(6) . ?
Nd1 C9 2.941(6) . ?
Nd1 Nd1 4.0454(6) 7_556 ?
S1 C19 1.923(15) . ?
S2 C22 1.834(19) . ?
N1 C8 1.221(11) 3_455 ?
N1 C12 1.415(8) . ?
O1 C1 1.254(9) . ?
O2 C1 1.278(10) . ?
O3 C9 1.253(8) . ?
O3 Nd1 2.390(5) 7_556 ?
O4 C9 1.251(7) . ?
O5 C16 1.253(8) . ?
O6 C16 1.264(9) 7_556 ?
O7 C17 1.457(17) . ?
O8 C20 1.474(14) . ?
O9 C18 1.369(16) . ?
O9 H9 0.8200 . ?
O10 C21 1.42(2) . ?
O10 H10 0.8200 . ?
C1 C2 1.476(9) . ?
C2 C3 1.368(11) . ?
C2 C7 1.386(12) . ?
C3 C4 1.380(10) . ?
C3 H3 0.9300 . ?
C4 C5 1.414(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.385(13) . ?
C5 C8 1.471(10) . ?
C6 C7 1.387(11) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 N1 1.221(11) 3_545 ?
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C8 H16 0.83(8) . ?
C9 C10 1.524(9) . ?
C10 C15 1.372(9) . ?
C10 C11 1.388(8) . ?
C11 C12 1.398(10) . ?
C11 H11 0.9300 . ?
C12 C13 1.411(9) 6_565 ?
C13 C14 1.382(8) . ?
C13 C12 1.411(9) 6_566 ?
C13 H13 0.9300 . ?
C14 C15 1.384(10) 6_566 ?
C14 C16 1.492(9) . ?
C15 C14 1.384(10) 6_565 ?
C15 H15 0.9300 . ?
C16 O6 1.264(9) 7_556 ?
C17 C18 1.445(18) . ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C18 C19 1.460(17) . ?
C18 H18 0.9800 . ?
C19 H19A 0.9700 . ?
C19 H19B 0.9700 . ?
C20 C21 1.46(2) . ?
C20 C22 1.56(2) . ?
C20 H20 0.9800 . ?
C21 H21A 0.9700 . ?
C21 H21B 0.9700 . ?
C22 H22A 0.9700 . ?
C22 H22B 0.9700 . ?

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O3 Nd1 O6 72.71(16) 7_556 . ?
O5 Nd1 O6 133.62(15) . . ?
O3 Nd1 O4 124.25(15) 7_556 . ?
O5 Nd1 O4 88.05(17) . . ?
O6 Nd1 O4 78.68(17) . . ?
O3 Nd1 O1 87.53(16) 7_556 . ?
O5 Nd1 O1 139.25(17) . . ?
O6 Nd1 O1 75.96(18) . . ?
O4 Nd1 O1 130.09(15) . . ?
O3 Nd1 O7 147.60(16) 7_556 . ?
O5 Nd1 O7 75.88(17) . . ?
O6 Nd1 O7 139.63(17) . . ?
O4 Nd1 O7 75.4(2) . . ?
O1 Nd1 O7 98.0(2) . . ?
O3 Nd1 O8 82.60(19) 7_556 . ?
O5 Nd1 O8 72.60(18) . . ?
O6 Nd1 O8 136.5(2) . . ?
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O4 Nd1 O8 143.84(19) . . ?
O1 Nd1 O8 67.54(19) . . ?
O7 Nd1 O8 70.5(2) . . ?
O3 Nd1 O2 131.81(16) 7_556 . ?
O5 Nd1 O2 148.09(18) . . ?
O6 Nd1 O2 72.78(15) . . ?
O4 Nd1 O2 79.72(15) . . ?
O1 Nd1 O2 51.97(17) . . ?
O7 Nd1 O2 72.55(17) . . ?
O8 Nd1 O2 100.64(17) . . ?
O3 Nd1 O3 75.41(17) 7_556 . ?
O5 Nd1 O3 67.33(14) . . ?
O6 Nd1 O3 70.29(14) . . ?
O4 Nd1 O3 49.93(14) . . ?
O1 Nd1 O3 145.36(18) . . ?
O7 Nd1 O3 112.57(19) . . ?
O8 Nd1 O3 137.04(16) . . ?
O2 Nd1 O3 121.57(15) . . ?
O3 Nd1 C1 109.6(2) 7_556 . ?
O5 Nd1 C1 154.11(17) . . ?
O6 Nd1 C1 71.69(17) . . ?
O4 Nd1 C1 105.10(19) . . ?
O1 Nd1 C1 25.7(2) . . ?
O7 Nd1 C1 85.8(2) . . ?
O8 Nd1 C1 84.18(19) . . ?
O2 Nd1 C1 26.3(2) . . ?
O3 Nd1 C1 137.87(16) . . ?
O3 Nd1 C9 100.17(17) 7_556 . ?
O5 Nd1 C9 76.39(16) . . ?
O6 Nd1 C9 73.28(17) . . ?
O4 Nd1 C9 24.74(16) . . ?
O1 Nd1 C9 144.25(17) . . ?
O7 Nd1 C9 93.8(2) . . ?
O8 Nd1 C9 147.77(18) . . ?
O2 Nd1 C9 100.97(16) . . ?
O3 Nd1 C9 25.19(16) . . ?
C1 Nd1 C9 123.67(19) . . ?
O3 Nd1 Nd1 40.54(11) 7_556 7_556 ?
O5 Nd1 Nd1 68.30(11) . 7_556 ?
O6 Nd1 Nd1 66.29(10) . 7_556 ?
O4 Nd1 Nd1 84.26(10) . 7_556 ?
O1 Nd1 Nd1 121.81(14) . 7_556 ?
O7 Nd1 Nd1 139.17(14) . 7_556 ?
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H19A C19 H19B 108.0 . . ?
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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Cryst</i>.
<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
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on F, and R-
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C18 C 0.3795(4) 0.4507(8) 0.8636(9) 0.064(3) Uani 1 1 d . . .
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C4 0.032(4) 0.042(5) 0.070(6) 0.006(4) 0.031(4) -0.005(4)
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 and torsion angles; correlations between esds in cell
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expression of
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C19 C 0.2066(6) 0.9263(6) 1.4600(6) 0.038(2) Uani 1 1 d . . .
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C20 C 0.2086(6) 0.8949(6) 1.5407(6) 0.040(2) Uani 1 1 d . . .
H20 H 0.2733 0.8849 1.5882 0.048 Uiso 1 1 calc R . .
C21 C 0.1139(6) 0.8783(5) 1.5507(5) 0.0231(17) Uani 1 1 d . . .
C22 C 0.0186(6) 0.8927(5) 1.4786(5) 0.0276(18) Uani 1 1 d . . .
H22 H -0.0455 0.8803 1.4838 0.033 Uiso 1 1 calc R . .
C23 C 0.0182(6) 0.9255(5) 1.3987(5) 0.0254(17) Uani 1 1 d . . .
H23 H -0.0463 0.9360 1.3513 0.030 Uiso 1 1 calc R . .
C24 C 0.1178(6) 0.8489(5) 1.6388(5) 0.0232(17) Uani 1 1 d . . .
C25 C 0.2134(5) 0.8065(5) 0.7892(5) 0.0176(15) Uani 1 1 d . . .
C26 C 0.2825(5) 0.7411(5) 0.8280(5) 0.0194(16) Uani 1 1 d . . .
H26 H 0.3139 0.7088 0.7926 0.023 Uiso 1 1 calc R . .
C27 C 0.3058(5) 0.7229(4) 0.9190(5) 0.0180(15) Uani 1 1 d . . .
C28 C 0.2615(5) 0.7742(5) 0.9727(5) 0.0202(16) Uani 1 1 d . . .
H28 H 0.2776 0.7638 1.0343 0.024 Uiso 1 1 calc R . .
C29 C 0.1932(5) 0.8412(4) 0.9344(5) 0.0144(14) Uani 1 1 d . . .
C30 C 0.1664(5) 0.8549(4) 0.8412(5) 0.0160(15) Uani 1 1 d . . .
H30 H 0.1168 0.8966 0.8141 0.019 Uiso 1 1 calc R . .
C31 C 0.3790(6) 0.6495(5) 0.9573(5) 0.0270(18) Uani 1 1 d . . .
C32 C 0.1574(5) 0.9029(4) 0.9966(5) 0.0155(15) Uani 1 1 d . . .
C33 C 0.7032(12) 0.3804(14) 0.8123(8) 0.150(9) Uani 1 1 d
DU . .
H33 H 0.6846 0.3359 0.8413 0.180 Uiso 1 1 calc R . .
C34 C 0.7911(13) 0.362(2) 0.7949(14) 0.183(12) Uani 1 1 d
DU . .
H34 H 0.8258 0.3087 0.8010 0.220 Uiso 1 1 calc R . .
C35 C 0.8200(15) 0.4429(17) 0.7648(13) 0.153(10) Uani 1 1 d
DU . .
H35 H 0.8844 0.4418 0.7578 0.183 Uiso 1 1 calc R . .
C36 C 0.7686(13) 0.5195(13) 0.7453(11) 0.141(8) Uani 1 1 d
DU . .
H36 H 0.7894 0.5681 0.7227 0.169 Uiso 1 1 calc R . .
C37 C 0.6774(9) 0.5118(10) 0.7658(8) 0.118(7) Uani 1 1 d DU . .
H37 H 0.6357 0.5615 0.7557 0.141 Uiso 1 1 calc R . .
C38 C 0.3942(6) 1.0309(5) 1.2141(5) 0.0298(19) Uani 1 1 d . . .
H38 H 0.3769 0.9712 1.2159 0.036 Uiso 1 1 calc R . .
C39 C 0.5008(6) 1.0583(6) 1.2392(6) 0.035(2) Uani 1 1 d . . .
H39 H 0.5537 1.0171 1.2561 0.042 Uiso 1 1 calc R . .
C40 C 0.5262(6) 1.1474(6) 1.2386(6) 0.037(2) Uani 1 1 d . . .
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H40 H 0.5967 1.1675 1.2565 0.045 Uiso 1 1 calc R . .
C41 C 0.4472(6) 1.2048(6) 1.2114(6) 0.035(2) Uani 1 1 d . . .
H41 H 0.4629 1.2648 1.2092 0.042 Uiso 1 1 calc R . .
C42 C 0.3441(6) 1.1750(5) 1.1872(5) 0.0246(17) Uani 1 1 d . . .
H42 H 0.2909 1.2158 1.1696 0.029 Uiso 1 1 calc R . .
C43 C 0.4545(7) 0.1591(8) 0.9085(7) 0.058(3) Uani 1 1 d . . .
H43 H 0.5223 0.1860 0.9274 0.069 Uiso 1 1 calc R . .
C44 C 0.4355(10) 0.1052(8) 0.9673(7) 0.063(3) Uani 1 1 d . . .
H44 H 0.4892 0.0964 1.0244 0.076 Uiso 1 1 calc R . .
C45 C 0.3385(10) 0.0657(6) 0.9408(8) 0.055(3) Uani 1 1 d . . .
H45 H 0.3244 0.0292 0.9797 0.066 Uiso 1 1 calc R . .
C46 C 0.2596(7) 0.0789(5) 0.8559(7) 0.042(2) Uani 1 1 d . . .
H46 H 0.1916 0.0519 0.8357 0.050 Uiso 1 1 calc R . .
C47 C 0.2861(6) 0.1334(5) 0.8032(6) 0.033(2) Uani 1 1 d . . .
H47 H 0.2331 0.1425 0.7458 0.040 Uiso 1 1 calc R . .
C48 C 0.0248(8) 1.3440(7) 1.0902(8) 0.059(3) Uani 1 1 d . . .
H48 H 0.0729 1.3141 1.0707 0.071 Uiso 1 1 calc R . .
C49 C -0.0406(9) 1.4036(8) 1.0329(9) 0.069(3) Uani 1 1 d . . .
H49 H -0.0373 1.4124 0.9761 0.082 Uiso 1 1 calc R . .
C50 C -0.1088(10) 1.4481(8) 1.0626(12) 0.092(5) Uani 1 1
d . . .
H50 H -0.1525 1.4891 1.0266 0.110 Uiso 1 1 calc R . .
C51 C -0.1138(9) 1.4328(7) 1.1462(11) 0.081(4) Uani 1 1 d . . .
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C52 C -0.0482(8) 1.3701(6) 1.1983(9) 0.064(3) Uani 1 1 d . . .
H52 H -0.0533 1.3575 1.2534 0.076 Uiso 1 1 calc R . .
C53 C 0.2458(11) 0.1653(9) 0.4768(9) 0.107(5) Uani 1 1 d DU . .
H53 H 0.2810 0.1166 0.4634 0.129 Uiso 1 1 calc R . .
C54 C 0.2563(14) 0.1984(13) 0.5725(14) 0.166(8) Uani 1 1 d
DU . .
H54 H 0.2859 0.1594 0.6175 0.200 Uiso 1 1 calc R . .
C55 C 0.2284(10) 0.2782(11) 0.6032(11) 0.118(6) Uani 1 1 d
DU . .
H55 H 0.2382 0.2970 0.6646 0.142 Uiso 1 1 calc R . .
C56 C 0.1843(12) 0.3255(12) 0.5299(12) 0.140(7) Uani 1 1 d
DU . .
H56 H 0.1664 0.3830 0.5445 0.168 Uiso 1 1 calc R . .
C57 C 0.1620(14) 0.3020(13) 0.4377(12) 0.148(7) Uani 1 1 d
DU . .
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H8 H 0.111(6) 0.732(6) 0.343(6) 0.04(2) Uiso 1 1 d . . .
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0.00386(15)
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0.00072(15)
O1 0.020(3) 0.036(3) 0.019(3) 0.007(2) 0.007(2) 0.004(2)
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O3 0.018(3) 0.042(3) 0.019(3) 0.011(2) 0.002(2) -0.007(2)
O4 0.019(3) 0.042(3) 0.034(3) 0.026(3) 0.003(3) -0.006(2)
O5 0.019(3) 0.025(3) 0.015(2) 0.006(2) 0.003(2) -0.002(2)
O6 0.019(3) 0.025(3) 0.012(2) 0.010(2) 0.002(2) -0.001(2)
O7 0.034(3) 0.020(3) 0.019(3) 0.001(2) 0.011(2) 0.011(2)
O8 0.070(4) 0.053(4) 0.015(3) 0.017(3) 0.022(3) 0.042(3)
O9 0.023(3) 0.028(3) 0.019(3) 0.011(2) 0.010(2) 0.007(2)
O10 0.025(3) 0.036(3) 0.016(3) 0.010(2) 0.005(2) 0.003(2)
O11 0.020(3) 0.024(3) 0.011(3) 0.000(2) 0.000(2) 0.007(2)
O12 0.014(2) 0.017(2) 0.020(2) 0.004(2) 0.011(2) 0.004(2)
O13 0.161(8) 0.022(3) 0.021(3) -0.002(3) 0.011(4) 0.011(4)
O14 0.049(4) 0.025(3) 0.038(3) -0.003(3) 0.027(3) -0.005(3)
N1 0.024(3) 0.025(3) 0.015(3) 0.006(3) 0.009(3) -0.001(3)
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N3 0.065(6) 0.171(11) 0.020(4) 0.014(5) 0.024(4) 0.064(7)
N4 0.024(3) 0.022(3) 0.015(3) 0.002(3) 0.002(3) -0.001(3)
N5 0.026(4) 0.040(4) 0.037(4) -0.009(3) 0.017(3) -0.002(3)
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C4 0.024(4) 0.033(5) 0.022(4) 0.003(3) 0.004(3) -0.003(3)
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C8 0.021(4) 0.033(5) 0.033(5) 0.014(4) 0.008(4) -0.007(4)
C9 0.025(4) 0.023(4) 0.018(4) 0.008(3) 0.009(3) 0.005(3)
C10 0.020(4) 0.017(4) 0.024(4) 0.008(3) 0.012(3) 0.001(3)
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C15 0.011(4) 0.030(4) 0.031(5) 0.019(4) 0.001(3) 0.001(3)
C16 0.016(4) 0.017(4) 0.027(4) 0.009(3) 0.013(3) 0.007(3)
C17 0.023(4) 0.017(4) 0.017(4) 0.001(3) 0.010(3) -0.006(3)
C18 0.022(4) 0.027(4) 0.019(4) 0.003(3) 0.009(3) 0.002(3)
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C22 0.024(4) 0.047(5) 0.021(4) 0.014(4) 0.016(4) 0.011(4)
C23 0.023(4) 0.034(5) 0.019(4) 0.006(3) 0.007(3) 0.004(3)
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C25 0.017(4) 0.020(4) 0.014(3) 0.005(3) 0.004(3) 0.001(3)
C26 0.022(4) 0.017(4) 0.022(4) 0.001(3) 0.012(3) 0.007(3)
C27 0.025(4) 0.017(4) 0.013(3) 0.006(3) 0.007(3) 0.010(3)
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C29 0.015(3) 0.011(3) 0.017(3) 0.000(3) 0.006(3) -0.002(3)
C30 0.016(4) 0.014(4) 0.018(4) 0.005(3) 0.007(3) 0.005(3)
C31 0.032(4) 0.031(5) 0.017(4) 0.005(3) 0.009(4) 0.014(4)
C32 0.014(4) 0.013(4) 0.021(4) 0.005(3) 0.008(3) 0.003(3)
C33 0.142(13) 0.29(2) 0.052(8) 0.054(11) 0.061(9) 0.170(15)
C34 0.148(18) 0.32(3) 0.100(14) 0.067(17) 0.057(13) 0.14(2)
C35 0.108(14) 0.24(2) 0.079(12) -0.030(14) 0.017(10) 0.099(16)
C36 0.089(11) 0.24(2) 0.104(13) -0.038(14) 0.059(11) -0.046(13)

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C37 0.041(7) 0.26(2) 0.045(7) -0.052(10) 0.029(6) -0.021(10)
C38 0.023(4) 0.030(4) 0.029(4) 0.001(4) 0.003(4) 0.000(3)
C39 0.024(4) 0.044(5) 0.034(5) 0.013(4) 0.006(4) 0.008(4)
C40 0.019(4) 0.064(6) 0.027(5) 0.008(4) 0.007(4) -0.004(4)
C41 0.032(5) 0.042(5) 0.031(5) 0.017(4) 0.009(4) -0.003(4)
C42 0.021(4) 0.028(4) 0.025(4) 0.006(3) 0.007(3) -0.003(3)
C43 0.030(5) 0.085(8) 0.043(6) -0.022(6) 0.006(5) -0.004(5)
C44 0.071(8) 0.074(8) 0.029(6) 0.003(5) 0.003(6) 0.029(7)
C45 0.090(9) 0.027(5) 0.061(7) 0.013(5) 0.043(7) 0.015(5)
C46 0.047(6) 0.022(5) 0.064(7) 0.005(4) 0.029(5) 0.000(4)
C47 0.032(5) 0.023(4) 0.038(5) 0.000(4) 0.007(4) -0.002(4)
C48 0.060(7) 0.049(6) 0.096(9) 0.006(6) 0.060(7) 0.005(5)
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C52 0.078(7) 0.023(5) 0.120(10) 0.004(6) 0.072(8) -0.005(5)
C53 0.154(12) 0.093(10) 0.065(8) 0.001(8) 0.036(9) -0.039(9)
C54 0.194(16) 0.178(16) 0.102(12) 0.036(12) 0.028(11) -
0.066(13)
C55 0.104(10) 0.106(11) 0.076(9) 0.019(9) -0.038(8) -0.063(9)
C56 0.118(11) 0.126(12) 0.171(15) -0.045(12) 0.066(11)
0.030(10)
C57 0.164(14) 0.151(14) 0.122(12) -0.027(11) 0.058(11)
0.058(12)

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;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Nd1 N3 2.673(9) . ?
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Nd2 N4 2.705(6) . ?
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O3 C15 1.265(9) . ?
O4 C15 1.275(9) . ?
O4 Nd1 2.366(5) 2_667 ?
O5 C16 1.246(8) . ?
O5 Nd2 2.407(5) 1_655 ?
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O8 C31 1.254(9) 2_667 ?
O9 C17 1.239(8) . ?
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O11 C32 1.257(8) . ?
O12 C32 1.273(7) . ?
O12 Nd2 2.416(4) 2_577 ?
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N1 C9 1.435(8) . ?
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C4 H4 0.9300 . ?
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C20 H20 0.9300 . ?
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Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
```

```
 'calc w=1/[\s^2^(Fo^2^)+(0.0517P)^2^+24.3365P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4741
_refine_ls_number_parameters      320
_refine_ls_number_restraints      59
_refine_ls_R_factor_all           0.0608
_refine_ls_R_factor_gt            0.0448
_refine_ls_wR_factor_ref          0.1255
_refine_ls_wR_factor_gt           0.1180
_refine_ls_goodness_of_fit_ref    1.096
_refine_ls_restrained_S_all       1.094
_refine_ls_shift/su_max           0.003
_refine_ls_shift/su_mean          0.000

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Nd1 Nd 0.818565(11) 0.28727(2) 0.54668(3) 0.01677(14) Uani 1 1
d . . .
N1 N 1.09704(18) 0.0780(4) 0.3500(4) 0.0231(13) Uani 1 1
d . . .
O1 O 0.88136(16) 0.1773(4) 0.5114(4) 0.0336(13) Uani 1 1
d . . .
O2 O 0.89145(16) 0.3256(4) 0.4787(4) 0.0346(13) Uani 1 1
d . . .
O3 O 0.79412(15) 0.4338(3) 0.4543(4) 0.0296(12) Uani 1 1
d . . .
O4 O 0.76836(14) 0.1525(3) 0.5381(3) 0.0209(10) Uani 1 1
d . . .
O5 O 0.79858(15) 0.2408(3) 0.3686(3) 0.0234(11) Uani 1 1
d . . .
O6 O 0.77125(15) 0.3298(4) 0.6731(4) 0.0287(12) Uani 1 1
d . . .
O7 O 0.8657(2) 0.4068(5) 0.6620(5) 0.070(2) Uani 1 1 d . . .
O8 O 0.8564(2) 0.2068(5) 0.7119(5) 0.0606(19) Uani 1 1 d . . .
O9 O 0.8696(6) 0.5909(13) 0.6356(16) 0.233(7) Uani 1 1 d DU . .
C1 C 0.9041(2) 0.2409(5) 0.4793(6) 0.0255(16) Uani 1 1 d . . .
C2 C 0.9479(2) 0.2181(5) 0.4389(6) 0.0269(16) Uani 1 1 d . . .
C3 C 0.9765(3) 0.2886(5) 0.4120(7) 0.040(2) Uani 1 1 d . . .
```

```
H3 H 0.9670 0.3503 0.4141 0.047 Uiso 1 1 calc R . .
C4 C 1.0186(3) 0.2680(6) 0.3824(7) 0.039(2) Uani 1 1 d . . .
H4 H 1.0377 0.3159 0.3662 0.047 Uiso 1 1 calc R . .
C5 C 1.0329(2) 0.1768(5) 0.3764(6) 0.0278(16) Uani 1 1 d . . .
C6 C 1.0036(2) 0.1057(5) 0.3997(6) 0.0293(17) Uani 1 1 d . . .
H6 H 1.0123 0.0439 0.3936 0.035 Uiso 1 1 calc R . .
C7 C 0.9621(2) 0.1263(5) 0.4314(6) 0.0306(17) Uani 1 1 d . . .
H7 H 0.9432 0.0784 0.4481 0.037 Uiso 1 1 calc R . .
C8 C 1.0791(2) 0.1582(6) 0.3511(5) 0.0279(17) Uani 1 1 d . . .
H16 H 1.094(3) 0.212(6) 0.341(6) 0.04(2) Uiso 1 1 d . . .
C9 C 0.7498(2) 0.4199(5) 0.4335(5) 0.0251(16) Uani 1 1 d . . .
C10 C 0.7191(2) 0.4934(5) 0.3748(5) 0.0191(14) Uani 1 1 d . . .
C11 C 1.1720(2) 0.0010(5) 0.3841(5) 0.0237(15) Uani 1 1 d . . .
H11 H 1.1592 -0.0408 0.4250 0.028 Uiso 1 1 calc R . .
C12 C 1.1439(2) 0.0713(5) 0.3320(5) 0.0196(14) Uani 1 1 d . . .
C13 C 1.1623(2) 0.1274(5) 0.2642(5) 0.0221(15) Uani 1 1 d . . .
H13 H 1.1432 0.1712 0.2252 0.026 Uiso 1 1 calc R . .
C14 C 0.7909(2) 0.1188(5) 0.2462(5) 0.0193(14) Uani 1 1 d . . .
C15 C 0.7627(2) 0.0537(5) 0.1900(5) 0.0207(15) Uani 1 1 d . . .
H15 H 0.7310 0.0498 0.1952 0.025 Uiso 1 1 calc R . .
C16 C 0.7712(2) 0.1822(5) 0.3201(5) 0.0225(15) Uani 1 1 d . . .
C17 C 0.9049(4) 0.1761(10) 0.7412(10) 0.094(4) Uani 1 1 d U . .
H17A H 0.9107 0.1244 0.6981 0.113 Uiso 1 1 calc R . .
H17B H 0.9261 0.2264 0.7314 0.113 Uiso 1 1 calc R . .
C18 C 0.9141(7) 0.1476(13) 0.8474(12) 0.147(7) Uani 1 1 d U . .
H18A H 0.9261 0.1990 0.8919 0.176 Uiso 1 1 calc R . .
H18B H 0.9367 0.0969 0.8585 0.176 Uiso 1 1 calc R . .
C19 C 0.8663(6) 0.1162(10) 0.8673(10) 0.119(6) Uani 1 1 d U . .
H19A H 0.8643 0.1226 0.9392 0.143 Uiso 1 1 calc R . .
H19B H 0.8598 0.0523 0.8461 0.143 Uiso 1 1 calc R . .
C20 C 0.8317(5) 0.1859(9) 0.7979(8) 0.087(4) Uani 1 1 d U . .
H20A H 0.8013 0.1571 0.7731 0.104 Uiso 1 1 calc R . .
H20B H 0.8270 0.2420 0.8355 0.104 Uiso 1 1 calc R . .
C21 C 0.8352(8) 0.607(2) 0.7010(17) 0.230(12) Uani 1 1 d DU . .
H21A H 0.8459 0.6554 0.7515 0.277 Uiso 1 1 calc R . .
H21B H 0.8288 0.5511 0.7362 0.277 Uiso 1 1 calc R . .
C22 C 0.7922(8) 0.639(2) 0.6257(19) 0.234(12) Uani 1 1 d DU . .
H22A H 0.7728 0.5848 0.6041 0.281 Uiso 1 1 calc R . .
H22B H 0.7740 0.6801 0.6613 0.281 Uiso 1 1 calc R . .
C23 C 0.8017(9) 0.6881(18) 0.531(2) 0.220(11) Uani 1 1 d DU . .
H23A H 0.7789 0.6740 0.4695 0.264 Uiso 1 1 calc R . .
H23B H 0.8059 0.7548 0.5399 0.264 Uiso 1 1 calc R . .
C24 C 0.8471(9) 0.635(2) 0.5399(18) 0.241(12) Uani 1 1 d DU . .
H24A H 0.8419 0.5866 0.4881 0.289 Uiso 1 1 calc R . .
H24B H 0.8701 0.6774 0.5203 0.289 Uiso 1 1 calc R . .

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Nd1 0.0115(2) 0.0198(2) 0.0206(2) -0.00140(16) 0.00706(14)
0.00087(15)
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N1 0.018(3) 0.029(3) 0.025(3) 0.002(3) 0.010(2) 0.006(3)
O1 0.026(3) 0.030(3) 0.050(3) 0.009(3) 0.021(2) 0.008(2)
O2 0.026(3) 0.029(3) 0.054(3) -0.004(3) 0.022(3) -0.003(2)
O3 0.018(2) 0.020(3) 0.052(3) 0.005(2) 0.011(2) -0.001(2)
O4 0.019(2) 0.015(2) 0.030(3) 0.005(2) 0.010(2) 0.0035(19)
O5 0.024(2) 0.026(3) 0.022(2) -0.008(2) 0.011(2) -0.006(2)
O6 0.019(2) 0.044(3) 0.026(3) -0.007(2) 0.011(2) -0.001(2)
O7 0.044(3) 0.100(6) 0.070(5) -0.039(4) 0.021(3) -0.026(4)
O8 0.059(4) 0.082(5) 0.035(3) 0.004(3) -0.005(3) 0.026(4)
O9 0.229(8) 0.237(9) 0.237(8) 0.001(5) 0.052(5) -0.004(5)
C1 0.012(3) 0.033(4) 0.031(4) 0.000(3) 0.004(3) -0.003(3)
C2 0.016(3) 0.037(4) 0.030(4) -0.001(3) 0.009(3) 0.000(3)
C3 0.032(4) 0.024(4) 0.071(6) 0.007(4) 0.031(4) 0.003(3)
C4 0.027(4) 0.042(5) 0.054(5) 0.009(4) 0.020(4) 0.002(4)
C5 0.022(4) 0.033(4) 0.030(4) 0.009(3) 0.011(3) 0.008(3)
C6 0.030(4) 0.024(4) 0.036(4) 0.001(3) 0.013(3) 0.008(3)
C7 0.021(3) 0.030(4) 0.044(5) 0.005(4) 0.015(3) 0.001(3)
C8 0.024(4) 0.036(5) 0.028(4) 0.003(4) 0.016(3) -0.002(4)
C9 0.022(4) 0.024(4) 0.033(4) -0.002(3) 0.015(3) 0.005(3)
C10 0.015(3) 0.016(3) 0.027(4) -0.006(3) 0.006(3) -0.001(3)
C11 0.019(3) 0.023(4) 0.032(4) 0.006(3) 0.015(3) 0.002(3)
C12 0.014(3) 0.025(4) 0.021(3) 0.002(3) 0.007(3) 0.001(3)
C13 0.022(3) 0.023(4) 0.023(4) 0.006(3) 0.008(3) 0.008(3)
C14 0.019(3) 0.023(4) 0.018(3) -0.002(3) 0.010(3) -0.005(3)
C15 0.013(3) 0.025(4) 0.027(4) 0.001(3) 0.010(3) 0.001(3)
C16 0.020(3) 0.026(4) 0.023(4) 0.002(3) 0.009(3) 0.004(3)
C17 0.075(8) 0.110(11) 0.084(9) -0.021(8) -0.020(7) 0.012(8)
C18 0.195(17) 0.113(13) 0.092(11) 0.036(10) -0.081(12)
0.005(13)
C19 0.193(16) 0.082(10) 0.059(8) -0.020(8) -0.041(10) 0.021(11)
C20 0.149(12) 0.068(8) 0.034(6) 0.000(6) -0.009(7) -0.006(8)
C21 0.235(12) 0.232(12) 0.230(12) -0.005(5) 0.056(5) -0.002(5)
C22 0.237(13) 0.232(13) 0.233(13) -0.003(5) 0.044(5) -0.004(5)
C23 0.223(12) 0.218(12) 0.218(12) -0.006(5) 0.036(5) -0.005(5)
C24 0.241(13) 0.241(13) 0.240(13) 0.000(5) 0.041(5) -0.006(5)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

loop_
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Nd1 O5 2.417(4) . ?
Nd1 O6 2.425(4) . ?
Nd1 O3 2.473(5) . ?
Nd1 O2 2.495(4) . ?
Nd1 O1 2.511(5) . ?
Nd1 O7 2.524(6) . ?
Nd1 O8 2.537(6) . ?
Nd1 O4 2.693(4) 7_656 ?
Nd1 C1 2.852(6) . ?
Nd1 C9 2.953(7) . ?
Nd1 Nd1 4.0629(7) 7_656 ?
N1 C8 1.264(9) . ?
N1 C12 1.417(7) . ?
O1 C1 1.244(8) . ?
O2 C1 1.271(9) . ?
O3 C9 1.271(8) . ?
O4 C9 1.255(8) 7_656 ?
O4 Nd1 2.693(4) 7_656 ?
O5 C16 1.248(8) . ?
O6 C16 1.256(7) 7_656 ?
O8 C17 1.451(13) . ?
O8 C20 1.482(13) . ?
O9 C21 1.453(5) . ?
O9 C24 1.458(5) . ?
C1 C2 1.496(9) . ?
C2 C7 1.390(10) . ?
C2 C3 1.394(10) . ?
C3 C4 1.376(10) . ?
C3 H3 0.9300 . ?
C4 C5 1.381(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.395(10) . ?
C5 C8 1.458(9) . ?
C6 C7 1.374(9) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.91(8) . ?
C9 O4 1.255(8) 7_656 ?
C9 C10 1.501(9) . ?
C10 C11 1.391(8) 3_455 ?
C10 C15 1.389(9) 4_655 ?
C11 C10 1.391(8) 3_545 ?
C11 C12 1.396(9) . ?
C11 H11 0.9300 . ?
C12 C13 1.384(9) . ?
C13 C14 1.387(8) 2_755 ?
C13 H13 0.9300 . ?
C14 C15 1.365(9) . ?
C14 C13 1.387(8) 2_755 ?
C14 C16 1.522(9) . ?
C15 C10 1.389(9) 4_645 ?
C15 H15 0.9300 . ?
C16 O6 1.256(7) 7_656 ?
```

```
C17 C18 1.442(18) . ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C18 C19 1.52(2) . ?
C18 H18A 0.9700 . ?
C18 H18B 0.9700 . ?
C19 C20 1.584(17) . ?
C19 H19A 0.9700 . ?
C19 H19B 0.9700 . ?
C20 H20A 0.9700 . ?
C20 H20B 0.9700 . ?
C21 C22 1.509(5) . ?
C21 H21A 0.9700 . ?
C21 H21B 0.9700 . ?
C22 C23 1.508(5) . ?
C22 H22A 0.9700 . ?
C22 H22B 0.9700 . ?
C23 C24 1.503(5) . ?
C23 H23A 0.9700 . ?
C23 H23B 0.9700 . ?
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C24 H24B 0.9700 . ?

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O4 Nd1 O5 72.46(15) . . ?
O4 Nd1 O6 79.97(15) . . ?
O5 Nd1 O6 132.87(15) . . ?
O4 Nd1 O3 123.23(14) . . ?
O5 Nd1 O3 75.98(17) . . ?
O6 Nd1 O3 88.92(16) . . ?
O4 Nd1 O2 134.37(15) . . ?
O5 Nd1 O2 76.95(16) . . ?
O6 Nd1 O2 144.26(17) . . ?
O3 Nd1 O2 79.38(16) . . ?
O4 Nd1 O1 86.14(15) . . ?
O5 Nd1 O1 72.23(17) . . ?
O6 Nd1 O1 143.51(17) . . ?
O3 Nd1 O1 126.42(16) . . ?
O2 Nd1 O1 52.25(16) . . ?
O4 Nd1 O7 145.92(19) . . ?
O5 Nd1 O7 141.62(19) . . ?
O6 Nd1 O7 73.70(17) . . ?
O3 Nd1 O7 78.0(2) . . ?
O2 Nd1 O7 70.87(18) . . ?
O1 Nd1 O7 102.4(2) . . ?
O4 Nd1 O8 80.4(2) . . ?
O5 Nd1 O8 134.67(19) . . ?
O6 Nd1 O8 74.14(18) . . ?
O3 Nd1 O8 148.6(2) . . ?
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O2 Nd1 O8 98.9(2) . . ?
O1 Nd1 O8 70.33(19) . . ?
O7 Nd1 O8 72.0(2) . . ?
O4 Nd1 O4 74.56(15) . 7_656 ?
O5 Nd1 O4 69.24(14) . 7_656 ?
O6 Nd1 O4 66.94(14) . 7_656 ?
O3 Nd1 O4 50.31(13) . 7_656 ?
O2 Nd1 O4 124.01(16) . 7_656 ?
O1 Nd1 O4 140.54(16) . 7_656 ?
O7 Nd1 O4 112.96(19) . 7_656 ?
O8 Nd1 O4 136.49(17) . 7_656 ?
O4 Nd1 C1 110.13(18) . . ?
O5 Nd1 C1 72.21(18) . . ?
O6 Nd1 C1 154.67(18) . . ?
O3 Nd1 C1 103.21(18) . . ?
O2 Nd1 C1 26.42(19) . . ?
O1 Nd1 C1 25.84(19) . . ?
O7 Nd1 C1 87.0(2) . . ?
O8 Nd1 C1 84.5(2) . . ?
O4 Nd1 C1 137.43(17) 7_656 . ?
O4 Nd1 C9 98.88(17) . . ?
O5 Nd1 C9 70.48(17) . . ?
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O1 Nd1 C9 138.72(17) . . ?
O7 Nd1 C9 96.0(2) . . ?
O8 Nd1 C9 150.95(19) . . ?
O4 Nd1 C9 25.15(15) 7_656 . ?
C1 Nd1 C9 122.02(19) . . ?
O4 Nd1 Nd1 39.72(10) . 7_656 ?
O5 Nd1 Nd1 65.57(10) . 7_656 ?
O6 Nd1 Nd1 68.72(11) . 7_656 ?
O3 Nd1 Nd1 84.34(10) . 7_656 ?
O2 Nd1 Nd1 141.75(13) . 7_656 ?
O1 Nd1 Nd1 118.16(12) . 7_656 ?
O7 Nd1 Nd1 138.55(14) . 7_656 ?
O8 Nd1 Nd1 112.44(16) . 7_656 ?
O4 Nd1 Nd1 34.85(9) 7_656 7_656 ?
C1 Nd1 Nd1 133.81(15) . 7_656 ?
C9 Nd1 Nd1 59.43(13) . 7_656 ?
C8 N1 C12 117.9(6) . . ?
C1 O1 Nd1 92.6(4) . . ?
C1 O2 Nd1 92.7(4) . . ?
C9 O3 Nd1 99.0(4) . . ?
C9 O4 Nd1 159.1(5) 7_656 . ?
C9 O4 Nd1 89.1(4) 7_656 7_656 ?
Nd1 O4 Nd1 105.43(15) . 7_656 ?
C16 O5 Nd1 134.7(4) . . ?
C16 O6 Nd1 134.0(4) 7_656 . ?
C17 O8 C20 108.0(8) . . ?
C17 O8 Nd1 127.6(7) . . ?
C20 O8 Nd1 124.3(6) . . ?
C21 O9 C24 101.8(18) . . ?
O1 C1 O2 122.5(6) . . ?
O1 C1 C2 119.6(7) . . ?
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O2 C1 C2 117.9(6) . . ?
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O2 C1 Nd1 60.9(3) . . ?
C2 C1 Nd1 177.2(5) . . ?
C7 C2 C3 118.5(6) . . ?
C7 C2 C1 120.8(6) . . ?
C3 C2 C1 120.7(7) . . ?
C4 C3 C2 120.8(7) . . ?
C4 C3 H3 119.6 . . ?
C2 C3 H3 119.6 . . ?
C3 C4 C5 120.5(7) . . ?
C3 C4 H4 119.8 . . ?
C5 C4 H4 119.8 . . ?
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C4 C5 C8 118.8(7) . . ?
C6 C5 C8 122.1(7) . . ?
C7 C6 C5 120.4(7) . . ?
C7 C6 H6 119.8 . . ?
C5 C6 H6 119.8 . . ?
C6 C7 C2 120.7(7) . . ?
C6 C7 H7 119.6 . . ?
C2 C7 H7 119.6 . . ?
N1 C8 C5 124.3(7) . . ?
N1 C8 H16 124(5) . . ?
C5 C8 H16 111(5) . . ?
O4 C9 O3 121.6(6) 7_656 . ?
O4 C9 C10 120.0(5) 7_656 . ?
O3 C9 C10 118.4(6) . . ?
O4 C9 Nd1 65.8(3) 7_656 . ?
O3 C9 Nd1 55.8(3) . . ?
C10 C9 Nd1 174.2(4) . . ?
C11 C10 C15 119.5(6) 3_455 4_655 ?
C11 C10 C9 120.2(6) 3_455 . ?
C15 C10 C9 120.3(5) 4_655 . ?
C10 C11 C12 120.0(6) 3_545 . ?
C10 C11 H11 120.0 3_545 . ?
C12 C11 H11 120.0 . . ?
C13 C12 C11 119.0(5) . . ?
C13 C12 N1 124.2(6) . . ?
C11 C12 N1 116.8(6) . . ?
C12 C13 C14 120.7(6) . 2_755 ?
C12 C13 H13 119.7 . . ?
C14 C13 H13 119.7 2_755 . ?
C15 C14 C13 119.9(6) . 2_755 ?
C15 C14 C16 120.4(5) . . ?
C13 C14 C16 119.6(6) 2_755 . ?
C14 C15 C10 120.6(5) . 4_645 ?
C14 C15 H15 119.7 . . ?
C10 C15 H15 119.7 4_645 . ?
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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G\"ottingen, Germany.

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Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
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We have applied several restraints to limit the disorder of
the
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DU . .
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PU A 2
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C10 C 0.2913(2) 0.1371(4) 0.5297(3) 0.0367(17) Uani 1 1 d . . .
C11 C 0.2749(2) 0.1848(3) 0.4768(3) 0.0333(16) Uani 1 1 d . . .
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C12 C 0.3038(2) 0.2253(3) 0.4614(3) 0.0348(17) Uani 1 1 d . . .
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
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d . . .
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DU . .
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DU . .
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H43B H 0.3608 0.8923 0.9221 0.265 Uiso 1 1 calc R . .
H43C H 0.3391 0.8922 0.8439 0.265 Uiso 1 1 calc R . .
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DU . .
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H44B H 0.4493 0.9659 0.8830 0.529 Uiso 1 1 calc R . .
H44C H 0.4549 0.9516 0.9555 0.529 Uiso 1 1 calc R . .
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H24 H 0.060(5) -0.117(15) 0.628(15) 0.423 Uiso 1 1 d D . .

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0.0034(2)
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0.0074(2)
Cd3 0.0247(3) 0.0380(3) 0.0442(3) 0.0019(2) 0.0025(2) -
0.0076(2)
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O2A 0.038(6) 0.042(6) 0.046(6) -0.001(5) 0.015(4) -0.007(4)
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O8 0.030(4) 0.145(8) 0.098(6) 0.033(5) 0.001(4) -0.022(4)
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O9 0.026(3) 0.027(3) 0.045(3) 0.012(2) 0.003(2) 0.000(2)
O10 0.023(3) 0.038(3) 0.050(3) 0.015(2) -0.001(2) -0.003(2)
O11 0.027(3) 0.041(3) 0.059(3) -0.006(3) -0.002(3) -0.006(2)
O12 0.033(3) 0.035(3) 0.043(3) -0.007(2) 0.007(2) -0.009(2)
O13 0.037(3) 0.070(4) 0.048(3) 0.008(3) -0.003(3) -0.009(3)
O14 0.096(6) 0.059(4) 0.096(5) -0.008(4) 0.013(4) 0.004(4)
O15 0.071(5) 0.100(5) 0.060(4) 0.027(4) -0.006(4) -0.039(4)
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N6 0.169(7) 0.167(7) 0.171(7) 0.013(5) 0.069(5) -0.008(5)
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C3A 0.034(7) 0.042(7) 0.036(7) -0.001(5) 0.014(5) 0.004(5)
C2 0.025(4) 0.060(6) 0.092(7) 0.019(5) -0.009(5) -0.006(4)
C4 0.035(4) 0.039(4) 0.042(4) 0.000(3) 0.016(3) -0.001(3)
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C37 0.246(8) 0.240(9) 0.229(9) -0.005(5) 0.107(5) 0.008(5)
C38 0.263(8) 0.265(9) 0.263(9) -0.001(5) 0.119(5) 0.005(5)

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C43 0.194(14) 0.213(18) 0.112(12) 0.055(12) 0.058(13) 0.045(12)
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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C26 C31 1.376(9) . ?
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H38A C38 H38B 109.5 . . ?
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H38B C38 H38C 109.5 . . ?
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H41B C41 H41C 109.5 . . ?
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# start Validation Reply Form
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;
RESPONSE: This is caused by the disordered structure
of UCY-3. We have applied several restraints including
DFIX to fix the positions of the imine H atoms.
Although the disorder has been limited, it cannot be
completely eliminated.
;
_vrf_CHEMW03_shelxl
;
```

```
RESPONSE: The reported formula, molecular weight, F000,
density etc include
the contribution of disordered solvents (10 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT043_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of disordered solvents (10 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT041_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of disordered solvents(10 H2O),
which were removed by SQUEEZE.
;
_vrf_FORMU01_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of disordered solvents(10 H2O),
which were removed by SQUEEZE.
;
_vrf_CELLZ01_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the contribution of disordered solvents(10 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT220_shelxl
;
RESPONSE: This is due to the disorder of the atoms. We had
applied
 several restraints to limit it and we have managed to
reduce it significantly. However, the disorder could
not be eliminated completely.
;
_vrf_PLAT241_shelxl
;
RESPONSE: This is due to the disorder of the atom. We had
 applied several restraints to limit it and we have managed
 to reduce it significantly. However, the disorder could not
 be eliminated completely.
;
_vrf_PLAT213_shelxl
;
RESPONSE:This is due to the disorder of the atoms. We had
applied
 several restraints to limit it and we have managed to
 reduce it significantly. However, the disorder could
not be eliminated completely.
;
```

```
_vrf_PLAT303_shelxl
;
RESPONSE: This is a highly disordered imine H atom.
We had applied DFIX to fix its position.
However, the disorder could
not be eliminated completely and thus, it appears erroneously
to be connected to 2 C atoms.
;

# end Validation Reply Form
```

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UCY-3/Benzene
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_chemical_name_common             ?
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


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 Refinement of F^2^ against ALL reflections.  The weighted R-
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
We have applied several restraints to limit the disorder of
the
```

```
CIP ligands and solvent molecules as well as to fix the
position
of imine H atoms.
;

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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_coef        ?
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d . . .
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A .
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d . . .
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d . . .
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d . . .
O12 O 0.26098(15) 0.8413(3) 0.7469(2) 0.0356(11) Uani 1 1
d . . .
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H4 H 0.5036 0.7621 0.5861 0.187 Uiso 1 1 calc R . .
C5 C 0.4824(4) 0.8458(7) 0.6215(6) 0.090(4) Uani 1 1 d D . .
C6 C 0.4961(3) 0.8996(7) 0.6693(5) 0.091(4) Uani 1 1 d D A 1
H6 H 0.4757 0.9248 0.6758 0.110 Uiso 1 1 calc R A 1
C8A C 0.4329(10) 0.8861(15) 0.6173(15) 0.031(6) Uani 0.25 1 d
PU A 2
C7 C 0.5407(3) 0.9161(8) 0.7081(6) 0.109(5) Uani 1 1 d DU . .
H7 H 0.5493 0.9542 0.7384 0.131 Uiso 1 1 calc R A 1
C8 C 0.4342(5) 0.8320(9) 0.5792(7) 0.082(5) Uani 0.75 1 d PU
A .
C9 C 0.2588(2) 0.9130(4) 0.5342(4) 0.0367(16) Uani 1 1 d . . .
C10 C 0.2897(2) 0.8669(4) 0.5232(3) 0.0322(15) Uani 1 1 d . A .
C11 C 0.2734(2) 0.8127(4) 0.4750(3) 0.0303(15) Uani 1 1 d . . .
H11 H 0.2434 0.8057 0.4491 0.036 Uiso 1 1 calc R . .
C12 C 0.3017(2) 0.7692(4) 0.4655(3) 0.0332(15) Uani 1 1 d . A .
C13 C 0.3467(2) 0.7809(4) 0.5025(4) 0.0375(16) Uani 1 1 d . . .
H13 H 0.3658 0.7521 0.4956 0.045 Uiso 1 1 calc R A .
C14 C 0.3630(2) 0.8367(4) 0.5503(4) 0.0406(18) Uani 1 1 d . A .
C15 C 0.3350(2) 0.8778(4) 0.5615(4) 0.0374(17) Uani 1 1 d . . .
H15 H 0.3460 0.9131 0.5946 0.045 Uiso 1 1 calc R A .
C16 C 0.2845(2) 0.7070(4) 0.4176(3) 0.0320(15) Uani 1 1 d . . .
C17 C 0.4033(2) 0.5813(5) 0.4428(4) 0.0433(19) Uani 1 1 d . . .
C18 C 0.4514(2) 0.5906(4) 0.4931(4) 0.0419(19) Uani 1 1 d . . .
C19 C 0.4722(3) 0.5446(5) 0.5451(4) 0.048(2) Uani 1 1 d . . .
H19 H 0.4565 0.5080 0.5518 0.057 Uiso 1 1 calc R . .
C20 C 0.5169(3) 0.5520(5) 0.5885(4) 0.048(2) Uani 1 1 d . . .
H20 H 0.5311 0.5188 0.6230 0.058 Uiso 1 1 calc R . .
C21 C 0.5403(3) 0.6075(4) 0.5811(4) 0.047(2) Uani 1 1 d . . .
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C22 C 0.5183(3) 0.6546(6) 0.5297(6) 0.090(4) Uani 1 1 d . . .
H22 H 0.5331 0.6944 0.5254 0.108 Uiso 1 1 calc R . .
C23 C 0.4748(3) 0.6449(6) 0.4842(6) 0.082(4) Uani 1 1 d . . .
H23 H 0.4611 0.6752 0.4473 0.099 Uiso 1 1 calc R . .
C24 C 0.5880(3) 0.6125(4) 0.6246(4) 0.046(2) Uani 1 1 d D . .
C25 C 0.2431(2) 1.0199(4) 0.6856(4) 0.0356(16) Uani 1 1 d . . .
C26 C 0.2217(2) 1.0892(4) 0.6878(4) 0.0361(17) Uani 1 1 d . . .
C27 C 0.1763(2) 1.0947(4) 0.6552(4) 0.0393(18) Uani 1 1 d . . .
H27 H 0.1592 1.0545 0.6323 0.047 Uiso 1 1 calc R . .
C28 C 0.1563(2) 1.1596(4) 0.6567(4) 0.0396(18) Uani 1 1 d . . .
C29 C 0.1822(2) 1.2209(4) 0.6887(4) 0.0425(18) Uani 1 1 d . . .
H29 H 0.1691 1.2655 0.6878 0.051 Uiso 1 1 calc R . .
C30 C 0.2276(2) 1.2149(4) 0.7219(3) 0.0356(16) Uani 1 1 d . . .
C31 C 0.2475(2) 1.1495(4) 0.7213(3) 0.0338(15) Uani 1 1 d . . .
H31 H 0.2779 1.1460 0.7431 0.041 Uiso 1 1 calc R . .
C32 C 0.2564(2) 0.7214(4) 0.2578(4) 0.0372(17) Uani 1 1 d . . .
C33 C 0.3667(6) 0.3908(8) 0.5107(7) 0.104(5) Uani 1 1 d . . .
C34 C 0.3565(10) 0.3020(13) 0.5807(15) 0.245(18) Uani 1 1
d . . .
H34A H 0.3684 0.2549 0.5994 0.367 Uiso 1 1 calc R . .
H34B H 0.3255 0.2977 0.5512 0.367 Uiso 1 1 calc R . .
H34C H 0.3620 0.3359 0.6154 0.367 Uiso 1 1 calc R . .
C35 C 0.4134(9) 0.2832(13) 0.5475(13) 0.214(14) Uani 1 1
d . . .
H35A H 0.4159 0.2398 0.5722 0.321 Uiso 1 1 calc R . .
H35B H 0.4405 0.3098 0.5691 0.321 Uiso 1 1 calc R . .
H35C H 0.4068 0.2698 0.5039 0.321 Uiso 1 1 calc R . .
C36 C 0.3696(3) 0.6395(5) 0.6001(4) 0.055(2) Uani 1 1 d . . .
C37 C 0.4459(4) 0.6590(9) 0.6814(7) 0.132(7) Uani 1 1 d . . .
H37A H 0.4625 0.6867 0.7212 0.197 Uiso 1 1 calc R . .
H37B H 0.4538 0.6738 0.6496 0.197 Uiso 1 1 calc R . .
H37C H 0.4519 0.6077 0.6907 0.197 Uiso 1 1 calc R . .
C38 C 0.3850(5) 0.7233(7) 0.6889(6) 0.100(5) Uani 1 1 d . . .
H38A H 0.4103 0.7417 0.7278 0.150 Uiso 1 1 calc R . .
H38B H 0.3663 0.6982 0.7012 0.150 Uiso 1 1 calc R . .
H38C H 0.3693 0.7634 0.6601 0.150 Uiso 1 1 calc R . .
C39 C 0.2697(3) 0.5316(5) 0.2018(4) 0.061(3) Uani 1 1 d . . .
C40 C 0.2927(3) 0.4242(6) 0.1676(5) 0.069(3) Uani 1 1 d . . .
H40A H 0.2793 0.3844 0.1371 0.103 Uiso 1 1 calc R . .
H40B H 0.3098 0.4050 0.2115 0.103 Uiso 1 1 calc R . .
H40C H 0.3113 0.4514 0.1563 0.103 Uiso 1 1 calc R . .
C41 C 0.2140(4) 0.4498(9) 0.1212(6) 0.101(5) Uani 1 1 d . . .
H41A H 0.2129 0.4058 0.0979 0.152 Uiso 1 1 calc R . .
H41B H 0.1989 0.4884 0.0901 0.152 Uiso 1 1 calc R . .
H41C H 0.2003 0.4413 0.1470 0.152 Uiso 1 1 calc R . .
C42 C 0.3288(6) 0.1406(10) 0.4314(8) 0.171(9) Uani 1 1 d DU . .
H42 H 0.3081 0.1715 0.3994 0.205 Uiso 1 1 calc R . .
C43 C 0.3228(7) 0.1194(10) 0.4834(8) 0.181(9) Uani 1 1 d DU . .
H43 H 0.2989 0.1352 0.4865 0.217 Uiso 1 1 calc R . .
C44 C 0.3545(7) 0.0732(9) 0.5304(9) 0.186(10) Uani 1 1 d DU . .
H44 H 0.3517 0.0578 0.5659 0.223 Uiso 1 1 calc R . .
C45 C 0.3902(7) 0.0495(9) 0.5255(10) 0.167(8) Uani 1 1 d DU . .
H45 H 0.4109 0.0185 0.5574 0.201 Uiso 1 1 calc R . .
C46 C 0.3947(6) 0.0725(9) 0.4729(9) 0.174(8) Uani 1 1 d DU . .
H46 H 0.4188 0.0569 0.4700 0.209 Uiso 1 1 calc R . .
C47 C 0.3640(6) 0.1183(9) 0.4246(10) 0.169(9) Uani 1 1 d DU . .
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H47 H 0.3668 0.1335 0.3891 0.202 Uiso 1 1 calc R . .
C48 C 0.2848(7) 0.2623(10) 0.6289(9) 0.155(7) Uani 1 1 d DU . .
H48 H 0.2759 0.3108 0.6255 0.186 Uiso 1 1 calc R . .
C49 C 0.3260(7) 0.2436(13) 0.6809(10) 0.197(10) Uani 1 1 d
DU . .
H49 H 0.3438 0.2790 0.7110 0.237 Uiso 1 1 calc R . .
C50 C 0.3404(7) 0.1714(12) 0.6875(9) 0.159(7) Uani 1 1 d DU . .
H50 H 0.3678 0.1578 0.7220 0.191 Uiso 1 1 calc R . .
C51 C 0.3131(5) 0.1200(11) 0.6417(7) 0.139(6) Uani 1 1 d DU . .
H51 H 0.3221 0.0715 0.6448 0.167 Uiso 1 1 calc R . .
C52 C 0.2722(5) 0.1415(8) 0.5909(7) 0.108(4) Uani 1 1 d DU . .
H52 H 0.2543 0.1059 0.5611 0.130 Uiso 1 1 calc R . .
C53 C 0.2563(6) 0.2128(8) 0.5818(8) 0.142(6) Uani 1 1 d DU . .
H53 H 0.2289 0.2262 0.5472 0.170 Uiso 1 1 calc R . .
C54 C 0.4111(5) 0.1876(10) 0.9041(9) 0.184(10) Uani 1 1 d
DU . .
H54 H 0.4034 0.2355 0.9077 0.221 Uiso 1 1 calc R . .
C55 C 0.4533(6) 0.1609(10) 0.9417(10) 0.299(19) Uani 1 1 d
DU . .
H55 H 0.4736 0.1942 0.9712 0.358 Uiso 1 1 calc R . .
C56 C 0.4696(6) 0.0917(9) 0.9419(10) 0.199(12) Uani 1 1 d
DU . .
H56 H 0.4987 0.0777 0.9689 0.239 Uiso 1 1 calc R . .
C57 C 0.4370(6) 0.0466(9) 0.8965(8) 0.135(6) Uani 1 1 d DU . .
H57 H 0.4447 -0.0011 0.8927 0.163 Uiso 1 1 calc R . .
C58 C 0.3937(6) 0.0666(9) 0.8561(8) 0.166(9) Uani 1 1 d DU . .
H58 H 0.3734 0.0333 0.8264 0.199 Uiso 1 1 calc R . .
C59 C 0.3813(5) 0.1372(9) 0.8608(8) 0.137(6) Uani 1 1 d DU . .
H59 H 0.3522 0.1511 0.8342 0.164 Uiso 1 1 calc R . .
C60 C 0.0149(12) 0.361(2) 0.3158(18) 0.236(14) Uani 1 1 d
DU . .
H60 H 0.0256 0.3629 0.3610 0.283 Uiso 1 1 calc R . .
C61 C 0.0451(9) 0.3607(15) 0.2943(14) 0.187(10) Uani 1 1 d
DU . .
H61 H 0.0749 0.3615 0.3255 0.224 Uiso 1 1 calc R . .
C62 C 0.0323(11) 0.359(2) 0.2277(15) 0.221(12) Uani 1 1 d
DU . .
H62 H 0.0520 0.3569 0.2125 0.265 Uiso 1 1 calc R . .
C63 C 0.4240(7) 0.4613(13) 0.6815(11) 0.223(13) Uani 1 1 d
DU . .
H63 H 0.4142 0.4938 0.6463 0.267 Uiso 1 1 calc R . .
C64 C 0.4634(8) 0.4242(16) 0.7042(17) 0.31(2) Uani 1 1 d DU . .
H64 H 0.4824 0.4279 0.6878 0.377 Uiso 1 1 calc R . .
C65 C 0.4688(15) 0.381(2) 0.7564(18) 0.36(2) Uani 1 1 d DU . .
H65 H 0.4949 0.3545 0.7734 0.426 Uiso 1 1 calc R . .
C66 C 0.4478(11) 0.3633(18) 0.7913(17) 0.48(3) Uani 1 1 d
DU . .
H66 H 0.4578 0.3307 0.8265 0.581 Uiso 1 1 calc R . .
C67 C 0.4091(11) 0.4032(10) 0.7646(6) 0.290(15) Uani 1 1 d
DU . .
H67 H 0.3904 0.3992 0.7814 0.348 Uiso 1 1 calc R . .
C68 C 0.399428(9) 0.449460(16) 0.711972(15) 0.201(11) Uani 1 1
d DU . .
H68 H 0.3734 0.4756 0.6951 0.242 Uiso 1 1 calc R . .
Cd1 Cd 0.291496(9) 0.896893(16) 0.686282(15) 0.03435(16) Uani
1 1 d R . .
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Cd2 Cd 0.323243(9) 0.546608(16) 0.471055(15) 0.03699(17) Uani
1 1 d R . .
Cd3 Cd 0.317343(9) 0.619594(16) 0.329819(15) 0.03455(16) Uani
1 1 d R . .
H24 H 0.602(2) 0.567(3) 0.650(3) 0.041 Uiso 1 1 d D . .

loop_
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 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
N1 0.026(4) 0.095(7) 0.045(4) -0.011(4) 0.004(3) -0.022(5)
N2 0.027(3) 0.024(3) 0.061(4) -0.008(3) -0.004(3) -0.001(3)
N3 0.176(14) 0.137(12) 0.212(15) 0.115(12) 0.147(13) 0.117(11)
N4 0.083(7) 0.065(6) 0.052(5) -0.009(4) 0.001(4) -0.014(5)
N5 0.060(5) 0.065(5) 0.054(5) -0.010(4) 0.013(4) 0.009(4)
O1 0.023(4) 0.041(5) 0.050(5) 0.001(4) 0.005(4) 0.001(4)
O1A 0.035(12) 0.069(16) 0.074(16) 0.013(13) -0.004(11)
0.013(11)
O2 0.042(5) 0.067(6) 0.063(5) -0.004(5) 0.023(4) -0.004(5)
O2A 0.034(14) 0.13(3) 0.053(17) 0.022(19) 0.004(13) -0.014(16)
O3 0.035(3) 0.036(3) 0.051(3) -0.003(2) 0.016(3) 0.003(2)
O4 0.055(3) 0.032(3) 0.043(3) -0.004(2) 0.019(3) 0.003(2)
O5 0.024(2) 0.026(3) 0.044(3) -0.009(2) 0.003(2) 0.001(2)
O6 0.023(2) 0.026(2) 0.043(3) -0.009(2) 0.004(2) -0.004(2)
O7 0.025(3) 0.037(3) 0.069(4) -0.013(3) 0.010(3) -0.002(2)
O8 0.024(3) 0.056(4) 0.053(3) -0.002(3) 0.005(3) 0.005(3)
O9 0.032(3) 0.023(2) 0.041(3) -0.004(2) 0.007(2) -0.003(2)
O10 0.026(3) 0.028(3) 0.048(3) -0.009(2) 0.005(2) 0.003(2)
O11 0.024(3) 0.030(3) 0.067(4) 0.015(3) -0.002(3) 0.001(2)
O12 0.027(2) 0.021(2) 0.046(3) 0.002(2) 0.009(2) 0.003(2)
O13 0.093(5) 0.033(3) 0.084(5) 0.010(3) 0.051(4) 0.016(3)
O14 0.039(3) 0.064(4) 0.047(3) -0.014(3) -0.005(3) 0.005(3)
O15 0.049(3) 0.039(3) 0.053(3) -0.007(3) 0.018(3) 0.001(3)
C1 0.031(5) 0.068(7) 0.074(7) 0.040(6) 0.014(5) 0.000(5)
C2 0.029(5) 0.075(7) 0.079(7) 0.035(6) 0.009(5) 0.007(5)
C3 0.072(7) 0.117(9) 0.131(9) 0.004(7) 0.019(6) -0.023(7)
C4 0.115(10) 0.162(11) 0.163(11) -0.033(8) 0.050(8) 0.009(8)
C5 0.091(9) 0.071(8) 0.107(9) -0.052(7) 0.049(8) -0.023(7)
C6 0.066(8) 0.138(13) 0.093(9) 0.015(8) 0.057(7) 0.009(8)
C8A 0.022(14) 0.022(13) 0.042(15) -0.002(12) 0.011(12)
0.009(11)
C7 0.084(7) 0.151(10) 0.097(8) 0.008(7) 0.048(6) 0.010(7)
C8 0.039(7) 0.092(11) 0.080(10) -0.053(9) 0.004(7) 0.008(7)
C9 0.038(4) 0.031(4) 0.035(4) -0.003(3) 0.013(3) -0.007(3)
C10 0.032(4) 0.023(3) 0.033(4) 0.002(3) 0.010(3) -0.002(3)
C11 0.023(3) 0.024(3) 0.030(3) 0.005(3) 0.003(3) -0.003(3)
C12 0.024(3) 0.023(3) 0.039(4) 0.000(3) 0.006(3) -0.003(3)
C13 0.025(3) 0.037(4) 0.045(4) -0.009(3) 0.013(3) -0.002(3)
C14 0.026(4) 0.042(4) 0.044(4) -0.010(3) 0.009(3) -0.012(3)
C15 0.035(4) 0.031(4) 0.036(4) -0.006(3) 0.010(3) -0.011(3)
C16 0.026(4) 0.021(3) 0.037(4) -0.002(3) 0.007(3) 0.000(3)
C17 0.023(4) 0.037(4) 0.049(5) -0.013(4) 0.003(3) 0.004(3)
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C18 0.022(4) 0.031(4) 0.051(5) -0.011(3) 0.002(3) 0.003(3)
C19 0.031(4) 0.040(5) 0.059(5) -0.001(4) 0.013(4) -0.001(3)
C20 0.029(4) 0.051(5) 0.045(5) -0.003(4) 0.004(3) -0.002(4)
C21 0.027(4) 0.031(4) 0.054(5) -0.008(3) -0.002(4) 0.000(3)
C22 0.033(5) 0.057(6) 0.113(9) 0.035(6) -0.013(5) -0.010(5)
C23 0.037(5) 0.057(6) 0.092(8) 0.034(6) -0.013(5) -0.003(5)
C24 0.028(4) 0.031(4) 0.051(5) -0.009(3) -0.001(4) 0.001(3)
C25 0.028(4) 0.027(4) 0.040(4) -0.004(3) 0.008(3) 0.000(3)
C26 0.024(3) 0.023(3) 0.040(4) 0.001(3) 0.000(3) -0.001(3)
C27 0.027(4) 0.027(4) 0.041(4) -0.007(3) 0.000(3) -0.004(3)
C28 0.025(4) 0.027(4) 0.043(4) 0.002(3) -0.001(3) 0.001(3)
C29 0.027(4) 0.024(4) 0.053(5) -0.004(3) 0.002(3) 0.000(3)
C30 0.025(3) 0.023(3) 0.037(4) -0.004(3) -0.001(3) -0.003(3)
C31 0.024(3) 0.024(4) 0.040(4) 0.000(3) 0.006(3) -0.003(3)
C32 0.029(4) 0.025(4) 0.041(4) 0.010(3) 0.005(3) 0.006(3)
C33 0.137(13) 0.072(9) 0.080(9) 0.015(7) 0.036(9) 0.017(9)
C34 0.33(4) 0.19(2) 0.39(4) 0.20(3) 0.30(4) 0.17(2)
C35 0.29(3) 0.17(2) 0.28(3) 0.13(2) 0.21(3) 0.16(2)
C36 0.057(6) 0.047(5) 0.038(4) -0.005(4) 0.005(4) -0.016(4)
C37 0.083(10) 0.096(11) 0.103(10) -0.012(9) -0.036(8) -0.014(8)
C38 0.154(14) 0.082(9) 0.062(7) -0.027(6) 0.053(8) -0.035(9)
C39 0.064(6) 0.054(6) 0.041(5) -0.010(4) 0.010(4) 0.006(5)
C40 0.062(6) 0.067(7) 0.068(6) -0.017(5) 0.026(5) 0.007(5)
C41 0.076(8) 0.125(12) 0.080(8) -0.042(8) 0.022(7) 0.001(8)
C42 0.21(2) 0.18(2) 0.137(14) 0.068(13) 0.100(15) 0.093(17)
C43 0.24(2) 0.18(2) 0.151(17) 0.057(14) 0.115(16) 0.067(17)
C44 0.30(3) 0.124(16) 0.131(14) 0.043(12) 0.108(17) 0.060(17)
C45 0.213(19) 0.081(12) 0.138(14) 0.016(10) 0.037(14) 0.038(13)
C46 0.149(16) 0.137(17) 0.21(2) 0.036(15) 0.070(15) 0.036(13)
C47 0.23(2) 0.118(15) 0.200(18) 0.058(13) 0.140(17) 0.075(15)
C48 0.228(19) 0.078(9) 0.23(2) -0.009(10) 0.168(15) -0.023(11)
C49 0.22(2) 0.196(17) 0.21(2) -0.051(19) 0.126(14) -0.067(17)
C50 0.115(12) 0.219(18) 0.141(14) 0.020(13) 0.063(10) -
0.041(12)
C51 0.138(13) 0.169(15) 0.133(14) 0.007(10) 0.084(10) 0.005(10)
C52 0.139(11) 0.096(8) 0.105(10) -0.010(8) 0.074(8) -0.021(9)
C53 0.205(17) 0.108(10) 0.137(13) 0.027(9) 0.105(11) 0.005(10)
C54 0.129(13) 0.122(14) 0.24(2) -0.046(14) 0.048(13) 0.038(10)
C55 0.149(15) 0.138(17) 0.35(3) -0.09(2) -0.064(18) 0.035(13)
C56 0.114(13) 0.120(14) 0.28(3) 0.027(15) 0.039(13) 0.033(10)
C57 0.213(16) 0.080(9) 0.147(15) 0.001(8) 0.115(12) 0.022(9)
C58 0.199(16) 0.111(11) 0.105(12) -0.005(10) 0.016(12) -
0.059(11)
C59 0.083(9) 0.145(12) 0.149(14) 0.055(11) 0.033(9) -0.007(8)
C60 0.21(3) 0.25(3) 0.25(2) -0.03(3) 0.12(2) 0.00(3)
C61 0.15(2) 0.17(2) 0.205(18) 0.04(2) 0.065(17) 0.019(17)
C62 0.16(2) 0.27(3) 0.20(2) 0.03(3) 0.064(18) 0.01(2)
C63 0.27(3) 0.20(2) 0.19(2) 0.040(18) 0.10(2) 0.10(2)
C64 0.33(4) 0.32(4) 0.35(4) 0.11(3) 0.21(3) 0.06(3)
C65 0.35(2) 0.36(2) 0.36(2) 0.001(5) 0.182(12) 0.003(5)
C66 0.56(4) 0.52(5) 0.40(4) 0.26(4) 0.26(3) 0.07(3)
C67 0.33(3) 0.39(4) 0.19(2) -0.18(2) 0.16(2) -0.18(2)
C68 0.094(13) 0.18(2) 0.29(3) -0.121(17) 0.071(15) -0.015(12)
Cd1 0.0192(3) 0.0256(3) 0.0414(3) -0.0064(2) 0.0027(2)
0.00082(19)

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Cd2 0.0255(3) 0.0283(3) 0.0412(3) -0.0026(2) 0.0049(2)
0.0042(2)
Cd3 0.0221(3) 0.0245(3) 0.0384(3) 0.0003(2) 0.0014(2)
0.00268(19)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

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O1A Cd1 2.42(2) . ?
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O3 Cd2 2.231(5) 7_566 ?
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O5 Cd3 2.340(5) . ?
O6 C16 1.239(8) . ?
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O7 Cd2 2.304(6) . ?
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O9 Cd2 2.377(5) 7_566 ?
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O2A C1 O1A 110(3) . 2_656 ?
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# start Validation Reply Form
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;
RESPONSE: This is caused by the disordered structure
of the compound. We have applied several restraints including
DFIX to fix the positions of the imine H atoms.
Although the disorder has been limited, it cannot be
completely eliminated.
;
_vrf_PLAT411_shelxl
;
RESPONSE: These H atoms belong to a disordered
benzene molecule and probably this causes these unusually
short H-H distances.
;
_vrf_PLAT220_shelxl
;
RESPONSE: This is due to the disorder of the atoms. We had
applied
 several restraints to limit it and we have managed to
reduce it significantly. However, the disorder could
not be eliminated completely.
;
_vrf_PLAT241_shelxl
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RESPONSE: This is due to the disorder of the atom. We had
 applied several restraints to limit it and we have managed
 to reduce it significantly. However, the disorder could not
 be eliminated completely.
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# end Validation Reply Form
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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 We have applied several restraints to limit the disorder of
the
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P=(Fo^2^+2Fc^2^)/3'
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PDU A 1
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PU A 2
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PDU A 1
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PU A 2
H3A H 0.0765 0.3406 0.1010 0.156 Uiso 0.50 1 calc PR A 2
C4 C 0.0066(8) 0.3316(16) 0.1439(12) 0.092(11) Uani 0.50 1 d
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PU A 2
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C10 C 0.3028(2) 0.2311(4) 0.4610(4) 0.0489(19) Uani 1 1 d U . .
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C15 C 0.2744(2) 0.1879(4) 0.4734(4) 0.049(2) Uani 1 1 d U . .
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C16 C 0.2395(3) 0.4080(5) 0.4607(6) 0.063(2) Uani 1 1 d U A .
C17 C 0.4041(4) 0.4125(9) 0.4362(9) 0.111(5) Uani 1 1 d U A .
C18 C 0.4520(4) 0.4025(6) 0.4850(6) 0.089(4) Uani 1 1 d U . .
C19 C 0.4770(5) 0.3447(10) 0.4754(9) 0.158(8) Uani 1 1 d U . .
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C20 C 0.5185(5) 0.3336(10) 0.5191(13) 0.198(12) Uani 1 1 d
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C24 C 0.0857(3) 0.1243(6) 0.1131(8) 0.112(6) Uani 1 1 d U . .
C25 C 0.2575(3) 0.5206(4) 0.3140(4) 0.055(2) Uani 1 1 d U A .
C26 C 0.2795(3) 0.5922(5) 0.3142(4) 0.053(2) Uani 1 1 d U . .
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C27 C 0.2527(3) 0.6533(4) 0.2842(4) 0.057(2) Uani 1 1 d U . .
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C28 C 0.2276(3) 0.2216(4) 0.2121(5) 0.062(2) Uani 1 1 d U . .
C29 C 0.1816(3) 0.2279(5) 0.1807(5) 0.071(3) Uani 1 1 d U . .
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A .
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DU . .
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H35C H 0.3160 0.5947 0.2159 0.290 Uiso 1 1 calc R . .
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H38C H 0.3679 0.3071 0.7020 0.190 Uiso 1 1 calc R . .
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DU . .
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H40B H 0.3062 0.6947 0.5078 0.448 Uiso 1 1 calc R . .
H40C H 0.3107 0.7024 0.4438 0.448 Uiso 1 1 calc R . .
C41 C 0.4086(10) 0.706(2) 0.5734(19) 0.37(2) Uani 1 1 d DU . .
H41A H 0.4068 0.7587 0.5753 0.551 Uiso 1 1 calc R . .
H41B H 0.4316 0.6933 0.5633 0.551 Uiso 1 1 calc R . .
H41C H 0.4149 0.6856 0.6151 0.551 Uiso 1 1 calc R . .
C42 C 0.4104(5) 0.4092(8) 0.2578(7) 0.154(9) Uani 0.50 1 d
PDU . .
H42 H 0.3989 0.4280 0.2862 0.185 Uiso 0.50 1 calc PR . .
C43 C 0.1682(5) 0.5768(7) 0.3575(7) 0.153(8) Uani 0.50 1 d
PDU . .
H43 H 0.1720 0.5308 0.3389 0.184 Uiso 0.50 1 calc PR . .
Cl1 Cl 0.3990(5) 0.4680(7) 0.1890(7) 0.184(5) Uani 0.50 1 d
PDU . .
Cl2 Cl 0.4688(5) 0.3949(8) 0.3001(7) 0.183(4) Uani 0.50 1 d
PDU . .
Cl3 Cl 0.3853(7) 0.3246(8) 0.2173(9) 0.243(8) Uani 0.50 1 d
PDU . .
Cl4 Cl 0.2143(5) 0.6356(7) 0.4057(7) 0.203(5) Uani 0.50 1 d
PDU . .
Cl5 Cl 0.1527(6) 0.6603(7) 0.3100(10) 0.232(6) Uani 0.50 1 d
PDU . .
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Cl6 Cl 0.1430(5) 0.5783(4) 0.4099(7) 0.184(5) Uani 0.50 1 d
PDU . .
N1 N -0.0894(3) 0.3396(5) 0.0879(4) 0.076(2) Uani 1 1 d U . .
N2 N 0.1111(4) 0.1754(6) 0.1116(7) 0.067(4) Uani 0.70 1 d
PU . .
N2A N 0.1049(10) 0.1624(18) 0.1393(14) 0.053(8) Uani 0.30 1 d
PU . .
N3 N 0.2595(6) 0.5409(9) 0.1672(10) 0.185(7) Uani 1 1 d DU . .
N4 N 0.4001(3) 0.3312(6) 0.6526(5) 0.117(4) Uani 1 1 d DU . .
N5 N 0.3671(7) 0.6776(7) 0.5228(10) 0.190(8) Uani 1 1 d DU . .
O1 O 0.1461(6) 0.3871(10) 0.2020(10) 0.107(6) Uani 0.50 1 d PU
A .
O1A O 0.1416(5) 0.3458(10) 0.2459(9) 0.068(4) Uani 0.50 1 d PU
A .
O2 O 0.1352(5) 0.4564(9) 0.2822(8) 0.102(4) Uani 0.60 1 d PU
A .
O2A O 0.1426(7) 0.3493(13) 0.2765(11) 0.076(6) Uani 0.40 1 d
PU A .
O3 O 0.24502(17) 0.2933(3) 0.3736(3) 0.0611(16) Uani 1 1 d
U . .
O4 O 0.31396(19) 0.3358(3) 0.4110(3) 0.0643(17) Uani 1 1 d
U . .
O5 O 0.2250(2) 0.4444(3) 0.4085(3) 0.0639(16) Uani 1 1 d U . .
O6 O 0.27931(19) 0.4046(3) 0.5023(4) 0.0702(18) Uani 1 1 d
U . .
O7 O 0.3808(2) 0.4559(4) 0.4408(5) 0.092(3) Uani 1 1 d U . .
O8 O 0.3899(3) 0.3749(7) 0.3803(6) 0.127(4) Uani 1 1 d U . .
O9 O 0.21806(17) 0.5122(3) 0.2794(3) 0.0646(17) Uani 1 1 d
U . .
O10 O 0.28253(17) 0.4689(3) 0.3499(3) 0.0562(15) Uani 1 1 d
U . .
O11 O 0.2393(2) 0.3467(3) 0.2444(3) 0.0663(17) Uani 1 1 d U . .
O12 O 0.2971(2) 0.2776(3) 0.2719(4) 0.0727(19) Uani 1 1 d U . .
O13 O 0.3159(3) 0.4573(5) 0.2463(5) 0.109(3) Uani 1 1 d DU . .
O14 O 0.3791(3) 0.4095(5) 0.5606(5) 0.115(3) Uani 1 1 d DU . .
O15 O 0.3283(3) 0.5668(4) 0.4884(5) 0.100(3) Uani 1 1 d DU . .

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0.0098(3)
Cd3 0.0430(4) 0.0444(4) 0.0836(5) -0.0046(3) 0.0100(4) -
0.0124(3)
C1 0.104(6) 0.107(6) 0.121(6) 0.021(4) 0.051(4) -0.009(4)
C2 0.042(12) 0.072(14) 0.070(13) -0.013(11) 0.018(11) -
0.019(10)
C2A 0.055(7) 0.059(7) 0.060(7) 0.004(4) 0.022(5) -0.003(5)
C3 0.040(13) 0.070(15) 0.100(19) 0.035(13) -0.002(13) 0.007(11)
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C3A 0.045(13) 0.10(2) 0.20(3) -0.09(2) 0.021(17) -0.018(12)
C4 0.031(13) 0.14(3) 0.079(19) 0.020(18) 0.008(13) -0.045(15)
C4A 0.034(10) 0.11(2) 0.13(2) -0.068(17) 0.027(12) -0.020(11)
C5 0.044(11) 0.048(11) 0.079(14) 0.031(10) 0.005(10) 0.020(8)
C5A 0.036(12) 0.057(12) 0.086(15) -0.037(11) 0.017(11) -
0.006(9)
C6 0.038(10) 0.064(14) 0.126(18) -0.033(12) 0.001(12) -0.023(9)
C6A 0.057(15) 0.20(4) 0.067(17) 0.009(19) 0.042(14) -0.038(18)
C7 0.023(9) 0.093(17) 0.102(16) 0.014(12) 0.009(10) 0.010(9)
C7A 0.035(13) 0.20(4) 0.064(14) -0.044(19) -0.008(12) -
0.027(18)
C8 0.046(11) 0.047(10) 0.086(13) -0.021(9) 0.020(10) -0.007(8)
C8A 0.038(11) 0.087(15) 0.072(12) -0.042(11) 0.003(10) -
0.002(10)
C9 0.030(4) 0.032(4) 0.073(5) 0.001(4) 0.001(4) 0.007(3)
C10 0.031(4) 0.039(4) 0.054(4) -0.001(3) 0.002(4) 0.000(3)
C11 0.033(4) 0.043(4) 0.059(5) 0.002(3) 0.009(4) 0.003(3)
C12 0.026(4) 0.046(5) 0.083(6) -0.009(4) 0.004(4) -0.010(3)
C13 0.035(4) 0.034(4) 0.062(5) -0.007(3) 0.003(4) -0.006(3)
C14 0.043(5) 0.032(4) 0.072(5) -0.001(4) 0.021(4) 0.003(3)
C15 0.024(4) 0.031(4) 0.066(5) -0.009(3) 0.000(3) 0.001(3)
C16 0.052(6) 0.033(4) 0.107(8) -0.011(5) 0.040(6) -0.003(4)
C17 0.046(7) 0.092(10) 0.154(13) 0.050(9) 0.014(8) -0.013(7)
C18 0.048(6) 0.060(6) 0.094(7) 0.004(5) -0.019(6) 0.006(5)
C19 0.078(10) 0.117(13) 0.154(13) -0.018(11) -0.046(10)
0.016(9)
C20 0.044(7) 0.109(13) 0.32(3) -0.055(16) -0.007(12) 0.024(8)
C21 0.040(5) 0.036(5) 0.135(9) -0.011(5) 0.017(6) 0.004(4)
C22 0.048(6) 0.111(11) 0.110(9) -0.013(8) 0.015(7) -0.018(7)
C23 0.061(8) 0.075(8) 0.155(12) 0.001(8) 0.025(8) 0.004(6)
C24 0.037(5) 0.054(6) 0.190(14) -0.045(8) 0.009(7) -0.004(5)
C25 0.037(4) 0.031(4) 0.077(5) 0.000(4) 0.012(4) -0.005(3)
C26 0.029(4) 0.039(4) 0.071(5) 0.005(4) 0.007(4) -0.002(3)
C27 0.027(4) 0.035(4) 0.078(5) 0.008(4) 0.000(4) 0.005(3)
C28 0.036(4) 0.026(4) 0.091(6) -0.011(4) 0.003(4) -0.008(3)
C29 0.040(5) 0.033(4) 0.100(7) -0.014(4) 0.001(5) 0.010(3)
C30 0.027(4) 0.045(5) 0.107(7) -0.022(5) -0.007(5) -0.002(4)
C31 0.047(5) 0.032(4) 0.101(7) 0.007(4) 0.000(5) 0.006(4)
C32 0.055(6) 0.030(4) 0.078(6) -0.012(4) 0.014(5) -0.011(4)
C33 0.152(14) 0.183(17) 0.175(17) 0.076(15) 0.011(13) -
0.041(12)
C34 0.229(14) 0.22(2) 0.158(16) 0.084(16) 0.118(14) 0.073(16)
C35 0.248(19) 0.18(2) 0.169(16) 0.065(16) 0.115(16) -0.014(16)
C36 0.094(9) 0.073(8) 0.112(8) -0.022(5) 0.007(6) 0.023(7)
C37 0.070(7) 0.26(2) 0.133(12) -0.060(13) 0.001(8) -0.011(10)
C38 0.136(12) 0.086(10) 0.115(10) 0.007(7) 0.025(9) 0.023(8)
C39 0.145(12) 0.085(8) 0.208(18) -0.024(11) 0.064(13) -0.039(9)
C40 0.34(2) 0.135(19) 0.37(3) -0.03(2) 0.13(2) 0.066(18)
C41 0.35(3) 0.21(3) 0.41(4) -0.12(3) 0.07(2) -0.15(2)
C42 0.147(12) 0.16(2) 0.19(2) 0.008(13) 0.115(16) -0.060(17)
C43 0.17(2) 0.20(2) 0.106(16) 0.059(14) 0.083(14) -0.036(15)
Cl1 0.194(11) 0.123(8) 0.235(12) 0.054(8) 0.103(9) 0.001(7)
Cl2 0.176(9) 0.194(12) 0.197(10) 0.014(8) 0.103(8) 0.006(8)
Cl3 0.289(17) 0.147(10) 0.249(14) 0.003(9) 0.092(12) -0.067(11)
Cl4 0.289(12) 0.165(10) 0.260(11) -0.093(9) 0.215(10) -0.089(9)
Cl5 0.290(14) 0.125(9) 0.384(16) 0.086(11) 0.245(12) 0.040(10)

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Cl6 0.313(14) 0.058(4) 0.307(13) -0.047(6) 0.251(13) -0.038(6)
N1 0.032(4) 0.086(7) 0.084(6) 0.006(5) 0.006(4) -0.015(4)
N2 0.035(6) 0.033(6) 0.093(9) -0.007(6) -0.001(6) 0.011(4)
N2A 0.053(9) 0.052(9) 0.056(9) -0.001(5) 0.026(6) 0.002(5)
N3 0.199(14) 0.130(13) 0.200(16) 0.036(11) 0.073(13) 0.000(10)
N4 0.080(6) 0.108(9) 0.111(7) -0.004(5) 0.005(6) 0.018(6)
N5 0.222(15) 0.098(8) 0.273(19) -0.096(11) 0.137(14) -0.057(9)
O1 0.080(12) 0.091(13) 0.113(13) -0.039(10) 0.016(10) 0.005(9)
O1A 0.067(6) 0.072(6) 0.068(5) -0.014(4) 0.035(4) -0.010(4)
O2 0.087(6) 0.102(6) 0.112(6) -0.005(4) 0.042(4) 0.002(4)
O2A 0.067(7) 0.081(7) 0.076(7) 0.009(5) 0.029(5) -0.003(4)
O3 0.030(3) 0.044(3) 0.075(4) 0.006(3) -0.003(3) 0.005(2)
O4 0.039(3) 0.034(3) 0.090(4) 0.005(3) 0.007(3) -0.004(2)
O5 0.062(4) 0.047(4) 0.086(4) 0.001(3) 0.038(4) 0.005(3)
O6 0.030(3) 0.048(3) 0.107(5) 0.000(3) 0.012(3) -0.003(2)
O7 0.041(4) 0.062(5) 0.151(7) 0.047(5) 0.027(4) 0.017(3)
O8 0.052(5) 0.158(11) 0.138(8) -0.003(8) 0.018(6) -0.026(6)
O9 0.027(3) 0.035(3) 0.099(4) -0.009(3) 0.004(3) -0.003(2)
O10 0.031(3) 0.034(3) 0.084(4) 0.004(3) 0.011(3) 0.007(2)
O11 0.061(4) 0.031(3) 0.087(4) -0.009(3) 0.019(3) -0.008(3)
O12 0.046(4) 0.046(3) 0.096(5) -0.011(3) 0.009(3) -0.014(3)
O13 0.111(7) 0.083(6) 0.135(7) -0.002(5) 0.060(6) -0.028(5)
O14 0.060(5) 0.069(5) 0.142(7) -0.007(5) -0.012(5) 0.004(4)
O15 0.100(6) 0.051(4) 0.122(6) -0.022(4) 0.032(5) -0.007(4)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Cd1 O1 2.417(17) . ?
Cd1 O10 2.607(6) . ?
Cd1 O2 2.616(16) . ?
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Cd2 O10 2.333(6) . ?
Cd2 O11 2.629(6) . ?
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Cd2 Cd3 3.4326(11) . ?
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Cd3 O4 2.343(6) . ?
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C1 O1 1.62(3) . ?
C2 C3 1.31(3) . ?
C2 C7 1.33(3) . ?
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C3 H3 0.9300 . ?
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C4 C5 1.45(3) . ?
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C13 C14 1.385(11) 2 ?
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C16 O6 1.251(11) . ?
C16 O5 1.254(12) . ?
C17 O7 1.172(19) . ?
C17 O8 1.33(2) . ?
C17 C18 1.509(16) . ?
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C19 C20 1.321(19) . ?
C19 H19 0.9300 . ?
C20 C21 1.35(2) 8_556 ?
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C21 C20 1.35(2) 8_455 ?
C21 C22 1.369(18) 8_455 ?
C21 C24 1.462(14) . ?
C22 C23 1.331(17) . ?
C22 C21 1.369(18) 8_556 ?
C22 H22 0.9300 . ?
C23 H23 0.9300 . ?
C24 N2A 0.95(3) . ?
C24 N2 1.29(2) . ?
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C25 O10 1.282(10) . ?
C25 C26 1.509(11) . ?
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C34 N3 1.451(2) . ?
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C34 H34C 0.9600 . ?
C35 N3 1.450(2) . ?
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C36 O14 1.251(2) . ?
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C37 N4 1.449(2) . ?
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C37 H37B 0.9600 . ?
C37 H37C 0.9600 . ?
C38 N4 1.450(2) . ?
C38 H38A 0.9600 . ?
C38 H38B 0.9600 . ?
C38 H38C 0.9600 . ?
C39 O15 1.249(5) . ?
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C40 H40B 0.9600 . ?
C40 H40C 0.9600 . ?
C41 N5 1.452(5) . ?
C41 H41A 0.9600 . ?
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C41 H41C 0.9600 . ?
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C43 H43 0.9800 . ?
Cl4 Cl5 2.27(2) . ?
N2 N2A 0.80(2) . ?
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O1A Cd1 O2 53.7(5) . . ?
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O1 Cd1 O2 57.3(6) . . ?
O10 Cd1 O2 122.3(4) . . ?
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O1A Cd1 C1 23.2(5) . . ?
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O3 Cd1 C1 116.3(4) . . ?
O9 Cd1 C1 97.3(4) . . ?
O11 Cd1 C1 111.9(4) . . ?
O1 Cd1 C1 36.3(6) . . ?
O10 Cd1 C1 149.2(4) . . ?
O2 Cd1 C1 30.6(5) . . ?
O8 Cd2 O12 108.2(4) . . ?
O8 Cd2 O13 100.3(4) . . ?
O12 Cd2 O13 103.3(3) . . ?
O8 Cd2 O4 89.9(4) . . ?
O12 Cd2 O4 89.5(3) . . ?
O13 Cd2 O4 160.0(3) . . ?
O8 Cd2 O10 120.1(4) . . ?
O12 Cd2 O10 127.7(2) . . ?
O13 Cd2 O10 87.1(3) . . ?
O4 Cd2 O10 72.9(2) . . ?
O8 Cd2 O11 161.3(4) . . ?
O12 Cd2 O11 53.0(2) . . ?
O13 Cd2 O11 86.3(3) . . ?
O4 Cd2 O11 89.4(2) . . ?
O10 Cd2 O11 77.4(2) . . ?
O8 Cd2 C32 134.9(4) . . ?
O12 Cd2 C32 26.7(3) . . ?
O13 Cd2 C32 96.9(3) . . ?
O4 Cd2 C32 87.7(3) . . ?
O10 Cd2 C32 102.0(2) . . ?
O11 Cd2 C32 26.4(2) . . ?
O8 Cd2 Cd3 86.2(4) . . ?
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O13 Cd2 Cd3 120.2(3) . . ?
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O11 Cd2 Cd3 105.77(16) . . ?
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O15 Cd3 O7 91.7(3) . . ?
O6 Cd3 O7 158.8(2) . . ?
O14 Cd3 O7 79.0(4) . . ?
O15 Cd3 O10 94.5(3) . . ?
O6 Cd3 O10 110.7(2) . . ?
O14 Cd3 O10 157.7(3) . . ?
O7 Cd3 O10 81.6(3) . . ?
O15 Cd3 O4 165.3(3) . . ?
O6 Cd3 O4 86.6(2) . . ?
O14 Cd3 O4 93.9(3) . . ?
O7 Cd3 O4 80.8(3) . . ?
O10 Cd3 O4 72.1(2) . . ?
O15 Cd3 Cd2 123.6(3) . . ?
O6 Cd3 Cd2 122.44(18) . . ?
O14 Cd3 Cd2 115.7(3) . . ?
O7 Cd3 Cd2 55.1(2) . . ?
O10 Cd3 Cd2 42.66(14) . . ?
O4 Cd3 Cd2 42.01(17) . . ?
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O2A C1 O2 106(2) . . ?
O1A C1 O2 126.8(18) . . ?
O2A C1 C2 127.9(19) . . ?
O1A C1 C2 130.3(19) . . ?
O2 C1 C2 102.2(16) . . ?
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O1A C1 C2A 103.4(19) . . ?
O2 C1 C2A 129.5(17) . . ?
C2 C1 C2A 30.6(10) . . ?
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O1A C1 O1 54.7(15) . . ?
O2 C1 O1 105.9(13) . . ?
C2 C1 O1 124.5(15) . . ?
C2A C1 O1 98.8(15) . . ?
O2A C1 Cd1 53.0(14) . . ?
O1A C1 Cd1 56.0(11) . . ?
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C2A C1 Cd1 157.1(15) . . ?
O1 C1 Cd1 62.0(8) . . ?
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C3 C2 C1 113(2) . . ?
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C4 C3 H3 117.0 . . ?
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C4 C5 C8 118.5(19) . . ?
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C6A C7A H7A 121.3 . . ?
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N1 C8A C5A 128.5(19) . . ?
O3 C9 O4 126.7(8) . . ?
O3 C9 C10 117.5(8) . . ?
O4 C9 C10 115.7(6) . . ?
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C15 C10 C9 120.7(7) . . ?
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C12 C11 H11 118.6 8_556 . ?
C10 C11 H11 118.6 . . ?
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C11 C12 C13 117.8(7) 8_455 . ?
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C14 C15 C10 119.7(7) 7_556 . ?
C14 C15 H15 120.1 7_556 . ?
C10 C15 H15 120.1 . . ?
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O6 C16 C14 114.9(9) . . ?
O5 C16 C14 121.2(8) . . ?
O7 C17 O8 118.9(13) . . ?
O7 C17 C18 125.0(17) . . ?
O8 C17 C18 115.5(16) . . ?
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C23 C18 C17 123.1(14) . . ?
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C20 C19 C18 120.5(16) . . ?
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C23 C22 C21 119.5(13) . 8_556 ?
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C18 C23 H23 118.3 . . ?
C22 C23 H23 118.3 . . ?
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N2 C24 C21 125.5(13) . . ?
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O9 C25 C26 121.0(7) . . ?
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C27 C26 C25 118.1(7) . . ?
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C28 C32 Cd2 166.1(6) . . ?
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N3 C34 H34B 109.5 . . ?
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N3 C34 H34C 109.5 . . ?
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N3 C35 H35B 109.5 . . ?
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H37B C37 H37C 109.5 . . ?
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N4 C38 H38B 109.5 . . ?
H38A C38 H38B 109.5 . . ?
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H38B C38 H38C 109.5 . . ?
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N5 C41 H41B 109.5 . . ?
H41A C41 H41B 109.5 . . ?
N5 C41 H41C 109.5 . . ?
H41A C41 H41C 109.5 . . ?
H41B C41 H41C 109.5 . . ?
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Cl2 C42 Cl1 106.5(10) . . ?
Cl3 C42 Cl1 101.7(9) . . ?
Cl2 C42 H42 113.4 . . ?
Cl3 C42 H42 113.4 . . ?
Cl1 C42 H42 113.4 . . ?
Cl4 C43 Cl6 98.4(8) . . ?
Cl4 C43 Cl5 78.2(10) . . ?
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Cl5 C43 H43 121.2 . . ?
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C43 Cl5 Cl4 50.8(5) . . ?
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C8A N1 C12 127.4(14) . . ?
C8 N1 C12 134.8(14) . . ?
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N2A N2 C30 94(3) . . ?
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C35 N3 C34 128.6(18) . . ?
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C1 O1 Cd1 81.7(10) . . ?
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O2A O1A O1 139(3) . . ?
C1 O1A O1 83.5(18) . . ?
O2A O1A Cd1 77(2) . . ?
C1 O1A Cd1 100.8(14) . . ?
O1 O1A Cd1 79.1(10) . . ?
C1 O2 Cd1 78.4(10) . . ?
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O1A O2A Cd1 85(2) . . ?
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C9 O3 Cd1 122.8(5) . . ?
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C9 O4 Cd3 118.5(6) . . ?
Cd2 O4 Cd3 95.2(2) . . ?
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C16 O6 Cd3 112.1(7) . . ?
C17 O7 Cd3 134.2(8) . . ?
C17 O8 Cd2 110.9(10) . . ?
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Cd2 O10 Cd3 94.49(18) . . ?
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Cd2 O10 Cd1 97.3(2) . . ?
Cd3 O10 Cd1 106.4(2) . . ?
C32 O11 Cd1 132.7(7) . . ?
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Cd1 O11 Cd2 96.6(2) . . ?
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  _platon_squeeze_void_count_electrons
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   2  0.000  0.025  0.250        12         1 ' '
   3  0.038  0.065  0.214         6         0 ' '
   4  0.962  0.065  0.286         6         0 ' '
   5  0.078  0.100  0.227         6         0 ' '
   6  0.922  0.100  0.273         5         0 ' '
   7  0.000  0.500  0.758      1493       260 ' '
   8  0.429  0.406  0.775         7         0 ' '
   9  0.571  0.406  0.725         7         0 ' '
  10  0.471  0.443  0.785         5         0 ' '
  11  0.529  0.443  0.715         5         0 ' '
  12  0.500  0.479  0.750        11         1 ' '
  13  0.500  0.525  0.250        12         1 ' '
  14  0.462  0.565  0.286         6         0 ' '
  15  0.538  0.565  0.214         6         0 ' '
  16  0.422  0.600  0.273         5         0 ' '
  17  0.578  0.600  0.227         6         0 ' '
  18  0.071  0.906  0.725         7         0 ' '
  19  0.929  0.906  0.775         7         0 ' '
  20  0.029  0.943  0.715         5         0 ' '
  21  0.971  0.943  0.785         5         0 ' '
  22  0.000  0.979  0.750        11         1 ' '

# start Validation Reply Form
_vrf_PLAT222_shelxl
;
RESPONSE: This is caused by the disordered structure
of the compound. We have applied several restraints
to limit this disorder.
Although the disorder has been reduced significantly,
it cannot be
completely eliminated.
;
_vrf_PLAT220_shelxl
;
RESPONSE: This is due to the disorder of the atoms. We had
applied
 several restraints to limit it and we have managed to
reduce it significantly. However, the disorder could
not be eliminated completely.
;
_vrf_PLAT241_shelxl
;
RESPONSE: This is due to the disorder of the atom. We had
 applied several restraints to limit it and we have managed
 to reduce it significantly. However, the disorder could not
 be eliminated completely.
;
_vrf_PLAT213_shelxl
;
RESPONSE:This is due to the disorder of the atoms. We had
applied
 several restraints to limit it and we have managed to
 reduce it significantly. However, the disorder could
not be eliminated completely.
```

```
;
_vrf_CHEMW03_shelxl
;
RESPONSE: The reported formula, molecular weight, F000,
density etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT043_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT042_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT068_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT041_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
;
_vrf_FORMU01_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
;
_vrf_CELLZ01_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (6.5 H2O),
which were removed by SQUEEZE.
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;

# end Validation Reply Form
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UCY-3/Toluene
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;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety
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 'C48 H56 Cd3 N5 O22'
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 'Cd'  'Cd'  -0.8075   1.2024
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_symmetry_space_group_name_H-M    'C 2/c'

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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_length_b                    18.4655(9)
_cell_length_c                    22.729(3)
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_cell_angle_beta                  118.603(12)
_cell_angle_gamma                 90.00
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_cell_measurement_temperature     100(2)
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Diffraction)'

_exptl_special_details
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 MERCURY (Bruno et al. 2002)
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;
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

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Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
 We have applied several restraints to limit the disorder of
the
 CIP ligands and solvent molecules.
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens    geom
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N3 N 0.1004(3) 0.1731(5) 0.3481(5) 0.086(3) Uani 1 1 d . . .
N4 N 0.1374(8) -0.1790(13) 0.4869(10) 0.188(7) Uani 1 1 d
DU . .
N5 N 0.2340(4) -0.0362(6) 0.8344(6) 0.099(3) Uani 1 1 d . . .
O1 O 0.3540(3) 0.1170(5) 0.8077(6) 0.113(4) Uani 1 1 d . . .
O2 O 0.3609(3) 0.1244(5) 0.7212(6) 0.104(3) Uani 1 1 d U . .
O3 O 0.2750(2) 0.0574(3) 0.5938(4) 0.0636(18) Uani 1 1 d . . .
O4 O 0.21965(17) 0.0978(3) 0.4965(3) 0.0643(18) Uani 1 1
d . . .
O5 O 0.18663(17) 0.1647(3) 0.5904(3) 0.0651(19) Uani 1 1
d . . .
O6 O 0.25488(16) 0.2062(3) 0.6302(3) 0.0603(17) Uani 1 1
d . . .
O7 O 0.11889(19) 0.0442(4) 0.5598(4) 0.073(2) Uani 1 1 d . . .
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O8 O 0.1089(2) 0.1301(5) 0.6175(5) 0.085(2) Uani 1 1 d . . .
O9 O 0.21775(16) 0.0333(3) 0.6528(3) 0.0592(17) Uani 1 1
d . . .
O10 O 0.28280(17) -0.0096(3) 0.7231(4) 0.071(2) Uani 1 1
d . . .
O11 O 0.20017(18) 0.2300(3) 0.7275(4) 0.072(2) Uani 1 1 d . . .
O12 O 0.25750(19) 0.1572(3) 0.7556(4) 0.0681(19) Uani 1 1
d . . .
O13 O 0.1206(2) 0.0993(4) 0.4374(4) 0.076(2) Uani 1 1 d . . .
O14 O 0.1725(3) -0.0626(4) 0.5080(5) 0.093(3) Uani 1 1 d D . .
O15 O 0.1852(3) 0.0458(4) 0.7620(5) 0.088(2) Uani 1 1 d . . .
C1 C 0.3770(4) 0.1207(6) 0.7799(8) 0.082(4) Uani 1 1 d . . .
C2 C -0.0739(3) 0.3705(6) 0.3213(7) 0.084(4) Uani 1 1 d . . .
C3 C -0.0559(4) 0.3547(8) 0.3903(9) 0.116(6) Uani 1 1 d . . .
H3 H -0.0732 0.3500 0.4112 0.139 Uiso 1 1 calc R . .
C4 C -0.0090(4) 0.3466(8) 0.4258(7) 0.098(4) Uani 1 1 d . . .
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C5 C 0.0168(3) 0.3500(6) 0.3965(7) 0.079(3) Uani 1 1 d . . .
C6 C -0.0033(4) 0.3685(8) 0.3299(6) 0.089(4) Uani 1 1 d . . .
H6 H 0.0137 0.3756 0.3087 0.107 Uiso 1 1 calc R . .
C7 C -0.0473(3) 0.3765(7) 0.2949(6) 0.082(3) Uani 1 1 d . . .
H7 H -0.0597 0.3869 0.2494 0.099 Uiso 1 1 calc R . .
C8 C 0.0637(3) 0.3436(5) 0.4365(5) 0.068(3) Uani 1 1 d . . .
C9 C 0.2391(3) 0.4063(5) 0.4586(5) 0.062(3) Uani 1 1 d . . .
C10 C 0.2092(3) 0.3619(5) 0.4745(5) 0.054(2) Uani 1 1 d . . .
C11 C 0.1651(3) 0.3706(5) 0.4393(5) 0.059(2) Uani 1 1 d . . .
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C12 C 0.1357(2) 0.3338(4) 0.4544(5) 0.056(2) Uani 1 1 d . . .
C13 C 0.1519(2) 0.2810(4) 0.5039(5) 0.057(2) Uani 1 1 d . . .
H13 H 0.1328 0.2530 0.5125 0.069 Uiso 1 1 calc R . .
C14 C 0.1972(2) 0.2704(4) 0.5403(4) 0.052(2) Uani 1 1 d . . .
C15 C 0.2250(2) 0.3107(4) 0.5258(5) 0.054(2) Uani 1 1 d . . .
H15 H 0.2553 0.3035 0.5509 0.065 Uiso 1 1 calc R . .
C16 C 0.2148(3) 0.2107(4) 0.5902(5) 0.060(3) Uani 1 1 d . . .
C17 C 0.0946(3) 0.0903(6) 0.5658(6) 0.073(3) Uani 1 1 d . . .
C18 C 0.0476(3) 0.1009(5) 0.5122(6) 0.066(3) Uani 1 1 d . . .
C19 C 0.0274(3) 0.0533(6) 0.4615(6) 0.076(3) Uani 1 1 d . . .
H19 H 0.0432 0.0155 0.4561 0.091 Uiso 1 1 calc R . .
C20 C -0.0164(3) 0.0611(6) 0.4182(6) 0.074(3) Uani 1 1 d . . .
H20 H -0.0305 0.0270 0.3845 0.089 Uiso 1 1 calc R . .
C21 C -0.0398(3) 0.1175(5) 0.4230(6) 0.075(3) Uani 1 1 d . . .
C22 C -0.0184(4) 0.1655(8) 0.4693(8) 0.112(5) Uani 1 1 d . . .
H22 H -0.0328 0.2079 0.4696 0.134 Uiso 1 1 calc R . .
C23 C 0.0247(4) 0.1561(8) 0.5179(8) 0.119(6) Uani 1 1 d . . .
H23 H 0.0376 0.1877 0.5540 0.143 Uiso 1 1 calc R . .
C24 C -0.0879(3) 0.1197(6) 0.3775(7) 0.087(4) Uani 1 1 d . . .
C25 C 0.2426(3) -0.0199(5) 0.6871(5) 0.064(3) Uani 1 1 d . . .
C26 C 0.2230(2) -0.0904(5) 0.6861(5) 0.058(2) Uani 1 1 d . . .
C27 C 0.1768(2) -0.0978(4) 0.6551(5) 0.057(2) Uani 1 1 d . . .
H27 H 0.1593 -0.0573 0.6362 0.068 Uiso 1 1 calc R . .
C28 C 0.1573(3) -0.1630(5) 0.6521(5) 0.068(3) Uani 1 1 d . . .
C29 C 0.1842(3) -0.2238(5) 0.6825(5) 0.063(3) Uani 1 1 d . . .
H29 H 0.1714 -0.2684 0.6812 0.075 Uiso 1 1 calc R . .
C30 C 0.2287(3) -0.2176(5) 0.7135(5) 0.065(3) Uani 1 1 d . . .
C31 C 0.2490(2) -0.1502(4) 0.7145(5) 0.053(2) Uani 1 1 d . . .
H31 H 0.2794 -0.1466 0.7342 0.063 Uiso 1 1 calc R . .
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C32 C 0.2414(3) 0.2194(5) 0.7550(5) 0.063(3) Uani 1 1 d . . .
C33 C 0.1291(3) 0.1435(6) 0.4017(5) 0.069(3) Uani 1 1 d . . .
C34 C 0.1155(6) 0.2240(9) 0.3166(8) 0.118(5) Uani 1 1 d U . .
H34A H 0.0908 0.2430 0.2772 0.177 Uiso 1 1 calc R . .
H34B H 0.1352 0.2004 0.3042 0.177 Uiso 1 1 calc R . .
H34C H 0.1306 0.2628 0.3471 0.177 Uiso 1 1 calc R . .
C35 C 0.0532(5) 0.1673(8) 0.3241(7) 0.109(4) Uani 1 1 d U . .
H35A H 0.0376 0.1943 0.2833 0.163 Uiso 1 1 calc R . .
H35B H 0.0463 0.1864 0.3573 0.163 Uiso 1 1 calc R . .
H35C H 0.0445 0.1173 0.3159 0.163 Uiso 1 1 calc R . .
C36 C 0.1355(10) -0.0976(16) 0.4926(14) 0.200(10) Uani 1 1 d
DU . .
C37 C 0.1846(10) -0.2142(17) 0.5142(14) 0.228(12) Uani 1 1 d
DU . .
H37A H 0.1816 -0.2657 0.5076 0.342 Uiso 1 1 calc R . .
H37B H 0.2019 -0.2039 0.5612 0.342 Uiso 1 1 calc R . .
H37C H 0.1988 -0.1944 0.4905 0.342 Uiso 1 1 calc R . .
C38 C 0.0945(10) -0.2210(17) 0.4675(15) 0.234(12) Uani 1 1 d
DU . .
H38A H 0.0995 -0.2718 0.4649 0.352 Uiso 1 1 calc R . .
H38B H 0.0719 -0.2044 0.4247 0.352 Uiso 1 1 calc R . .
H38C H 0.0853 -0.2131 0.5007 0.352 Uiso 1 1 calc R . .
C39 C 0.2229(5) 0.0222(8) 0.7962(7) 0.091(4) Uani 1 1 d U . .
C40 C 0.2818(5) -0.0564(8) 0.8716(8) 0.112(5) Uani 1 1 d U . .
H40A H 0.2852 -0.0998 0.8970 0.167 Uiso 1 1 calc R . .
H40B H 0.2982 -0.0179 0.9015 0.167 Uiso 1 1 calc R . .
H40C H 0.2925 -0.0646 0.8403 0.167 Uiso 1 1 calc R . .
C41 C 0.2017(5) -0.0865(9) 0.8311(8) 0.115(5) Uani 1 1 d U . .
H41A H 0.2160 -0.1254 0.8620 0.172 Uiso 1 1 calc R . .
H41B H 0.1858 -0.1055 0.7864 0.172 Uiso 1 1 calc R . .
H41C H 0.1817 -0.0624 0.8426 0.172 Uiso 1 1 calc R . .
C42 C 0.4501(8) 0.0577(14) 0.4019(12) 0.187(9) Uani 1 1 d
DU . .
H42 H 0.4410 0.0119 0.4069 0.224 Uiso 1 1 calc R . .
C43 C 0.4938(9) 0.0675(17) 0.4176(14) 0.223(12) Uani 1 1 d
DU . .
H43 H 0.5136 0.0295 0.4361 0.267 Uiso 1 1 calc R . .
C44 C 0.5084(10) 0.1335(15) 0.4060(14) 0.218(12) Uani 1 1 d
DU . .
H44 H 0.5368 0.1440 0.4139 0.262 Uiso 1 1 calc R . .
C45 C 0.4729(8) 0.1810(19) 0.3805(16) 0.243(14) Uani 1 1 d
DU . .
H45 H 0.4807 0.2246 0.3685 0.292 Uiso 1 1 calc R . .
C46 C 0.4293(8) 0.1834(12) 0.3674(11) 0.168(8) Uani 1 1 d
DU . .
H46 H 0.4106 0.2233 0.3538 0.202 Uiso 1 1 calc R . .
C47 C 0.4196(8) 0.1137(12) 0.3789(12) 0.171(8) Uani 1 1 d
DU . .
C48 C 0.3754(10) 0.1059(16) 0.3696(15) 0.227(13) Uani 1 1 d
DU . .
H48A H 0.3711 0.0572 0.3801 0.340 Uiso 1 1 calc R . .
H48B H 0.3545 0.1164 0.3238 0.340 Uiso 1 1 calc R . .
H48C H 0.3712 0.1390 0.3986 0.340 Uiso 1 1 calc R . .
Cd1 Cd 0.289856(17) 0.10808(3) 0.69520(4) 0.0567(3) Uani 1 1
d . . .

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Cd2 Cd 0.175985(18) 0.05373(3) 0.53504(4) 0.0620(3) Uani 1 1
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Cd3 Cd 0.178975(19) 0.11957(3) 0.68024(4) 0.0628(3) Uani 1 1
d . . .

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N2 0.018(3) 0.038(4) 0.124(7) 0.013(4) -0.011(4) -0.001(3)
N3 0.055(5) 0.071(6) 0.084(6) 0.025(5) -0.006(5) 0.002(5)
N4 0.189(9) 0.187(9) 0.189(8) -0.004(5) 0.091(6) -0.003(5)
N5 0.087(8) 0.071(6) 0.136(9) 0.027(6) 0.050(7) -0.011(6)
O1 0.032(4) 0.080(6) 0.181(10) -0.054(6) 0.015(5) -0.012(4)
O2 0.077(4) 0.112(5) 0.109(5) 0.011(4) 0.033(4) -0.014(4)
O3 0.043(4) 0.031(3) 0.084(5) 0.004(3) 0.005(3) -0.001(3)
O4 0.014(3) 0.043(3) 0.095(5) -0.003(3) -0.007(3) -0.003(2)
O5 0.018(3) 0.030(3) 0.110(5) 0.000(3) 0.001(3) -0.005(2)
O6 0.014(2) 0.035(3) 0.089(4) 0.006(3) -0.010(3) 0.002(2)
O7 0.024(3) 0.051(4) 0.117(6) 0.020(4) 0.013(3) 0.009(3)
O8 0.027(3) 0.082(5) 0.117(6) -0.018(5) 0.010(4) -0.004(4)
O9 0.015(2) 0.026(3) 0.095(4) 0.004(3) -0.007(3) 0.002(2)
O10 0.014(3) 0.039(3) 0.109(5) 0.004(3) -0.012(3) -0.004(2)
O11 0.024(3) 0.042(3) 0.114(5) -0.019(3) 0.003(3) -0.009(3)
O12 0.030(3) 0.041(4) 0.102(5) -0.016(3) 0.007(3) -0.008(3)
O13 0.023(3) 0.065(4) 0.095(5) 0.006(4) -0.007(3) -0.001(3)
O14 0.068(5) 0.044(4) 0.132(7) -0.010(4) 0.019(5) -0.014(4)
O15 0.058(5) 0.054(4) 0.138(7) 0.019(4) 0.035(5) 0.001(4)
C1 0.036(6) 0.063(7) 0.120(11) 0.014(7) 0.014(7) -0.017(5)
C2 0.025(5) 0.058(6) 0.121(10) -0.016(6) -0.003(6) 0.007(4)
C3 0.028(5) 0.096(10) 0.169(14) 0.047(10) 0.003(7) 0.008(6)
C4 0.043(6) 0.115(11) 0.098(9) 0.019(8) 0.004(6) -0.005(7)
C5 0.032(5) 0.072(7) 0.115(10) 0.009(7) 0.021(6) 0.013(5)
C6 0.047(6) 0.116(11) 0.084(8) 0.012(7) 0.015(6) 0.022(7)
C7 0.026(5) 0.092(9) 0.092(8) -0.007(6) -0.001(5) 0.002(5)
C8 0.032(5) 0.049(5) 0.093(7) 0.006(5) 0.006(5) 0.006(4)
C9 0.021(4) 0.045(5) 0.091(7) 0.005(5) 0.004(4) 0.006(4)
C10 0.023(4) 0.041(5) 0.078(6) 0.006(4) 0.008(4) 0.002(4)
C11 0.020(4) 0.040(4) 0.084(6) -0.004(4) -0.001(4) 0.004(4)
C12 0.020(4) 0.035(4) 0.080(6) 0.004(4) -0.004(4) 0.001(3)
C13 0.020(4) 0.033(4) 0.091(7) 0.008(4) 0.003(4) 0.005(3)
C14 0.021(4) 0.031(4) 0.072(6) 0.003(4) -0.003(4) -0.002(3)
C15 0.014(3) 0.027(4) 0.088(6) 0.002(4) -0.004(4) -0.002(3)
C16 0.023(4) 0.031(4) 0.096(7) -0.001(4) 0.004(4) 0.011(4)
C17 0.031(5) 0.064(7) 0.100(9) 0.025(6) 0.011(5) -0.006(5)
C18 0.024(4) 0.044(5) 0.094(7) 0.012(5) 0.000(5) 0.005(4)
C19 0.029(5) 0.062(6) 0.117(9) 0.013(6) 0.019(5) 0.012(5)
C20 0.032(5) 0.066(7) 0.101(8) 0.006(6) 0.013(5) 0.001(5)
C21 0.023(5) 0.037(5) 0.128(10) 0.015(5) 0.006(5) 0.004(4)
C22 0.030(5) 0.078(8) 0.173(13) 0.000(9) 0.005(7) 0.013(6)
C23 0.036(6) 0.091(10) 0.152(12) -0.041(9) -0.017(7) -0.008(6)
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C24 0.021(5) 0.062(7) 0.128(10) 0.026(6) -0.006(5) -0.007(4)
C25 0.020(4) 0.055(6) 0.093(7) 0.013(5) 0.008(4) 0.002(4)
C26 0.015(4) 0.036(4) 0.085(6) -0.007(4) -0.006(4) -0.003(3)
C27 0.014(4) 0.025(4) 0.093(7) 0.000(4) -0.006(4) 0.002(3)
C28 0.018(4) 0.040(5) 0.098(7) 0.005(5) -0.011(4) -0.005(4)
C29 0.027(4) 0.031(4) 0.096(7) 0.015(4) 0.001(4) 0.003(3)
C30 0.024(4) 0.033(4) 0.101(7) 0.005(5) 0.001(4) -0.003(4)
C31 0.015(3) 0.026(4) 0.084(6) 0.005(4) -0.004(4) 0.001(3)
C32 0.031(4) 0.029(4) 0.100(7) -0.011(4) 0.009(4) -0.009(4)
C33 0.046(6) 0.057(6) 0.074(7) -0.004(5) 0.004(5) -0.001(5)
C34 0.119(6) 0.118(7) 0.114(6) 0.004(4) 0.054(5) 0.003(5)
C35 0.100(6) 0.100(6) 0.111(6) 0.001(4) 0.038(4) 0.003(4)
C36 0.202(11) 0.199(11) 0.199(11) 0.000(5) 0.095(7) 0.002(5)
C37 0.230(13) 0.226(13) 0.226(12) -0.002(5) 0.108(7) 0.002(5)
C38 0.235(13) 0.236(13) 0.234(13) -0.001(5) 0.113(7) -0.003(5)
C39 0.090(5) 0.084(5) 0.091(5) 0.007(4) 0.036(4) 0.000(4)
C40 0.108(6) 0.104(6) 0.113(6) -0.001(4) 0.045(5) 0.005(4)
C41 0.110(6) 0.115(6) 0.121(6) 0.007(4) 0.056(5) -0.006(4)
C42 0.189(10) 0.185(11) 0.186(10) -0.004(5) 0.089(6) 0.007(5)
C43 0.225(13) 0.222(13) 0.222(13) 0.000(5) 0.107(7) -0.002(5)
C44 0.218(13) 0.220(13) 0.219(12) 0.001(5) 0.106(7) -0.002(5)
C45 0.244(14) 0.240(14) 0.243(14) 0.000(5) 0.114(8) 0.003(5)
C46 0.170(9) 0.164(9) 0.168(9) -0.001(5) 0.079(6) -0.005(5)
C47 0.172(10) 0.173(10) 0.168(9) 0.003(5) 0.081(6) 0.003(5)
C48 0.226(13) 0.228(14) 0.225(13) -0.004(5) 0.107(8) -0.002(5)
Cd1 0.0112(3) 0.0337(4) 0.0895(6) 0.0060(3) -0.0046(3) -
0.0011(2)
Cd2 0.0187(3) 0.0363(4) 0.0948(6) 0.0072(3) -0.0021(3) -
0.0044(2)
Cd3 0.0208(3) 0.0344(4) 0.1016(6) -0.0059(3) 0.0038(3) -
0.0049(2)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

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N5 C40 1.499(18) . ?
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O2 C1 1.175(15) . ?
O2 Cd1 2.256(10) . ?
O3 C9 1.246(12) 7_556 ?
O3 Cd1 2.305(7) . ?
O4 C9 1.300(10) 7_556 ?
O4 Cd2 2.231(7) . ?
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O5 Cd3 2.335(7) . ?
O5 Cd2 2.339(6) . ?
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O6 Cd1 2.285(5) . ?
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C1 C2 1.508(14) 8_556 ?
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N2 C28 C29 119.3(8) 5_556 . ?
C30 C29 C28 120.5(8) . . ?
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N3 C34 H34B 109.5 . . ?
H34A C34 H34B 109.5 . . ?
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;
RESPONSE: This is due to the disorder of the atoms. We had
applied
 several restraints to limit it and we have managed to
reduce it significantly. However, the disorder could
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not be eliminated completely.
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RESPONSE: This is due to the disorder of the atom. We had
 applied several restraints to limit it and we have managed
 to reduce it significantly. However, the disorder could not
 be eliminated completely.
;
_vrf_CHEMW03_shelxl
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RESPONSE: The reported formula, molecular weight, F000,
density etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (7 H2O),
which were removed by SQUEEZE.
;
_vrf_PLAT043_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
etc include
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and the contribution of disordered solvents (7 H2O),
which were removed by SQUEEZE.
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_vrf_PLAT042_shelxl
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RESPONSE:The reported formula, molecular weight, F000, density
etc include
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and the contribution of disordered solvents (7 H2O),
which were removed by SQUEEZE.
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RESPONSE:The reported formula, molecular weight, F000, density
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which were removed by SQUEEZE.
;
_vrf_PLAT041_shelxl
;
RESPONSE:The reported formula, molecular weight, F000, density
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and the contribution of disordered solvents (7 H2O),
which were removed by SQUEEZE.
;
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RESPONSE:The reported formula, molecular weight, F000, density
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and the contribution of disordered solvents (7 H2O),
which were removed by SQUEEZE.

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_vrf_CELLZ01_shelxl
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RESPONSE:The reported formula, molecular weight, F000, density
etc include
the imine H atoms that could not be located
and the contribution of disordered solvents (7 H2O),
which were removed by SQUEEZE.
;

end Validation Reply Form

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 'Eu'  'Eu'  -0.1578   3.6682
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 '-x, -y, -z'
 'x, -y, z-1/2'
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 'x+1/2, -y+1/2, z-1/2'

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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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C2 C 0.4441(4) 0.2112(10) 0.9278(9) 0.059(4) Uani 1 1 d . . .
C3 C 0.4575(4) 0.1146(11) 0.9304(10) 0.077(5) Uani 1 1 d . . .
H3 H 0.4380 0.0676 0.9513 0.092 Uiso 1 1 calc R . .
C4 C 0.4994(4) 0.0903(11) 0.5989(11) 0.084(5) Uani 1 1 d . . .
H4 H 0.4904 0.0264 0.5965 0.101 Uiso 1 1 calc R . .
C5 C 0.4700(4) 0.1570(10) 0.6311(9) 0.056(3) Uani 1 1 d . . .
C6 C 0.5152(4) 0.2508(11) 0.8625(11) 0.077(4) Uani 1 1 d . . .
H6 H 0.5342 0.2967 0.8381 0.093 Uiso 1 1 calc R . .
C7 C 0.4716(4) 0.2792(10) 0.8920(11) 0.068(4) Uani 1 1 d . . .
H7 H 0.4620 0.3427 0.8870 0.082 Uiso 1 1 calc R . .
C8 C 0.4240(4) 0.1394(11) 0.6596(10) 0.063(4) Uani 1 1 d D . .
C9 C 0.2459(3) 0.4109(8) 0.9115(8) 0.046(3) Uani 1 1 d . . .
C10 C 0.2160(4) 0.4776(9) 0.8551(8) 0.051(3) Uani 1 1 d . . .
C11 C 0.2660(4) 0.0389(8) 0.7120(9) 0.055(3) Uani 1 1 d . . .
H11 H 0.2347 0.0363 0.7214 0.066 Uiso 1 1 calc R . .
C12 C 0.2938(4) 0.1024(9) 0.7639(8) 0.051(3) Uani 1 1 d . . .
C13 C 0.3421(3) 0.1066(9) 0.7501(8) 0.055(3) Uani 1 1 d . . .
H13 H 0.3614 0.1470 0.7868 0.067 Uiso 1 1 calc R . .
C14 C 0.3593(4) 0.0497(9) 0.6815(10) 0.062(4) Uani 1 1 d . . .
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C15 C 0.3311(4) -0.0177(9) 0.6315(8) 0.053(3) Uani 1 1 d . . .
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C16 C 0.2763(4) 0.1657(9) 0.8393(9) 0.047(3) Uani 1 1 d . . .
C17 C 0.3402(4) 0.5412(9) 1.0792(12) 0.110(5) Uani 1 1 d DU . .
H17 H 0.3311 0.5496 1.0157 0.132 Uiso 1 1 calc R . .
C18 C 0.3462(5) 0.6221(13) 1.1359(11) 0.124(5) Uani 1 1 d
DU . .
H18 H 0.3415 0.6829 1.1101 0.149 Uiso 1 1 calc R . .
C19 C 0.3593(4) 0.6118(11) 1.2310(11) 0.102(4) Uani 1 1 d
DU . .
H19 H 0.3631 0.6652 1.2700 0.122 Uiso 1 1 calc R . .
C20 C 0.3667(4) 0.5203(9) 1.2668(10) 0.092(4) Uani 1 1 d DU . .
H20 H 0.3758 0.5101 1.3300 0.110 Uiso 1 1 calc R . .
C21 C 0.3598(3) 0.4445(9) 1.2041(7) 0.080(4) Uani 1 1 d DU . .
C22 C 0.3609(7) 0.3461(8) 1.2457(9) 0.110(5) Uani 1 1 d DU . .
H22A H 0.3886 0.3385 1.2873 0.132 Uiso 1 1 calc R . .
H22B H 0.3345 0.3375 1.2828 0.132 Uiso 1 1 calc R . .
N1 N 0.4063(3) 0.0547(9) 0.6584(8) 0.072(4) Uani 1 1 d . . .
N2 N 0.3469(3) 0.4510(8) 1.1117(7) 0.065(3) Uani 1 1 d D . .
O1 O 0.3760(3) 0.1797(6) 1.0075(6) 0.064(3) Uani 1 1 d . . .
O2 O 0.3870(2) 0.3281(6) 0.9566(5) 0.0442(18) Uani 1 1 d . . .
O3 O 0.2882(2) 0.4299(5) 0.9234(6) 0.051(2) Uani 1 1 d . . .
O4 O 0.2702(2) 0.1603(5) 1.0511(5) 0.0419(17) Uani 1 1 d . . .
O5 O 0.3023(2) 0.2271(6) 0.8754(5) 0.0471(19) Uani 1 1 d . . .
O6 O 0.2349(3) 0.1489(6) 0.8569(6) 0.061(2) Uani 1 1 d . . .
O7 O 0.3600(4) 0.2745(7) 1.1723(6) 0.080(3) Uani 1 1 d DU . .
H16 H 0.402(4) 0.191(7) 0.671(11) 0.096 Uiso 1 1 d D . .
Eu1 Eu 0.313795(15) 0.30007(4) 1.02528(3) 0.0365(2) Uani 1 1
d . . .

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C2 0.033(6) 0.093(11) 0.054(7) 0.014(7) 0.025(5) 0.009(7)
C3 0.030(6) 0.102(11) 0.102(11) 0.057(9) 0.037(7) 0.026(7)
C4 0.054(8) 0.086(10) 0.118(12) -0.042(10) 0.049(8) -0.026(8)
C5 0.023(5) 0.067(8) 0.081(9) -0.024(7) 0.021(6) -0.023(6)
C6 0.042(7) 0.083(10) 0.112(12) 0.017(9) 0.047(8) 0.009(8)
C7 0.045(7) 0.068(9) 0.097(11) 0.011(8) 0.038(7) 0.019(7)
C8 0.031(6) 0.082(10) 0.078(9) -0.022(8) 0.029(6) -0.014(7)
C9 0.024(5) 0.056(7) 0.059(7) 0.002(6) 0.019(5) 0.010(5)
C10 0.041(6) 0.057(7) 0.059(7) 0.014(6) 0.026(5) 0.011(6)
C11 0.030(5) 0.066(8) 0.072(8) -0.013(7) 0.024(5) -0.019(6)
C12 0.043(6) 0.059(7) 0.056(7) -0.019(6) 0.031(5) -0.013(6)
C13 0.033(6) 0.065(8) 0.072(8) -0.031(7) 0.036(5) -0.028(6)
C14 0.038(6) 0.063(8) 0.089(9) -0.031(7) 0.040(6) -0.018(6)
C15 0.039(6) 0.060(8) 0.063(7) -0.024(6) 0.028(6) -0.009(6)
C16 0.028(6) 0.053(7) 0.061(7) -0.013(6) 0.024(5) -0.001(5)
C17 0.114(7) 0.106(7) 0.110(6) -0.001(4) 0.007(5) -0.005(5)
C18 0.131(7) 0.119(7) 0.121(6) -0.002(4) 0.001(5) -0.002(5)
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C19 0.102(6) 0.100(5) 0.105(5) -0.005(4) 0.011(5) 0.001(5)
C20 0.089(6) 0.097(5) 0.090(5) -0.013(4) 0.012(4) -0.003(5)
C21 0.071(5) 0.092(5) 0.078(5) -0.006(4) 0.010(4) -0.003(4)
C22 0.112(7) 0.107(5) 0.110(6) -0.004(4) 0.009(5) 0.001(5)
N1 0.036(5) 0.094(9) 0.090(8) -0.052(7) 0.035(5) -0.024(6)
N2 0.046(6) 0.074(8) 0.077(8) -0.014(6) 0.020(5) -0.011(6)
O1 0.045(5) 0.073(6) 0.078(6) 0.028(5) 0.037(5) 0.025(4)
O2 0.018(3) 0.059(5) 0.058(5) -0.006(4) 0.019(3) -0.002(3)
O3 0.031(4) 0.059(5) 0.067(5) 0.010(4) 0.020(4) 0.007(4)
O4 0.032(4) 0.038(4) 0.058(5) 0.019(4) 0.019(3) -0.003(3)
O5 0.030(4) 0.063(5) 0.050(4) -0.010(4) 0.020(3) -0.011(4)
O6 0.042(4) 0.074(6) 0.072(6) -0.030(5) 0.039(4) -0.023(4)
O7 0.089(7) 0.096(6) 0.050(5) 0.016(5) -0.026(5) 0.005(6)
Eu1 0.0226(3) 0.0470(4) 0.0418(4) -0.0008(2) 0.0158(2)
0.0009(2)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C4 H4 0.9300 . ?
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C5 C8 1.447(14) . ?
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C6 C7 1.423(15) . ?
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C7 H7 0.9300 . ?
C8 N1 1.290(16) . ?
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C10 C11 1.411(15) 4_556 ?
C11 C12 1.377(15) . ?
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C11 H11 0.9300 . ?
C12 C13 1.433(14) . ?
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C13 C14 1.380(15) . ?
C13 H13 0.9300 . ?
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C21 C22 1.494(5) . ?
C22 O7 1.445(5) . ?
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C22 H22B 0.9700 . ?
N2 Eu1 2.588(10) . ?
O1 Eu1 2.496(8) . ?
O2 Eu1 2.439(6) . ?
O3 Eu1 2.404(8) . ?
O4 C9 1.235(13) 7_557 ?
O4 Eu1 2.369(7) . ?
O4 Eu1 2.660(7) 7_557 ?
O5 Eu1 2.364(8) . ?
O6 Eu1 2.382(7) 7_557 ?
O7 Eu1 2.429(8) . ?
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O1 C1 Eu1 62.4(5) . . ?
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O4 C9 O3 120.6(10) 7_557 . ?
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O4 C9 Eu1 66.1(6) 7_557 . ?
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C14 C15 H15 119.9 . . ?
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H22A C22 H22B 108.1 . . ?
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C21 N2 C17 114.9(13) . . ?
C21 N2 Eu1 118.5(8) . . ?
C17 N2 Eu1 123.8(9) . . ?
C1 O1 Eu1 90.7(6) . . ?
C1 O2 Eu1 93.5(6) . . ?
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C9 O4 Eu1 162.3(8) 7_557 . ?
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Eu1 O4 Eu1 104.6(3) . 7_557 ?
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C16 O6 Eu1 134.9(8) . 7_557 ?
C22 O7 Eu1 120.1(9) . . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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C3 C 0.4785(5) 0.2185(8) 0.9033(11) 0.101(5) Uani 1 1 d . . .
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C5 C 0.5351(4) 0.3338(9) 0.8727(8) 0.081(3) Uani 1 1 d . . .
C6 C 0.5050(4) 0.4022(9) 0.9018(9) 0.088(4) Uani 1 1 d . . .
H6 H 0.5130 0.4634 0.8987 0.105 Uiso 1 1 calc R . .
C7 C 0.4623(4) 0.3751(8) 0.9357(8) 0.080(3) Uani 1 1 d . . .
H7 H 0.4429 0.4191 0.9577 0.096 Uiso 1 1 calc R . .
C8 C 0.5826(4) 0.3507(9) 0.8455(9) 0.084(4) Uani 1 1 d D . .
C9 C 0.2509(3) 0.0968(5) 0.9082(6) 0.045(2) Uani 1 1 d . . .
C10 C 0.2199(3) 0.0276(5) 0.8506(6) 0.0401(18) Uani 1 1 d . . .
C11 C 0.2378(3) -0.0280(5) 0.7845(6) 0.0426(19) Uani 1 1
d . . .
H11 H 0.2695 -0.0217 0.7752 0.051 Uiso 1 1 calc R . .
C12 C 0.2090(3) -0.0932(6) 0.7316(6) 0.052(2) Uani 1 1 d . . .
C13 C 0.1606(3) -0.1035(7) 0.7456(6) 0.061(3) Uani 1 1 d . . .
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C14 C 0.6432(3) 0.4513(6) 0.8166(7) 0.059(3) Uani 1 1 d . . .
C15 C 0.1719(3) 0.0180(6) 0.8648(6) 0.048(2) Uani 1 1 d . . .
H15 H 0.1595 0.0574 0.9076 0.057 Uiso 1 1 calc R . .
C16 C 0.2275(3) -0.1538(7) 0.6597(7) 0.061(3) Uani 1 1 d . . .
C20 C 0.3802(14) 0.010(3) 1.098(3) 0.307(11) Uani 1 1 d DU . .
H20A H 0.4127 0.0055 1.1340 0.369 Uiso 1 1 calc R . .
H20B H 0.3827 0.0157 1.0281 0.369 Uiso 1 1 calc R . .
C21 C 0.3553(12) -0.078(2) 1.111(3) 0.305(9) Uani 1 1 d DU . .
C22 C 0.3494(11) -0.114(2) 1.203(3) 0.291(9) Uani 1 1 d DU . .
C23 C 0.3118(11) -0.1752(19) 1.180(3) 0.299(9) Uani 1 1 d
DU . .
H23 H 0.3054 -0.2024 1.2384 0.359 Uiso 1 1 calc R . .
C24 C 0.2806(13) -0.209(2) 1.099(3) 0.328(10) Uani 1 1 d DU . .
H24 H 0.2567 -0.2528 1.1010 0.393 Uiso 1 1 calc R . .
C25 C 0.2917(14) -0.167(2) 1.015(3) 0.325(10) Uani 1 1 d DU . .
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C26 C 0.3283(14) -0.103(3) 1.020(3) 0.314(10) Uani 1 1 d DU . .
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O1 O 0.3874(2) 0.1807(4) 0.9539(5) 0.0631(18) Uani 1 1 d . . .
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O3 O 0.29551(19) 0.0846(4) 0.9245(4) 0.0498(14) Uani 1 1
d . . .
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O6 O 0.2697(2) 0.1433(4) 1.1460(5) 0.0632(18) Uani 1 1 d . . .
O7 O 0.3546(14) 0.265(2) 1.208(3) 0.101(9) Uani 0.50 1 d
PDU . .
O7A O 0.3503(13) 0.255(3) 1.2028(16) 0.108(10) Uani 0.50 1 d
PU . .
O8 O 0.3632(3) 0.0836(6) 1.1235(6) 0.098(3) Uani 1 1 d . . .
O9 O 0.3769(8) -0.0627(16) 1.2836(17) 0.285(8) Uani 1 1 d
DU . .
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A .
N2 N 0.3606(11) 0.345(2) 1.352(2) 0.150(7) Uani 0.50 1 d
PDU . .
C18 C 0.3788(14) 0.393(2) 1.443(2) 0.159(10) Uani 0.50 1 d PDU
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H18B H 0.3932 0.3505 1.4922 0.239 Uiso 0.50 1 calc PR A 1
H18C H 0.3530 0.4241 1.4665 0.239 Uiso 0.50 1 calc PR A 1
C19 C 0.3234(13) 0.391(3) 1.395(3) 0.168(10) Uani 0.50 1 d PDU
A 2
H19A H 0.3380 0.4294 1.4486 0.251 Uiso 0.50 1 calc PR A 2
H19B H 0.3034 0.3468 1.4200 0.251 Uiso 0.50 1 calc PR A 2
H19C H 0.3043 0.4276 1.3453 0.251 Uiso 0.50 1 calc PR A 2
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C12 0.049(5) 0.058(5) 0.058(5) -0.022(4) 0.034(4) -0.015(4)
C13 0.047(5) 0.089(7) 0.053(5) -0.043(5) 0.027(4) -0.026(5)
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C15 0.038(4) 0.054(5) 0.059(5) -0.021(4) 0.031(4) -0.005(4)
C16 0.043(5) 0.083(7) 0.062(6) -0.030(5) 0.025(5) -0.017(5)
C20 0.308(12) 0.306(11) 0.309(12) 0.002(5) 0.053(5) -0.001(5)
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C22 0.291(10) 0.291(10) 0.292(9) -0.003(5) 0.052(5) 0.003(5)
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C24 0.329(11) 0.329(11) 0.324(11) 0.000(5) 0.050(5) -0.006(5)
C25 0.327(11) 0.326(11) 0.323(10) 0.002(5) 0.052(5) -0.004(5)
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O1 0.061(4) 0.049(3) 0.090(5) 0.007(3) 0.044(4) 0.005(3)
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O4 0.041(3) 0.047(3) 0.070(4) -0.019(3) 0.020(3) -0.004(3)
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O6 0.042(3) 0.083(4) 0.075(4) 0.033(4) 0.040(3) 0.013(3)
O7 0.10(2) 0.055(11) 0.14(2) -0.004(12) -0.006(15) 0.006(11)
O7A 0.096(18) 0.19(3) 0.026(8) 0.003(11) -0.022(9) -0.055(16)
O8 0.100(6) 0.091(6) 0.112(6) 0.039(5) 0.045(5) 0.051(5)
O9 0.284(9) 0.291(9) 0.281(8) 0.009(5) 0.048(5) -0.001(5)
C17 0.146(10) 0.148(10) 0.145(9) 0.001(5) 0.023(5) -0.001(5)
N2 0.158(9) 0.148(9) 0.143(8) -0.007(5) 0.021(5) -0.001(5)
C18 0.159(11) 0.162(11) 0.157(10) -0.004(5) 0.025(5) -0.003(5)
C19 0.168(11) 0.168(11) 0.166(11) -0.001(5) 0.026(5) 0.002(5)
Eu1 0.0263(2) 0.0398(3) 0.0427(3) 0.00179(17) 0.01518(17) -
0.00275(16)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
```

```
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

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C1 O1 1.265(12) . ?
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C1 Eu1 2.822(9) . ?
C2 C7 1.356(14) . ?
C2 C3 1.417(15) . ?
C3 C4 1.354(15) . ?
C3 H3 0.9300 . ?
C4 C5 1.424(18) . ?
C4 H4 0.9300 . ?
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C5 C8 1.472(14) . ?
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C7 H7 0.9300 . ?
C8 N1 1.360(14) . ?
C8 H16 1.01(2) . ?
C9 O3 1.256(10) . ?
C9 O4 1.257(9) 7_557 ?
C9 C10 1.482(11) . ?
C9 Eu1 2.898(9) . ?
C10 C11 1.373(10) . ?
C10 C15 1.406(10) . ?
C11 C12 1.383(11) . ?
C11 H11 0.9300 . ?
C12 C13 1.417(11) . ?
C12 C16 1.482(11) . ?
C13 C14 1.408(11) 3_445 ?
C13 H13 0.9300 . ?
C14 C15 1.369(11) 3 ?
C14 N1 1.405(10) . ?
C14 C13 1.408(11) 3 ?
C15 C14 1.369(11) 3_445 ?
C15 H15 0.9300 . ?
C16 O6 1.244(10) 6 ?
C16 O5 1.267(10) 4_546 ?
C20 O8 1.25(4) . ?
C20 C21 1.506(5) . ?
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C20 H20B 0.9700 . ?
C21 C26 1.391(5) . ?
C21 C22 1.394(5) . ?
C22 C23 1.388(5) . ?
C22 O9 1.449(5) . ?
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C24 C25 1.392(5) . ?
C24 H24 0.9300 . ?
C25 C26 1.390(5) . ?
C25 H25 0.9300 . ?
C26 H26 0.9300 . ?
O1 Eu1 2.465(6) . ?
O2 Eu1 2.471(6) . ?
O3 Eu1 2.426(5) . ?
O4 C9 1.257(9) 7_557 ?
O4 Eu1 2.360(6) . ?
O4 Eu1 2.627(6) 7_557 ?
O5 C16 1.267(10) 4_556 ?
O5 Eu1 2.366(6) . ?
O6 C16 1.244(10) 6_556 ?
O6 Eu1 2.382(5) . ?
O7 C17 1.251(5) . ?
O7 Eu1 2.52(4) . ?
O7A C17 1.29(6) . ?
O7A Eu1 2.38(2) . ?
O8 Eu1 2.451(7) . ?
O9 H9 0.8200 . ?
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N2 C18 1.449(5) . ?
N2 C19 1.452(5) . ?
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C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
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C19 H19B 0.9600 . ?
C19 H19C 0.9600 . ?
Eu1 O4 2.627(6) 7_557 ?

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O2 C1 C2 119.1(10) . . ?
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O1 C1 Eu1 60.7(4) . . ?
C2 C1 Eu1 177.0(7) . . ?
C7 C2 C3 119.9(9) . . ?
C7 C2 C1 120.7(9) . . ?
C3 C2 C1 119.4(9) . . ?
C4 C3 C2 120.7(11) . . ?
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C2 C3 H3 119.7 . . ?
C3 C4 C5 120.3(12) . . ?
C3 C4 H4 119.9 . . ?
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C6 C5 C4 119.3(9) . . ?
C6 C5 C8 124.4(11) . . ?
C4 C5 C8 116.2(11) . . ?
C5 C6 C7 118.3(11) . . ?
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C7 C6 H6 120.9 . . ?
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C2 C7 H7 119.3 . . ?
C6 C7 H7 119.3 . . ?
N1 C8 C5 118.0(11) . . ?
N1 C8 H16 116(10) . . ?
C5 C8 H16 91(10) . . ?
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O3 C9 C10 119.1(7) . . ?
O4 C9 C10 120.1(7) 7_557 . ?
O3 C9 Eu1 55.8(4) . . ?
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C11 C10 C9 120.4(6) . . ?
C15 C10 C9 119.8(7) . . ?
C10 C11 C12 120.4(7) . . ?
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C12 C11 H11 119.8 . . ?
C11 C12 C13 120.2(7) . . ?
C11 C12 C16 121.3(7) . . ?
C13 C12 C16 118.5(8) . . ?
C14 C13 C12 118.9(8) 3_445 . ?
C14 C13 H13 120.6 3_445 . ?
C12 C13 H13 120.6 . . ?
C15 C14 N1 119.3(7) 3 . ?
C15 C14 C13 119.5(7) 3 3 ?
N1 C14 C13 121.2(8) . 3 ?
C14 C15 C10 121.0(7) 3_445 . ?
C14 C15 H15 119.5 3_445 . ?
C10 C15 H15 119.5 . . ?
O6 C16 O5 124.6(8) 6 4_546 ?
O6 C16 C12 118.4(8) 6 . ?
O5 C16 C12 116.9(7) 4_546 . ?
O8 C20 C21 120(3) . . ?
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C21 C20 H20A 107.3 . . ?
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C26 C21 C20 108(4) . . ?
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C23 C22 C21 104(3) . . ?
C23 C22 O9 143(4) . . ?
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C22 C23 C24 141(4) . . ?
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C24 C23 H23 109.6 . . ?
C25 C24 C23 107(4) . . ?
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C21 C26 H26 119.4 . . ?
C8 N1 C14 115.9(8) . . ?
C1 O1 Eu1 92.7(5) . . ?
C1 O2 Eu1 92.8(6) . . ?
C9 O3 Eu1 98.9(5) . . ?
C9 O4 Eu1 162.2(6) 7_557 . ?
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Eu1 O4 Eu1 105.7(2) . 7_557 ?
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C16 O6 Eu1 134.4(6) 6_556 . ?
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C20 O8 Eu1 135.7(19) . . ?
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O7 C17 O7A 9(3) . . ?
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O7A C17 N2 122(3) . . ?
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N2 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N2 C19 H19A 109.5 . . ?
N2 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N2 C19 H19C 109.5 . . ?
H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
O4 Eu1 O5 72.2(2) . . ?
O4 Eu1 O6 80.7(2) . . ?
O5 Eu1 O6 134.1(2) . . ?
O4 Eu1 O3 124.1(2) . . ?
O5 Eu1 O3 78.3(2) . . ?
O6 Eu1 O3 87.8(2) . . ?
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O5 Eu1 O7A 134.9(9) . . ?
O6 Eu1 O7A 72.4(9) . . ?
O3 Eu1 O7A 146.3(10) . . ?
O4 Eu1 O7 79.6(7) . . ?
O5 Eu1 O7 132.0(8) . . ?
O6 Eu1 O7 75.5(9) . . ?
O3 Eu1 O7 148.7(7) . . ?
O7A Eu1 O7 3.2(17) . . ?
O4 Eu1 O8 144.7(2) . . ?
O5 Eu1 O8 143.1(2) . . ?
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O3 Eu1 O8 77.6(3) . . ?
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O7 Eu1 O8 72.2(7) . . ?
O4 Eu1 O1 136.8(2) . . ?
O5 Eu1 O1 74.4(2) . . ?
O6 Eu1 O1 142.4(2) . . ?
O3 Eu1 O1 73.5(2) . . ?
O7A Eu1 O1 105.9(9) . . ?
O7 Eu1 O1 104.2(9) . . ?
O8 Eu1 O1 72.1(2) . . ?
O4 Eu1 O2 91.2(2) . . ?
O5 Eu1 O2 72.8(3) . . ?
O6 Eu1 O2 145.2(2) . . ?
O3 Eu1 O2 123.7(2) . . ?
O7A Eu1 O2 72.9(9) . . ?
O7 Eu1 O2 69.7(9) . . ?
O8 Eu1 O2 98.3(3) . . ?
O1 Eu1 O2 52.8(2) . . ?
O4 Eu1 O4 74.3(2) . 7_557 ?
O5 Eu1 O4 69.4(2) . 7_557 ?
O6 Eu1 O4 67.9(2) . 7_557 ?
O3 Eu1 O4 51.00(17) . 7_557 ?
O7A Eu1 O4 135.5(9) . 7_557 ?
O7 Eu1 O4 137.7(9) . 7_557 ?
O8 Eu1 O4 113.9(3) . 7_557 ?
O1 Eu1 O4 117.7(2) . 7_557 ?
O2 Eu1 O4 142.1(3) . 7_557 ?
O4 Eu1 C1 114.1(3) . . ?
O5 Eu1 C1 70.8(2) . . ?
O6 Eu1 C1 155.1(2) . . ?
O3 Eu1 C1 98.6(3) . . ?
O7A Eu1 C1 89.9(9) . . ?
O7 Eu1 C1 87.3(9) . . ?
O8 Eu1 C1 85.6(3) . . ?
O1 Eu1 C1 26.6(3) . . ?
O2 Eu1 C1 26.2(3) . . ?
O4 Eu1 C1 133.8(2) 7_557 . ?
O4 Eu1 C9 99.6(2) . . ?
O5 Eu1 C9 73.1(2) . . ?
O6 Eu1 C9 75.9(2) . . ?
O3 Eu1 C9 25.35(19) . . ?
O7A Eu1 C9 147.9(9) . . ?
O7 Eu1 C9 151.1(9) . . ?
O8 Eu1 C9 95.2(3) . . ?
O1 Eu1 C9 96.1(2) . . ?
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C1 Eu1 C9 118.3(3) . . ?

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  _platon_squeeze_void_count_electrons
  _platon_squeeze_void_content
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   2  0.500  1.000 -0.014       548        91 ' '

# start Validation Reply Form
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;
RESPONSE: This is due to the severe disorder of this
atom, which could not eliminated although
we have applied several restaints to limit it.
;
_vrf_PLAT411_UCY-8-2hp
;
RESPONSE:These H atoms are attached to severely disordered C
atoms,
for which the disorder could not eliminated although
we have applied several restaints to limit it,
and this disorder results in unusual H-H distances.
;
```

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data_UCY-8-2-mIm

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 'C23 H19 Eu N4 O7'
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 'C23 H19 Eu N4 O7'
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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
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 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Eu'  'Eu'  -0.1578   3.6682
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loop_
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 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    29.974(3)
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_cell_angle_gamma                 90.00
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_cell_formula_units_Z             8
_cell_measurement_temperature     100(2)
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Source'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
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_refine_ls_number_reflns          5507
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d . . .
C1 C 0.3968(2) 0.2686(7) 0.4714(5) 0.0282(17) Uani 1 1 d . . .
C2 C 0.4417(2) 0.2455(7) 0.4358(5) 0.0294(17) Uani 1 1 d . . .
C3 C 0.4567(3) 0.1395(8) 0.4285(5) 0.041(2) Uani 1 1 d . . .
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C4 C 0.4991(3) 0.1181(8) 0.3994(6) 0.043(2) Uani 1 1 d . . .
H4 H 0.5086 0.0473 0.3932 0.051 Uiso 1 1 calc R . .
C5 C 0.5273(3) 0.2016(7) 0.3795(5) 0.0359(19) Uani 1 1 d . . .
C6 C 0.5124(3) 0.3082(7) 0.3854(6) 0.039(2) Uani 1 1 d . . .
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H7 H 0.4602 0.4009 0.4204 0.045 Uiso 1 1 calc R . .
C8 C 0.5739(3) 0.1851(7) 0.3570(6) 0.038(2) Uani 1 1 d D . .
C9 C 0.2428(2) 0.4433(6) 0.4377(4) 0.0188(14) Uani 1 1 d . . .
C10 C 0.2111(2) 0.5139(6) 0.3808(4) 0.0220(15) Uani 1 1 d . . .
C11 C 0.1653(2) 0.5168(6) 0.3928(4) 0.0227(15) Uani 1 1 d . . .
H11 H 0.1530 0.4720 0.4366 0.027 Uiso 1 1 calc R . .
C12 C 0.1382(2) 0.5861(6) 0.3396(5) 0.0259(16) Uani 1 1 d . . .
C13 C 0.1557(2) 0.6426(6) 0.2672(5) 0.0269(16) Uani 1 1 d . . .
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C15 C 0.2288(2) 0.5753(5) 0.3114(4) 0.0186(13) Uani 1 1 d . . .
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C16 C 0.2208(2) 0.6932(6) 0.1726(4) 0.0225(15) Uani 1 1 d . . .
C17 C 0.3383(4) 0.2843(11) 0.7647(9) 0.081(2) Uani 1 1 d U . .
C18 C 0.3453(4) 0.2901(10) 0.9371(8) 0.087(2) Uani 1 1 d U . .
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H18B H 0.3152 0.3153 0.9407 0.130 Uiso 1 1 calc R . .
H18C H 0.3653 0.3505 0.9376 0.130 Uiso 1 1 calc R . .
C19 C 0.3613(4) 0.1119(11) 0.8527(9) 0.091(2) Uani 1 1 d U . .
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 and torsion angles; correlations between esds in cell
parameters are only
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approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
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_exptl_crystal_density_diffrn     1.606
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'
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_diffrn_radiation_wavelength      0.71073
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_diffrn_radiation_source          'SuperNova (Mo) X-ray
Source'
_diffrn_radiation_monochromator   'mirror'
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Atlas'
_diffrn_measurement_method        '\w scans'
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_diffrn_standards_number          ?
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
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_refine_ls_R_factor_all           0.0354
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C2 C 0.44350(15) 0.7343(4) 0.9316(3) 0.0204(10) Uani 1 1
d . . .
C3 C 0.45815(17) 0.6339(4) 0.9203(4) 0.0335(13) Uani 1 1
d . . .
H3 H 0.4385 0.5794 0.9289 0.040 Uiso 1 1 calc R . .
C4 C 0.50154(17) 0.6135(4) 0.8964(4) 0.0364(13) Uani 1 1
d . . .
H4 H 0.5110 0.5457 0.8893 0.044 Uiso 1 1 calc R . .
C5 C 0.47332(16) 0.8148(4) 0.9190(4) 0.0260(11) Uani 1 1
d . . .
H5 H 0.4641 0.8825 0.9272 0.031 Uiso 1 1 calc R . .
C6 C 0.46898(17) 0.6945(4) 0.6170(4) 0.0279(12) Uani 1 1
d . . .
C7 C 0.48340(16) 0.7950(4) 0.6056(4) 0.0282(12) Uani 1 1
d . . .
H7 H 0.4639 0.8495 0.6146 0.034 Uiso 1 1 calc R . .
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C8 C 0.42188(16) 0.6763(4) 0.6376(4) 0.0276(11) Uani 1 1 d
D . .
C9 C 0.24425(14) 0.9378(3) 0.9450(3) 0.0126(9) Uani 1 1 d . . .
C10 C 0.28525(14) 0.5103(3) 0.6152(3) 0.0127(8) Uani 1 1
d . . .
C11 C 0.26577(14) 0.5766(3) 0.6790(3) 0.0132(9) Uani 1 1
d . . .
H11 H 0.2346 0.5779 0.6812 0.016 Uiso 1 1 calc R . .
C12 C 0.29325(14) 0.6407(3) 0.7394(3) 0.0125(9) Uani 1 1
d . . .
C13 C 0.33916(14) 0.6447(3) 0.7303(3) 0.0170(9) Uani 1 1
d . . .
H13 H 0.3574 0.6891 0.7695 0.020 Uiso 1 1 calc R . .
C14 C 0.35826(14) 0.5825(3) 0.6627(3) 0.0173(9) Uani 1 1
d . . .
C15 C 0.33155(14) 0.5121(3) 0.6080(3) 0.0161(9) Uani 1 1
d . . .
H15 H 0.3446 0.4664 0.5669 0.019 Uiso 1 1 calc R . .
C16 C 0.27269(14) 0.7019(3) 0.8175(3) 0.0124(9) Uani 1 1
d . . .
C17 C 0.32000(16) 1.0159(4) 1.1855(3) 0.0218(10) Uani 1 1
d . . .
H17 H 0.2887 1.0138 1.1731 0.026 Uiso 1 1 calc R . .
C18 C 0.38680(16) 1.0602(4) 1.2478(3) 0.0250(11) Uani 1 1
d . . .
H18 H 0.4103 1.0934 1.2844 0.030 Uiso 1 1 calc R . .
C19 C 0.39070(15) 0.9825(4) 1.1834(3) 0.0227(10) Uani 1 1
d . . .
C20 C 0.43299(17) 0.9318(5) 1.1566(4) 0.0377(14) Uani 1 1
d . . .
H20A H 0.4254 0.8794 1.1088 0.057 Uiso 1 1 calc R . .
H20B H 0.4486 0.9011 1.2133 0.057 Uiso 1 1 calc R . .
H20C H 0.4521 0.9824 1.1305 0.057 Uiso 1 1 calc R . .
C21 C 0.3618(3) 0.1439(6) 0.9099(5) 0.0614(17) Uani 1 1 d U . .
H21 H 0.3820 0.0928 0.8947 0.074 Uiso 1 1 calc R . .
C22 C 0.3159(3) 0.2338(7) 0.9879(6) 0.0652(17) Uani 1 1 d U . .
H22 H 0.2978 0.2550 1.0356 0.078 Uiso 1 1 calc R . .
C23 C 0.3241(3) 0.2843(6) 0.9089(6) 0.0676(19) Uani 1 1 d U . .
C24 C 0.3078(4) 0.3873(8) 0.8720(7) 0.102(3) Uani 1 1 d U . .
H24A H 0.3205 0.4023 0.8122 0.154 Uiso 1 1 calc R . .
H24B H 0.3169 0.4393 0.9191 0.154 Uiso 1 1 calc R . .
H24C H 0.2754 0.3865 0.8610 0.154 Uiso 1 1 calc R . .
N1 N 0.40512(12) 0.5877(3) 0.6464(3) 0.0231(9) Uani 1 1 d . . .
N2 N 0.34772(12) 0.9550(3) 1.1423(3) 0.0172(8) Uani 1 1 d . . .
N3 N 0.34153(13) 1.0805(3) 1.2485(3) 0.0222(9) Uani 1 1 d D . .
N4 N 0.3515(2) 0.2288(5) 0.8568(5) 0.0715(17) Uani 1 1 d U . .
N5 N 0.3394(2) 0.1446(4) 0.9852(5) 0.0609(15) Uani 1 1 d U . .
O1 O 0.38365(10) 0.8477(2) 0.9634(2) 0.0169(6) Uani 1 1 d . . .
O2 O 0.37298(10) 0.6810(2) 0.9835(2) 0.0188(7) Uani 1 1 d . . .
O3 O 0.27225(9) 0.6454(2) 1.0254(2) 0.0141(6) Uani 1 1 d . . .
O4 O 0.28493(9) 0.9598(2) 0.9648(2) 0.0154(6) Uani 1 1 d . . .
O5 O 0.23316(10) 0.6816(2) 0.8333(2) 0.0154(6) Uani 1 1 d . . .
O6 O 0.29786(9) 0.7696(2) 0.8624(2) 0.0133(6) Uani 1 1 d . . .
O7 O 0.35767(11) 0.7274(3) 1.1729(2) 0.0257(8) Uani 1 1 d . . .
H16 H 0.4033(15) 0.739(3) 0.645(4) 0.031 Uiso 1 1 d D . .
H24 H 0.3268(15) 1.129(3) 1.290(3) 0.031 Uiso 1 1 d D . .
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0.00013(8)
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C2 0.017(2) 0.023(2) 0.022(2) 0.003(2) 0.0066(19) 0.0012(19)
C3 0.023(3) 0.026(3) 0.053(3) 0.005(3) 0.016(2) -0.001(2)
C4 0.028(3) 0.026(3) 0.059(4) 0.008(3) 0.021(3) 0.008(2)
C5 0.022(3) 0.026(3) 0.031(3) 0.002(2) 0.008(2) 0.002(2)
C6 0.019(3) 0.032(3) 0.034(3) -0.008(2) 0.011(2) -0.003(2)
C7 0.018(3) 0.026(3) 0.041(3) -0.005(2) 0.009(2) 0.000(2)
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C9 0.017(2) 0.011(2) 0.0106(19) -0.0022(17) 0.0052(16)
0.0020(17)
C10 0.018(2) 0.010(2) 0.0110(19) 0.0013(17) 0.0048(16) -
0.0013(17)
C11 0.013(2) 0.014(2) 0.013(2) 0.0032(17) 0.0052(16) -
0.0011(17)
C12 0.017(2) 0.011(2) 0.0096(19) -0.0009(17) 0.0036(16) -
0.0004(17)
C13 0.018(2) 0.016(2) 0.018(2) -0.0032(18) 0.0050(18) -
0.0040(18)
C14 0.015(2) 0.018(2) 0.020(2) -0.0011(19) 0.0073(18) -
0.0035(18)
C15 0.015(2) 0.015(2) 0.019(2) -0.0025(18) 0.0073(17) -
0.0006(18)
C16 0.015(2) 0.014(2) 0.0091(19) 0.0051(17) 0.0013(16) -
0.0001(17)
C17 0.022(2) 0.019(2) 0.025(2) 0.001(2) 0.0046(19) -0.002(2)
C18 0.024(3) 0.026(3) 0.024(2) -0.006(2) -0.001(2) -0.004(2)
C19 0.023(3) 0.023(3) 0.022(2) -0.004(2) 0.0023(19) -0.004(2)
C20 0.021(3) 0.043(3) 0.049(3) -0.020(3) 0.000(2) 0.000(2)
C21 0.082(4) 0.047(3) 0.056(3) 0.000(3) 0.015(3) 0.003(3)
C22 0.066(5) 0.070(4) 0.060(4) -0.014(3) 0.007(3) -0.003(4)
C23 0.084(4) 0.068(3) 0.050(3) -0.011(3) 0.004(3) 0.019(3)
C24 0.129(5) 0.095(4) 0.083(4) 0.006(3) 0.009(4) 0.037(4)
N1 0.0133(19) 0.027(2) 0.030(2) -0.0111(18) 0.0079(16) -
0.0037(17)
N2 0.0149(18) 0.0155(19) 0.0217(19) -0.0016(16) 0.0047(15) -
0.0024(15)
N3 0.026(2) 0.018(2) 0.025(2) -0.0066(17) 0.0092(17) -
0.0019(17)
N4 0.092(4) 0.067(3) 0.058(3) 0.009(2) 0.019(3) 0.012(3)
N5 0.073(4) 0.043(3) 0.069(4) -0.002(3) 0.020(3) -0.020(3)
O1 0.0152(15) 0.0174(16) 0.0190(15) -0.0014(13) 0.0056(12) -
0.0011(13)
O2 0.0143(16) 0.0210(17) 0.0221(16) 0.0030(13) 0.0067(13)
0.0027(13)
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O4 0.0142(16) 0.0110(15) 0.0208(15) 0.0005(13) 0.0004(12) -
0.0028(12)
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0.0033(12)
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0.0022(12)
O7 0.0336(19) 0.0227(18) 0.0198(17) 0.0014(14) -0.0029(14)
0.0032(15)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O5 2.398(3) 7_567 ?
Eu1 O4 2.425(3) . ?
Eu1 O6 2.446(3) . ?
Eu1 O1 2.453(3) . ?
Eu1 O2 2.488(3) . ?
Eu1 N2 2.626(4) . ?
Eu1 O3 2.730(3) 7_567 ?
Eu1 C1 2.825(4) . ?
Eu1 C9 2.942(4) . ?
C1 O2 1.261(5) . ?
C1 O1 1.268(6) . ?
C1 C2 1.489(6) . ?
C2 C3 1.387(7) . ?
C2 C5 1.390(7) . ?
C3 C4 1.385(7) . ?
C3 H3 0.9300 . ?
C4 C6 1.391(7) 2_656 ?
C4 H4 0.9300 . ?
C5 C7 1.384(7) 2_656 ?
C5 H5 0.9300 . ?
C6 C7 1.385(7) . ?
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C6 C4 1.391(7) 2_656 ?
C6 C8 1.473(7) . ?
C7 C5 1.384(7) 2_656 ?
C7 H7 0.9300 . ?
C8 N1 1.262(6) . ?
C8 H16 0.99(2) . ?
C9 O4 1.248(5) . ?
C9 O3 1.269(5) 7_567 ?
C9 C10 1.487(6) 4_556 ?
C10 C15 1.388(6) . ?
C10 C11 1.396(6) . ?
C10 C9 1.487(6) 4_546 ?
C11 C12 1.389(6) . ?
C11 H11 0.9300 . ?
C12 C13 1.382(6) . ?
C12 C16 1.514(6) . ?
C13 C14 1.394(6) . ?
C13 H13 0.9300 . ?
C14 C15 1.388(6) . ?
C14 N1 1.432(5) . ?
C15 H15 0.9300 . ?
C16 O5 1.242(5) . ?
C16 O6 1.277(5) . ?
C17 N2 1.322(6) . ?
C17 N3 1.330(6) . ?
C17 H17 0.9300 . ?
C18 C19 1.358(7) . ?
C18 N3 1.371(6) . ?
C18 H18 0.9300 . ?
C19 N2 1.395(6) . ?
C19 C20 1.494(7) . ?
C20 H20A 0.9600 . ?
C20 H20B 0.9600 . ?
C20 H20C 0.9600 . ?
C21 N5 1.287(9) . ?
C21 N4 1.343(9) . ?
C21 H21 0.9300 . ?
C22 C23 1.316(11) . ?
C22 N5 1.353(10) . ?
C22 H22 0.9300 . ?
C23 N4 1.344(10) . ?
C23 C24 1.495(11) . ?
C24 H24A 0.9600 . ?
C24 H24B 0.9600 . ?
C24 H24C 0.9600 . ?
N3 H24 0.98(2) . ?
O3 C9 1.269(5) 7_567 ?
O3 Eu1 2.730(3) 7_567 ?
O5 Eu1 2.398(3) 7_567 ?

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O3 Eu1 O4 121.99(9) . . ?
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O5 Eu1 O4 90.42(10) 7_567 . ?
O3 Eu1 O6 75.00(10) . . ?
O7 Eu1 O6 139.66(10) . . ?
O5 Eu1 O6 132.53(10) 7_567 . ?
O4 Eu1 O6 72.71(10) . . ?
O3 Eu1 O1 130.26(10) . . ?
O7 Eu1 O1 90.76(11) . . ?
O5 Eu1 O1 149.07(10) 7_567 . ?
O4 Eu1 O1 84.32(10) . . ?
O6 Eu1 O1 74.64(9) . . ?
O3 Eu1 O2 80.45(10) . . ?
O7 Eu1 O2 69.25(11) . . ?
O5 Eu1 O2 139.35(10) 7_567 . ?
O4 Eu1 O2 130.20(10) . . ?
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O7 Eu1 O3 141.03(10) . 7_567 ?
O5 Eu1 O3 66.86(9) 7_567 7_567 ?
O4 Eu1 O3 49.91(9) . 7_567 ?
O6 Eu1 O3 68.56(9) . 7_567 ?
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O7 Eu1 C1 77.59(12) . . ?
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O4 Eu1 C1 108.59(11) . . ?
O6 Eu1 C1 72.86(11) . . ?
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N2 Eu1 C1 93.81(12) . . ?
O3 Eu1 C1 140.04(10) 7_567 . ?
O3 Eu1 C9 97.92(11) . . ?
O7 Eu1 C9 153.18(11) . . ?
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O6 Eu1 C9 66.66(10) . . ?
O1 Eu1 C9 104.91(11) . . ?
O2 Eu1 C9 137.49(10) . . ?
N2 Eu1 C9 89.49(11) . . ?
O3 Eu1 C9 25.50(10) 7_567 . ?
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C1 Eu1 C9 124.98(12) . . ?
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O7 Eu1 Eu1 119.83(8) . 7_567 ?
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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RED</i>. Oxford
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Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
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factors based
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A .
C2 C 0.9435(2) 0.2617(5) 0.4315(5) 0.0265(13) Uani 1 1 d . . .
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d . . .
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C15 C 0.73267(19) -0.0645(4) 0.3155(4) 0.0204(12) Uani 1 1
d . . .
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H18C H 0.8431 0.4474 0.8214 0.192 Uiso 0.50 1 calc PR A 1
C18A C 0.9050(8) 0.3908(17) 0.9138(16) 0.082(6) Uani 0.50 1 d
PU A 2
H18D H 0.8776 0.3712 0.9404 0.123 Uiso 0.50 1 calc PR A 2
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H18F H 0.9300 0.3517 0.9445 0.123 Uiso 0.50 1 calc PR A 2
C17 C 0.8822(6) 0.3141(13) 0.7122(14) 0.129(3) Uani 1 1 d DU A
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C19 C 0.9337(10) 0.394(2) 0.710(2) 0.126(4) Uani 0.50 1 d PDU
A 2
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N5 0.081(5) 0.046(4) 0.062(4) 0.007(4) 0.027(4) 0.020(4)
N6 0.016(4) 0.022(5) 0.013(4) 0.001(4) 0.006(3) 0.006(4)
N6A 0.104(6) 0.104(6) 0.104(6) 0.0000(10) 0.0121(13) 0.0001(10)
O1 0.018(2) 0.022(2) 0.028(2) 0.0015(17) 0.0106(16) 0.0026(16)
O2 0.024(2) 0.028(2) 0.050(3) -0.013(2) 0.024(2) -0.0094(18)
O3 0.0176(19) 0.0148(18) 0.024(2) -0.0013(15) 0.0089(15)
0.0012(15)
O4 0.015(2) 0.020(2) 0.031(2) -0.0038(17) 0.0050(16) -
0.0014(16)
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0.0045(18)
O6 0.015(2) 0.037(2) 0.024(2) 0.0110(18) 0.0118(16) 0.0018(18)
O7 0.038(3) 0.049(3) 0.037(3) 0.004(2) -0.009(2) -0.019(2)
C18 0.128(3) 0.128(4) 0.128(3) 0.0004(10) 0.0143(11) 0.0000(10)
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0.0001(10)
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0.0004(10)

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l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O4 2.431(4) . ?
Eu1 O2 2.455(4) . ?
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C9 O4 1.253(7) . ?
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N4 N5 1.359(9) . ?
N4 H17 1.00(2) . ?
O3 Eu1 2.357(4) 7_656 ?
O5 C16 1.257(7) 4_655 ?
O6 C16 1.246(7) 6_556 ?
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H18A C18 H18B 109.5 . . ?
N2 C18 H18C 109.5 . . ?
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H18E C18A H18F 109.5 . . ?
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O7 C17 Eu1 35.1(8) . . ?
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N2 C19 H19B 109.5 . . ?
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 MERCURY (Bruno et al. 2002)
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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Cryst</i>.
<b>30</b>, 565.

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Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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1 d . . .
C1 C 0.1023(2) 0.7447(6) 1.0406(5) 0.0330(15) Uani 1 1 d . . .
C2 C 0.0573(2) 0.7682(6) 1.0776(5) 0.0360(16) Uani 1 1 d U . .
C3 C 0.0310(3) 0.6894(7) 1.1084(7) 0.060(3) Uani 1 1 d . . .
H3 H 0.0428 0.6229 1.1131 0.072 Uiso 1 1 calc R . .
C4 C -0.0131(3) 0.7075(7) 1.1328(7) 0.060(3) Uani 1 1 d . . .
H4 H -0.0312 0.6532 1.1505 0.072 Uiso 1 1 calc R . .
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C7 C 0.0406(2) 0.8674(6) 1.0762(6) 0.0436(19) Uani 1 1 d . . .
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DU . .
C9 C 0.2548(2) 0.5656(5) 1.0651(4) 0.0258(14) Uani 1 1 d . . .
C10 C 0.28444(19) 0.4939(5) 1.1245(4) 0.0237(13) Uani 1 1
d . . .
C11 C 0.3305(2) 0.4882(5) 1.1120(4) 0.0284(14) Uani 1 1 d . . .
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H13 H 0.3564 0.3139 1.2699 0.036 Uiso 1 1 calc R . .
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d . . .
C15 C 0.2654(2) 0.4345(5) 1.1916(4) 0.0253(13) Uani 1 1 d . . .
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C16 C 0.2727(2) 0.3089(5) 1.3251(4) 0.0257(14) Uani 1 1 d . . .
C17 C 0.1940(7) 0.8794(17) 0.6096(13) 0.185(5) Uani 1 1 d
DU . .
H17 H 0.2170 0.9267 0.6260 0.222 Uiso 1 1 calc R . .
C18 C 0.1496(7) 0.9119(17) 0.6168(10) 0.177(5) Uani 1 1 d
DU . .
H18 H 0.1471 0.9817 0.6304 0.212 Uiso 1 1 calc R . .
C19 C 0.1081(7) 0.8612(16) 0.6077(11) 0.191(4) Uani 1 1 d
DU . .
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DU . .
C22 C 0.2071(7) 0.7824(16) 0.5802(14) 0.185(4) Uani 1 1 d
DU . .
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O8 O 0.14709(19) 0.7696(5) 0.8250(4) 0.0549(15) Uani 1 1
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C13 0.024(3) 0.041(4) 0.026(3) 0.013(3) 0.011(3) 0.009(3)
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C16 0.021(3) 0.035(4) 0.021(3) 0.004(3) 0.005(3) 0.003(3)
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N2 0.186(5) 0.192(5) 0.192(7) 0.002(5) 0.014(5) 0.004(4)
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O2 0.027(3) 0.035(3) 0.074(4) -0.010(3) 0.022(2) -0.001(2)
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
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N1 C12 1.421(8) 3_455 ?
O4 C9 1.271(7) 7_567 ?
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_cell_formula_units_Z             8
_cell_measurement_temperature     100(2)
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_exptl_crystal_size_mid           0.07
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_exptl_crystal_density_diffrn     1.565
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2448
_exptl_absorpt_coefficient_mu     2.443
_exptl_absorpt_correction_type    'multi-scan'
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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_diffrn_radiation_wavelength      0.71073
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_diffrn_radiation_source          'SuperNova (Mo) X-ray
Source'
_diffrn_radiation_monochromator   'mirror'
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Atlas'
_diffrn_measurement_method        '\w scans'
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_diffrn_standards_decay_%         ?
_diffrn_reflns_number             11119
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_diffrn_reflns_av_sigmaI/netI     0.0646
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_diffrn_reflns_limit_k_max        17
_diffrn_reflns_limit_l_min        -9
_diffrn_reflns_limit_l_max        14
_diffrn_reflns_theta_min          3.25
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_reflns_number_total              4591
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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Cryst</i>.
<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0887P)^2^+60.1560P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4591
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_refine_ls_number_restraints      19
_refine_ls_R_factor_all           0.0779
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_refine_ls_wR_factor_ref          0.1719
_refine_ls_wR_factor_gt           0.1609
_refine_ls_goodness_of_fit_ref    1.062
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d . . .
O1 O 0.8780(2) 0.1873(4) 0.5137(6) 0.0457(17) Uani 1 1 d . . .
O2 O 0.8864(2) 0.3292(4) 0.4571(5) 0.0395(15) Uani 1 1 d . . .
O3 O 0.78959(19) 0.4325(4) 0.4563(5) 0.0325(13) Uani 1 1
d . . .
O4 O 0.77156(18) 0.1558(4) 0.5362(5) 0.0292(13) Uani 1 1
d . . .
O5 O 0.76964(19) 0.3222(4) 0.6819(5) 0.0344(14) Uani 1 1
d . . .
O6 O 0.7982(2) 0.2490(4) 0.3567(5) 0.0375(14) Uani 1 1 d . . .
O7 O 0.8524(3) 0.2129(4) 0.7166(6) 0.0506(18) Uani 1 1 d U . .
C1 C 0.9006(3) 0.2478(7) 0.4700(8) 0.039(2) Uani 1 1 d . . .
C2 C 0.9457(3) 0.2210(6) 0.4367(8) 0.037(2) Uani 1 1 d . . .
C3 C 0.9584(3) 0.1294(7) 0.4337(9) 0.051(3) Uani 1 1 d . . .
H3 H 0.9380 0.0839 0.4479 0.061 Uiso 1 1 calc R . .
C4 C 1.0017(3) 0.1060(7) 0.4091(9) 0.050(3) Uani 1 1 d . . .
H4 H 1.0101 0.0450 0.4041 0.061 Uiso 1 1 calc R . .
C5 C 1.0325(3) 0.1759(7) 0.3920(9) 0.042(2) Uani 1 1 d . . .
```

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C6 C 1.0192(4) 0.2645(8) 0.3918(11) 0.064(3) Uani 1 1 d . . .
H6 H 1.0391 0.3104 0.3755 0.077 Uiso 1 1 calc R . .
C7 C 0.9760(4) 0.2871(7) 0.4158(11) 0.056(3) Uani 1 1 d . . .
H7 H 0.9676 0.3483 0.4177 0.067 Uiso 1 1 calc R . .
C8 C 1.0796(3) 0.1551(7) 0.3708(9) 0.046(2) Uani 1 1 d D . .
H16 H 1.102(3) 0.203(5) 0.374(9) 0.055 Uiso 1 1 d D . .
C9 C 0.7457(3) 0.4187(5) 0.4383(7) 0.0299(18) Uani 1 1 d . . .
C10 C 0.7160(3) 0.4928(5) 0.3859(7) 0.0288(18) Uani 1 1 d . . .
C11 C 0.6695(3) 0.4975(6) 0.3959(7) 0.0331(19) Uani 1 1 d . . .
H11 H 0.6564 0.4532 0.4359 0.040 Uiso 1 1 calc R . .
C12 C 0.6428(3) 0.5689(6) 0.3454(8) 0.037(2) Uani 1 1 d . . .
C13 C 0.6616(3) 0.6306(6) 0.2790(7) 0.0335(19) Uani 1 1 d . . .
H13 H 0.6432 0.6758 0.2419 0.040 Uiso 1 1 calc R . .
C14 C 0.7073(3) 0.6257(6) 0.2676(7) 0.0302(18) Uani 1 1 d . . .
C15 C 0.7354(3) 0.5582(6) 0.3239(7) 0.0313(19) Uani 1 1 d . . .
H15 H 0.7667 0.5571 0.3200 0.038 Uiso 1 1 calc R . .
C16 C 0.7277(3) 0.3100(6) 0.6936(8) 0.032(2) Uani 1 1 d . . .
C17 C 0.8516(4) 0.4961(8) 0.7104(10) 0.059(3) Uani 1 1 d . . .
C18 C 0.9194(5) 0.4538(9) 0.7995(14) 0.095(5) Uani 1 1 d U . .
C19 C 0.9039(4) 0.3926(9) 0.7232(12) 0.079(4) Uani 1 1 d . . .
H19 H 0.9197 0.3398 0.7097 0.094 Uiso 1 1 calc R . .
C20 C 0.9635(6) 0.4583(13) 0.8787(15) 0.117(6) Uani 1 1 d U . .
H20A H 0.9639 0.5130 0.9221 0.175 Uiso 1 1 calc R . .
H20B H 0.9890 0.4590 0.8382 0.175 Uiso 1 1 calc R . .
H20C H 0.9657 0.4059 0.9262 0.175 Uiso 1 1 calc R . .
C21 C 0.8114(4) 0.5560(9) 0.6755(10) 0.062(3) Uani 1 1 d . . .
H21A H 0.8037 0.5885 0.7391 0.075 Uiso 1 1 calc R . .
H21B H 0.7853 0.5183 0.6465 0.075 Uiso 1 1 calc R . .
C22 C 0.8202(5) 0.6250(8) 0.5882(13) 0.083(4) Uani 1 1 d . . .
H22A H 0.7932 0.6615 0.5677 0.124 Uiso 1 1 calc R . .
H22B H 0.8275 0.5932 0.5247 0.124 Uiso 1 1 calc R . .
H22C H 0.8454 0.6638 0.6172 0.124 Uiso 1 1 calc R . .
C23 C 0.8479(5) 0.2209(9) 0.8315(11) 0.075(4) Uani 1 1 d U . .
H23A H 0.8347 0.2799 0.8447 0.090 Uiso 1 1 calc R . .
H23B H 0.8781 0.2175 0.8755 0.090 Uiso 1 1 calc R . .
C24 C 0.8187(6) 0.1479(11) 0.8657(13) 0.097(5) Uani 1 1 d U . .
H24A H 0.8159 0.1555 0.9420 0.146 Uiso 1 1 calc R . .
H24B H 0.8322 0.0895 0.8550 0.146 Uiso 1 1 calc R . .
H24C H 0.7888 0.1511 0.8222 0.146 Uiso 1 1 calc R . .
N1 N 1.0960(2) 0.0747(5) 0.3624(7) 0.0424(19) Uani 1 1 d . . .
N2 N 0.8609(3) 0.4165(5) 0.6651(7) 0.0445(19) Uani 1 1 d . . .
N3 N 0.8855(4) 0.5219(7) 0.7927(9) 0.076(3) Uani 1 1 d U . .

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0.00046(15)
O1 0.032(4) 0.032(4) 0.076(5) 0.012(3) 0.018(3) 0.009(3)
O2 0.032(3) 0.025(3) 0.063(4) -0.004(3) 0.009(3) 0.002(3)
O3 0.026(3) 0.022(3) 0.048(4) 0.000(3) 0.000(2) 0.002(2)
```

```
O4 0.024(3) 0.019(3) 0.044(3) 0.001(2) 0.003(2) 0.002(2)
O5 0.022(3) 0.033(3) 0.048(4) -0.005(3) 0.005(2) -0.003(2)
O6 0.030(3) 0.027(3) 0.058(4) -0.011(3) 0.013(3) -0.005(3)
O7 0.054(5) 0.047(4) 0.046(4) -0.001(3) -0.007(3) 0.008(3)
C1 0.033(5) 0.034(5) 0.049(6) -0.004(4) 0.004(4) 0.011(4)
C2 0.031(5) 0.027(5) 0.055(6) 0.007(4) 0.007(4) -0.006(4)
C3 0.035(5) 0.035(5) 0.089(8) 0.008(5) 0.027(5) -0.002(4)
C4 0.040(6) 0.037(6) 0.078(8) 0.008(5) 0.019(5) 0.010(4)
C5 0.021(5) 0.034(5) 0.073(7) 0.009(5) 0.013(4) 0.007(4)
C6 0.038(6) 0.047(7) 0.111(10) 0.011(7) 0.030(6) 0.001(5)
C7 0.031(6) 0.030(5) 0.112(10) 0.008(5) 0.023(6) 0.013(4)
C8 0.030(5) 0.039(6) 0.068(7) 0.009(5) 0.008(5) 0.002(4)
C9 0.025(4) 0.018(4) 0.046(5) -0.006(4) 0.003(4) -0.001(3)
C10 0.026(4) 0.023(4) 0.037(5) -0.001(3) 0.003(3) 0.000(3)
C11 0.033(5) 0.030(5) 0.035(5) 0.009(4) 0.004(4) 0.002(4)
C12 0.014(4) 0.028(5) 0.069(6) 0.001(4) 0.008(4) 0.000(3)
C13 0.026(4) 0.024(4) 0.051(5) 0.005(4) 0.006(4) 0.007(4)
C14 0.022(4) 0.023(4) 0.046(5) 0.002(4) 0.006(3) -0.002(3)
C15 0.024(4) 0.028(4) 0.042(5) 0.003(4) 0.006(3) 0.000(3)
C16 0.023(5) 0.027(4) 0.047(5) 0.001(4) 0.008(4) 0.001(3)
C17 0.036(6) 0.051(7) 0.087(9) -0.003(6) 0.004(5) -0.004(5)
C18 0.086(10) 0.050(7) 0.126(13) -0.014(8) -0.056(9) 0.004(7)
C19 0.050(7) 0.049(7) 0.128(12) -0.024(7) -0.018(7) -0.002(6)
C20 0.115(7) 0.112(7) 0.117(7) -0.001(5) -0.001(5) 0.002(5)
C21 0.049(7) 0.070(8) 0.071(8) -0.002(6) 0.018(6) 0.002(6)
C22 0.072(9) 0.037(6) 0.141(13) 0.008(8) 0.023(8) -0.018(6)
C23 0.077(10) 0.073(9) 0.068(9) 0.004(7) -0.011(7) 0.012(7)
C24 0.100(6) 0.095(6) 0.096(6) 0.005(5) 0.014(4) -0.006(5)
N1 0.027(4) 0.034(4) 0.069(6) 0.013(4) 0.017(4) 0.006(3)
N2 0.036(4) 0.036(4) 0.061(5) -0.010(4) 0.005(4) -0.001(4)
N3 0.080(8) 0.059(7) 0.079(8) -0.002(6) -0.018(6) -0.010(6)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O4 2.368(5) . ?
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Eu1 O3 2.405(5) . ?
Eu1 O1 2.459(6) . ?
Eu1 O7 2.497(7) . ?
Eu1 O2 2.544(6) . ?
Eu1 N2 2.584(8) . ?
Eu1 O4 2.730(5) 7_656 ?
Eu1 C1 2.863(9) . ?
Eu1 C9 2.939(8) . ?
O1 C1 1.272(12) . ?
O2 C1 1.264(11) . ?
O3 C9 1.295(10) . ?
O4 C9 1.262(9) 7_656 ?
O4 Eu1 2.730(5) 7_656 ?
O5 C16 1.277(10) . ?
O6 C16 1.252(11) 7_656 ?
O7 C23 1.442(16) . ?
C1 C2 1.501(13) . ?
C2 C7 1.365(13) . ?
C2 C3 1.392(13) . ?
C3 C4 1.398(13) . ?
C3 H3 0.9300 . ?
C4 C5 1.401(13) . ?
C4 H4 0.9300 . ?
C5 C6 1.353(15) . ?
C5 C8 1.481(13) . ?
C6 C7 1.388(14) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 N1 1.280(12) . ?
C8 H16 0.95(2) . ?
C9 O4 1.262(9) 7_656 ?
C9 C10 1.478(11) . ?
C10 C11 1.395(12) . ?
C10 C15 1.396(11) . ?
C11 C12 1.397(12) . ?
C11 H11 0.9300 . ?
C12 C13 1.385(12) . ?
C12 N1 1.428(11) 3_455 ?
C13 C14 1.376(11) . ?
C13 H13 0.9300 . ?
C14 C15 1.402(11) . ?
C14 C16 1.494(12) 6_565 ?
C15 H15 0.9300 . ?
C16 O6 1.252(11) 7_656 ?
C16 C14 1.494(12) 6_566 ?
C17 N2 1.336(13) . ?
C17 N3 1.364(14) . ?
C17 C21 1.484(15) . ?
C18 C19 1.327(17) . ?
C18 N3 1.403(17) . ?
C18 C20 1.50(2) . ?
C19 N2 1.403(14) . ?
C19 H19 0.9300 . ?
C20 H20A 0.9600 . ?
C20 H20B 0.9600 . ?
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C20 H20C 0.9600 . ?
C21 C22 1.522(17) . ?
C21 H21A 0.9700 . ?
C21 H21B 0.9700 . ?
C22 H22A 0.9600 . ?
C22 H22B 0.9600 . ?
C22 H22C 0.9600 . ?
C23 C24 1.47(2) . ?
C23 H23A 0.9700 . ?
C23 H23B 0.9700 . ?
C24 H24A 0.9600 . ?
C24 H24B 0.9600 . ?
C24 H24C 0.9600 . ?
N1 C12 1.428(11) 3_545 ?

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O5 Eu1 O6 132.7(2) . . ?
O4 Eu1 O6 72.2(2) . . ?
O5 Eu1 O3 89.0(2) . . ?
O4 Eu1 O3 123.97(19) . . ?
O6 Eu1 O3 76.8(2) . . ?
O5 Eu1 O1 138.9(2) . . ?
O4 Eu1 O1 83.7(2) . . ?
O6 Eu1 O1 75.1(2) . . ?
O3 Eu1 O1 130.9(2) . . ?
O5 Eu1 O7 73.2(2) . . ?
O4 Eu1 O7 79.6(2) . . ?
O6 Eu1 O7 134.7(2) . . ?
O3 Eu1 O7 147.9(2) . . ?
O1 Eu1 O7 66.9(2) . . ?
O5 Eu1 O2 149.1(2) . . ?
O4 Eu1 O2 129.72(19) . . ?
O6 Eu1 O2 73.5(2) . . ?
O3 Eu1 O2 81.29(19) . . ?
O1 Eu1 O2 52.5(2) . . ?
O7 Eu1 O2 100.3(2) . . ?
O5 Eu1 N2 76.3(2) . . ?
O4 Eu1 N2 148.5(2) . . ?
O6 Eu1 N2 139.3(2) . . ?
O3 Eu1 N2 76.0(2) . . ?
O1 Eu1 N2 101.3(2) . . ?
O7 Eu1 N2 74.1(2) . . ?
O2 Eu1 N2 72.9(2) . . ?
O5 Eu1 O4 66.13(19) . 7_656 ?
O4 Eu1 O4 74.70(19) . 7_656 ?
O6 Eu1 O4 70.05(19) . 7_656 ?
O3 Eu1 O4 51.00(17) . 7_656 ?
O1 Eu1 O4 143.1(2) . 7_656 ?
```

```
O7 Eu1 O4 134.8(2) . 7_656 ?
O2 Eu1 O4 124.65(19) . 7_656 ?
N2 Eu1 O4 112.8(2) . 7_656 ?
O5 Eu1 C1 153.8(2) . . ?
O4 Eu1 C1 107.3(2) . . ?
O6 Eu1 C1 72.6(2) . . ?
O3 Eu1 C1 106.3(2) . . ?
O1 Eu1 C1 26.3(2) . . ?
O7 Eu1 C1 83.1(3) . . ?
O2 Eu1 C1 26.2(2) . . ?
N2 Eu1 C1 86.7(3) . . ?
O4 Eu1 C1 139.9(2) 7_656 . ?
O5 Eu1 C9 76.0(2) . . ?
O4 Eu1 C9 99.4(2) . . ?
O6 Eu1 C9 72.1(2) . . ?
O3 Eu1 C9 25.6(2) . . ?
O1 Eu1 C9 144.2(2) . . ?
O7 Eu1 C9 148.8(2) . . ?
O2 Eu1 C9 103.7(2) . . ?
N2 Eu1 C9 94.4(2) . . ?
O4 Eu1 C9 25.38(19) 7_656 . ?
C1 Eu1 C9 125.8(3) . . ?
O5 Eu1 Eu1 67.89(14) . 7_656 ?
O4 Eu1 Eu1 40.45(13) . 7_656 ?
O6 Eu1 Eu1 65.94(14) . 7_656 ?
O3 Eu1 Eu1 84.42(13) . 7_656 ?
O1 Eu1 Eu1 118.29(17) . 7_656 ?
O7 Eu1 Eu1 111.68(18) . 7_656 ?
O2 Eu1 Eu1 139.05(15) . 7_656 ?
N2 Eu1 Eu1 139.28(18) . 7_656 ?
O4 Eu1 Eu1 34.25(11) 7_656 7_656 ?
C1 Eu1 Eu1 133.41(19) . 7_656 ?
C9 Eu1 Eu1 59.18(15) . 7_656 ?
C1 O1 Eu1 94.9(5) . . ?
C1 O2 Eu1 91.1(5) . . ?
C9 O3 Eu1 100.9(5) . . ?
C9 O4 Eu1 162.1(5) 7_656 . ?
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O4 C9 C10 120.5(7) 7_656 . ?
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H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
C8 N1 C12 116.8(8) . 3_545 ?
C17 N2 C19 103.3(9) . . ?
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
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C10 C 0.7945(3) 0.6431(7) 0.7397(7) 0.018(2) Uani 1 1 d . . .
C11 C 0.8409(3) 0.6453(7) 0.7303(7) 0.021(2) Uani 1 1 d . . .
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C14 C 0.7864(3) 0.4872(7) 1.1125(7) 0.017(2) Uani 1 1 d . . .
C15 C 0.7674(3) 0.5778(7) 0.6776(7) 0.018(2) Uani 1 1 d . . .
H15 H 0.7364 0.5786 0.6806 0.022 Uiso 1 1 calc R . .
C16 C 0.7566(3) 0.5587(7) 1.0515(7) 0.020(2) Uani 1 1 d . . .
C17 C 0.6127(4) 0.5285(9) 0.8253(9) 0.041(3) Uani 1 1 d U . .
H17 H 0.5877 0.5626 0.8467 0.050 Uiso 1 1 calc R . .
C18 C 0.6114(4) 0.4538(10) 0.7529(10) 0.045(3) Uani 1 1 d U . .
H18 H 0.5863 0.4302 0.7155 0.054 Uiso 1 1 calc R . .
C19 C 0.6797(4) 0.4770(8) 0.8148(8) 0.028(2) Uani 1 1 d U . .
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C20 C 0.6391(7) 0.8025(15) 0.5842(14) 0.088(4) Uani 1 1 d U . .
H20 H 0.6381 0.8733 0.6001 0.106 Uiso 1 1 calc R . .
C21 C 0.6029(7) 0.7378(15) 0.5787(13) 0.082(4) Uani 1 1 d U . .
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O9 O 0.0288(5) 0.3415(11) 0.6386(10) 0.105(4) Uani 1 1 d U . .
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H24 H 0.599(5) 0.580(10) 0.543(14) 0.126 Uiso 1 1 d D . .
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C2 0.025(4) 0.017(4) 0.020(4) 0.014(3) 0.009(3) -0.001(3)
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C7 0.026(6) 0.034(6) 0.031(6) -0.003(5) 0.002(5) -0.003(5)
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C15 0.015(5) 0.023(5) 0.017(5) 0.000(4) 0.007(4) 0.000(4)
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O2 0.021(4) 0.026(4) 0.029(4) 0.001(3) 0.012(3) 0.005(3)
O3 0.019(4) 0.034(4) 0.014(3) -0.003(3) 0.005(3) -0.002(3)
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O5 0.018(4) 0.013(3) 0.027(4) -0.001(3) 0.000(3) -0.002(3)
O6 0.018(3) 0.019(3) 0.020(4) 0.002(3) 0.006(3) 0.001(3)
O7 0.034(4) 0.034(4) 0.029(4) 0.002(3) -0.005(3) 0.005(3)
O8 0.033(5) 0.060(6) 0.051(6) -0.005(5) -0.009(4) 0.007(4)
O9 0.104(6) 0.115(6) 0.097(6) -0.006(4) 0.010(4) 0.011(4)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O5 2.452(6) . ?
Eu1 O2 2.478(6) . ?
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Eu1 O6 2.695(6) 7_667 ?
Eu1 C1 2.812(10) . ?
Eu1 C16 2.937(10) . ?
C1 O2 1.240(11) . ?
C1 O1 1.267(12) . ?
C1 C2 1.502(13) . ?
C2 C3 1.348(14) . ?
C2 C7 1.419(14) . ?
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C3 H3 0.9300 . ?
C4 C5 1.392(15) . ?
C4 H4 0.9300 . ?
C5 C6 1.391(15) . ?
C5 C8 1.461(14) . ?
C6 C7 1.380(15) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 N1 1.271(13) . ?
C8 H16 0.95(2) . ?
C9 O3 1.255(11) . ?
C9 O4 1.323(11) 7_667 ?
C9 C10 1.504(13) . ?
C10 C11 1.403(13) . ?
C10 C15 1.408(13) . ?
C11 C12 1.384(13) 8_565 ?
C11 H11 0.9300 . ?
C12 C13 1.382(14) . ?
C12 C11 1.384(14) 8_466 ?
C12 N1 1.427(12) . ?
C13 C14 1.389(13) 3_455 ?
C13 H13 0.9300 . ?
C14 C15 1.374(13) 6_566 ?
C14 C13 1.389(13) 3_545 ?
C14 C16 1.490(13) . ?
C15 C14 1.374(13) 6_565 ?
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C16 O5 1.247(11) . ?
C16 O6 1.266(11) 7_667 ?
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C20 N5 1.39(2) . ?
C20 H20 0.9300 . ?
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C21 H21 0.9300 . ?
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C22 N5 1.39(2) . ?
C22 H22 0.9300 . ?
N3 H23 0.95(2) . ?
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N4 H24 0.97(2) . ?
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O3 Eu1 O7 73.9(2) . . ?
O4 Eu1 O7 140.2(2) . . ?
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O6 Eu1 O5 121.3(2) . . ?
O3 Eu1 O5 91.8(2) . . ?
O4 Eu1 O5 72.5(2) . . ?
O7 Eu1 O5 143.9(2) . . ?
O1 Eu1 O5 86.4(2) . . ?
O6 Eu1 O2 80.0(2) . . ?
O3 Eu1 O2 137.2(2) . . ?
O4 Eu1 O2 71.9(2) . . ?
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O4 Eu1 N2 133.1(2) . . ?
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O5 Eu1 N2 70.7(2) . . ?
O2 Eu1 N2 113.8(2) . . ?
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O3 Eu1 O6 67.4(2) . 7_667 ?
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O4 Eu1 C1 72.8(2) . . ?
O7 Eu1 C1 77.2(3) . . ?
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O2 Eu1 C1 26.1(3) . . ?
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C13 C12 N1 118.1(9) . . ?
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C15 C14 C16 118.6(8) 6_566 . ?
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C14 C15 H15 119.8 6_565 . ?
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N5 C22 H22 125.2 . . ?
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C19 N2 C17 104.9(9) . . ?
C19 N2 Eu1 125.8(7) . . ?
C17 N2 Eu1 128.0(7) . . ?
C18 N3 C19 107.4(9) . . ?
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   2  0.000  0.083  0.750        94        18 ' '
   3  0.281  0.085  0.331        19         3 ' '
   4  0.719  0.085  0.169        19         3 ' '
   5  0.500  0.418  0.250        94        17 ' '
   6  0.219  0.415  0.669        19         3 ' '
   7  0.781  0.415  0.831        19         3 ' '
   8  0.500  0.583  0.750        94        18 ' '
   9  0.219  0.585  0.169        19         3 ' '
  10  0.781  0.585  0.331        19         3 ' '
  11  0.281  0.915  0.831        19         3 ' '
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 MERCURY (Bruno et al. 2002)
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_computing_publication_material   'WINGX (Farrugia, 1999)'
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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d . . .
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d . . .
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O5 O 0.30178(17) 0.7616(4) -0.1318(4) 0.0389(11) Uani 1 1
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O6 O 0.26682(18) 0.8130(4) 0.1732(4) 0.0482(14) Uani 1 1
d . . .
O7 O 0.3636(3) 0.7479(7) 0.1976(5) 0.085(2) Uani 1 1 d U . .
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N3 N 0.3416(3) 1.0746(7) 0.2653(7) 0.079(2) Uani 1 1 d U . .
C1 C 0.3992(3) 0.7561(7) -0.0189(6) 0.0474(19) Uani 1 1 d . . .
C2 C 0.4436(3) 0.7337(8) -0.0580(7) 0.054(2) Uani 1 1 d . . .
C3 C 0.4708(4) 0.8081(8) -0.0861(11) 0.080(4) Uani 1 1 d . . .
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C6 C 0.5012(4) 0.6150(8) -0.0944(9) 0.077(3) Uani 1 1 d . . .
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C7 C 0.4582(3) 0.6346(8) -0.0626(8) 0.073(3) Uani 1 1 d . . .
H7 H 0.4398 0.5826 -0.0450 0.087 Uiso 1 1 calc R . .
C8 C 0.5751(4) 0.6705(9) -0.1480(8) 0.067(3) Uani 1 1 d D . .
C9 C 0.2452(3) 0.9323(5) -0.0623(5) 0.0390(16) Uani 1 1 d . . .
C10 C 0.2138(2) 1.0020(5) -0.1226(5) 0.0357(15) Uani 1 1
d . . .
C11 C 0.2324(2) 1.0678(5) -0.1874(5) 0.0382(16) Uani 1 1
d . . .
H11 H 0.2640 1.0659 -0.1911 0.046 Uiso 1 1 calc R . .
C12 C 0.2047(2) 0.8649(5) 0.2544(5) 0.0379(15) Uani 1 1 d . . .
C13 C 0.6671(3) 0.5086(6) -0.1159(5) 0.0430(17) Uani 1 1
d . . .
H13 H 0.6540 0.4644 -0.0749 0.052 Uiso 1 1 calc R . .
C14 C 0.6394(3) 0.5793(6) -0.1687(6) 0.0487(19) Uani 1 1
d . . .
C15 C 0.6576(3) 0.6399(6) -0.2373(6) 0.0462(18) Uani 1 1
d . . .
H15 H 0.6383 0.6835 -0.2775 0.055 Uiso 1 1 calc R . .
C16 C 0.2244(3) 0.8007(5) 0.1811(6) 0.0382(17) Uani 1 1 d . . .
C17 C 0.3256(5) 1.0384(10) 0.1776(10) 0.092(3) Uani 1 1 d U . .
H17 H 0.3037 1.0716 0.1328 0.111 Uiso 1 1 calc R . .
C18 C 0.3628(5) 1.0052(11) 0.3142(11) 0.097(3) Uani 1 1 d U . .
H18 H 0.3774 1.0065 0.3799 0.117 Uiso 1 1 calc R . .
C19 C 0.3597(5) 0.9289(10) 0.2500(9) 0.089(3) Uani 1 1 d U . .
C20 C 0.3776(6) 0.8232(11) 0.2599(12) 0.108(4) Uani 1 1 d U . .
H20A H 0.4109 0.8276 0.2615 0.129 Uiso 1 1 calc R . .
H20B H 0.3724 0.8009 0.3256 0.129 Uiso 1 1 calc R . .
H16 H 0.588(5) 0.732(7) -0.176(11) 0.129 Uiso 1 1 d D . .
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d . . .

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O3 0.023(3) 0.041(3) 0.057(3) -0.002(2) 0.017(2) 0.001(2)
O4 0.026(3) 0.043(3) 0.053(3) 0.003(2) 0.022(2) 0.004(2)
O5 0.033(3) 0.045(3) 0.042(3) -0.003(2) 0.017(2) -0.006(2)
O6 0.025(3) 0.075(4) 0.050(3) -0.017(3) 0.024(2) -0.010(2)
O7 0.089(4) 0.098(4) 0.068(3) 0.000(3) 0.007(3) 0.028(3)
N1 0.032(4) 0.081(5) 0.072(5) 0.030(4) 0.028(3) 0.026(4)
N2 0.068(4) 0.062(3) 0.067(3) -0.003(3) 0.013(3) -0.008(3)
N3 0.076(4) 0.082(4) 0.080(4) -0.011(3) 0.019(3) -0.009(3)
C1 0.027(4) 0.065(5) 0.054(4) 0.005(4) 0.019(3) 0.010(4)
C2 0.035(5) 0.072(5) 0.060(5) 0.008(5) 0.021(4) 0.013(4)
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C5 0.041(5) 0.083(7) 0.087(7) 0.024(5) 0.040(5) 0.022(5)
C6 0.057(6) 0.077(7) 0.106(8) 0.036(6) 0.048(6) 0.026(5)
C7 0.050(6) 0.078(6) 0.100(7) 0.030(6) 0.047(5) 0.025(5)
C8 0.047(6) 0.088(7) 0.072(6) 0.018(6) 0.029(5) 0.011(5)
C9 0.037(4) 0.045(4) 0.039(4) -0.004(3) 0.022(3) 0.007(3)
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C19 0.093(5) 0.088(4) 0.084(4) -0.001(4) 0.010(4) -0.009(4)
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Eu1 0.0202(3) 0.0422(3) 0.0422(3) -0.00085(14) 0.01657(16)
0.00168(12)

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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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O4 Eu1 2.362(5) . ?
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C4 H4 0.9300 . ?
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C5 C8 1.480(13) . ?
C6 C7 1.403(12) . ?
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C10 C11 1.404(9) . ?
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C12 C11 1.379(10) 6_576 ?
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
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Netherlands.
;


_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.1480P)^2^+22.5312P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
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_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
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_refine_ls_number_parameters      316
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d . . .
C1 C 0.0984(4) 0.7522(9) 0.5260(8) 0.054(3) Uani 1 1 d . . .
C2 C 0.0540(4) 0.7768(9) 0.5652(9) 0.055(3) Uani 1 1 d . . .
C3 C 0.0382(5) 0.8704(10) 0.5643(12) 0.086(4) Uani 1 1 d . . .
H3 H 0.0569 0.9183 0.5446 0.104 Uiso 1 1 calc R . .
C4 C -0.0029(5) 0.8931(10) 0.5908(11) 0.076(4) Uani 1 1 d . . .
H4 H -0.0132 0.9555 0.5866 0.091 Uiso 1 1 calc R . .
C5 C -0.0305(5) 0.8220(10) 0.6251(10) 0.067(3) Uani 1 1 d . . .
C6 C -0.0154(6) 0.7325(12) 0.6289(15) 0.100(6) Uani 1 1 d . . .
H6 H -0.0335 0.6856 0.6526 0.120 Uiso 1 1 calc R . .
C7 C 0.0275(5) 0.7072(10) 0.5978(14) 0.088(5) Uani 1 1 d . . .
H7 H 0.0374 0.6444 0.5996 0.106 Uiso 1 1 calc R . .
C8 C -0.0782(5) 0.8392(13) 0.6508(12) 0.086(4) Uani 1 1 d . . .
C9 C 0.2537(3) 0.5796(7) 0.5748(7) 0.044(2) Uani 1 1 d . . .
C10 C 0.2838(3) 0.5082(7) 0.6284(7) 0.041(2) Uani 1 1 d . . .
C11 C 0.3304(3) 0.5002(7) 0.6185(7) 0.045(2) Uani 1 1 d . . .
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H11 H 0.3433 0.5425 0.5773 0.054 Uiso 1 1 calc R . .
C12 C 0.3578(3) 0.4323(7) 0.6672(8) 0.047(2) Uani 1 1 d . . .
C13 C 0.3397(4) 0.3744(7) 0.7394(7) 0.046(2) Uani 1 1 d . . .
H13 H 0.3587 0.3314 0.7780 0.055 Uiso 1 1 calc R . .
C14 C 0.2938(3) 0.3835(7) 0.7506(6) 0.039(2) Uani 1 1 d . . .
C15 C 0.2655(3) 0.4497(7) 0.6966(7) 0.042(2) Uani 1 1 d . . .
H15 H 0.2345 0.4552 0.7057 0.050 Uiso 1 1 calc R . .
C16 C 0.2738(3) 0.3234(8) 0.8272(7) 0.044(2) Uani 1 1 d . . .
C17 C 0.1192(15) 0.486(2) 0.380(3) 0.278(8) Uani 1 1 d DU . .
H17A H 0.0869 0.5017 0.3827 0.333 Uiso 1 1 calc R . .
H17B H 0.1315 0.4583 0.4438 0.333 Uiso 1 1 calc R . .
C18 C 0.1207(13) 0.412(3) 0.300(2) 0.290(7) Uani 1 1 d DU . .
H18 H 0.1029 0.3554 0.3136 0.348 Uiso 1 1 calc R . .
C19 C 0.1719(13) 0.392(3) 0.311(3) 0.295(8) Uani 1 1 d DU . .
H19A H 0.1860 0.4525 0.2993 0.354 Uiso 1 1 calc R . .
H19B H 0.1759 0.3527 0.2541 0.354 Uiso 1 1 calc R . .
C20 C 0.1587(8) 0.803(2) 0.2277(18) 0.194(6) Uani 1 1 d DU . .
C21 C 0.0698(9) 0.860(2) 0.178(2) 0.213(7) Uani 1 1 d DU . .
H21A H 0.0603 0.8093 0.2186 0.319 Uiso 1 1 calc R . .
H21B H 0.0523 0.8567 0.1126 0.319 Uiso 1 1 calc R . .
H21C H 0.0644 0.9195 0.2084 0.319 Uiso 1 1 calc R . .
C22 C 0.1298(9) 0.9295(19) 0.110(2) 0.202(7) Uani 1 1 d DU . .
H22A H 0.1016 0.9545 0.0744 0.303 Uiso 1 1 calc R . .
H22B H 0.1498 0.9089 0.0636 0.303 Uiso 1 1 calc R . .
H22C H 0.1451 0.9779 0.1527 0.303 Uiso 1 1 calc R . .
N1 N -0.0953(3) 0.9220(7) 0.6471(7) 0.056(2) Uani 1 1 d . . .
N2 N 0.1190(9) 0.8500(17) 0.1709(19) 0.201(6) Uani 1 1 d DU . .
O1 O 0.1136(3) 0.6689(6) 0.5411(6) 0.062(2) Uani 1 1 d . . .
O2 O 0.1202(3) 0.8137(6) 0.4860(7) 0.066(2) Uani 1 1 d . . .
O3 O 0.2107(2) 0.5648(5) 0.5536(5) 0.0497(17) Uani 1 1 d . . .
O4 O 0.2288(2) 0.8444(4) 0.4545(5) 0.0437(15) Uani 1 1 d . . .
O5 O 0.2327(2) 0.6591(5) 0.3428(5) 0.0505(18) Uani 1 1 d . . .
O6 O 0.1997(2) 0.7616(5) 0.6271(5) 0.0457(16) Uani 1 1 d . . .
O7 O 0.1441(4) 0.5738(17) 0.3685(7) 0.171(5) Uani 1 1 d DU . .
O8 O 0.1098(12) 0.443(2) 0.194(2) 0.295(8) Uani 1 1 d DU . .
H8 H 0.1335 0.4412 0.1668 0.442 Uiso 1 1 calc R . .
O9 O 0.1464(5) 0.7637(11) 0.3026(11) 0.125(4) Uani 1 1 d DU . .
S1 S 0.2096(7) 0.3408(14) 0.4142(13) 0.315(6) Uani 1 1 d DU . .

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0.00200(17)
C1 0.034(6) 0.062(7) 0.069(7) -0.004(6) 0.025(5) 0.006(5)
C2 0.031(6) 0.063(7) 0.075(7) 0.001(6) 0.022(5) 0.003(5)
C3 0.060(8) 0.067(8) 0.139(12) 0.023(9) 0.039(9) 0.009(7)
C4 0.053(7) 0.072(8) 0.109(10) 0.010(8) 0.035(7) 0.012(7)
C5 0.049(7) 0.066(8) 0.088(9) 0.011(7) 0.014(6) 0.009(6)
C6 0.072(10) 0.082(10) 0.161(16) 0.047(11) 0.063(11) 0.022(9)
C7 0.055(9) 0.080(10) 0.140(14) 0.018(9) 0.053(10) 0.010(7)
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C8 0.052(8) 0.105(12) 0.110(11) 0.014(10) 0.038(8) 0.015(9)
C9 0.034(5) 0.044(5) 0.061(6) 0.001(5) 0.026(4) 0.004(4)
C10 0.032(5) 0.035(5) 0.060(5) 0.010(4) 0.018(4) 0.002(4)
C11 0.038(5) 0.044(5) 0.059(5) 0.007(5) 0.025(4) 0.008(4)
C12 0.026(5) 0.052(6) 0.069(6) 0.012(5) 0.022(4) 0.006(4)
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C14 0.032(5) 0.043(5) 0.046(5) 0.004(4) 0.017(4) 0.001(4)
C15 0.029(5) 0.038(5) 0.062(5) -0.004(4) 0.022(4) 0.001(4)
C16 0.033(5) 0.048(5) 0.053(5) 0.007(5) 0.014(4) -0.003(5)
C17 0.277(9) 0.273(9) 0.282(9) 0.003(5) 0.039(5) -0.012(5)
C18 0.294(8) 0.284(8) 0.292(8) -0.006(4) 0.042(5) -0.006(5)
C19 0.296(8) 0.294(9) 0.296(9) -0.001(5) 0.044(4) 0.002(5)
C20 0.197(7) 0.196(8) 0.190(7) 0.014(5) 0.032(5) -0.005(5)
C21 0.208(7) 0.213(9) 0.217(9) 0.004(5) 0.028(5) 0.003(5)
C22 0.209(8) 0.199(8) 0.196(8) 0.008(5) 0.022(5) 0.001(5)
N1 0.031(4) 0.071(6) 0.071(5) 0.012(5) 0.022(4) 0.014(5)
N2 0.206(7) 0.201(7) 0.194(7) 0.015(5) 0.019(4) 0.004(5)
O1 0.047(5) 0.054(5) 0.091(6) -0.013(4) 0.033(4) -0.008(4)
O2 0.040(4) 0.067(5) 0.100(6) 0.033(5) 0.040(4) 0.023(4)
O3 0.032(4) 0.044(4) 0.076(4) 0.012(3) 0.015(3) 0.002(3)
O4 0.037(4) 0.029(3) 0.068(4) 0.007(3) 0.020(3) 0.004(3)
O5 0.030(4) 0.057(4) 0.071(4) -0.016(4) 0.028(3) -0.003(3)
O6 0.033(4) 0.050(4) 0.058(4) -0.009(3) 0.020(3) -0.004(3)
O7 0.060(6) 0.386(15) 0.071(6) -0.057(9) 0.027(5) -0.065(11)
O8 0.296(9) 0.299(9) 0.290(8) -0.005(5) 0.043(5) 0.001(5)
O9 0.117(6) 0.127(5) 0.131(5) -0.035(4) 0.012(4) 0.006(4)
S1 0.321(7) 0.306(8) 0.312(7) -0.004(5) 0.026(5) 0.008(5)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O3 2.417(7) . ?
Eu1 O7 2.451(17) . ?
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C1 O2 1.240(14) . ?
C1 O1 1.262(15) . ?
C1 C2 1.501(14) . ?
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C2 C3 1.399(17) . ?
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C7 H7 0.9300 . ?
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C9 O3 1.258(12) . ?
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C9 C10 1.459(14) . ?
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C10 C15 1.394(13) . ?
C11 C12 1.356(14) . ?
C11 H11 0.9300 . ?
C12 C13 1.425(13) . ?
C12 N1 1.433(12) 3_545 ?
C13 C14 1.368(13) . ?
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C14 C15 1.385(13) . ?
C14 C16 1.515(13) . ?
C15 H15 0.9300 . ?
C16 O5 1.263(12) 6_566 ?
C16 O6 1.268(13) 4_546 ?
C17 O7 1.454(5) . ?
C17 C18 1.505(5) . ?
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C17 H17B 0.9700 . ?
C18 C19 1.501(5) . ?
C18 O8 1.501(5) . ?
C18 H18 0.9800 . ?
C19 S1 1.800(5) . ?
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C19 H19B 0.9700 . ?
C20 O9 1.249(5) . ?
C20 N2 1.452(5) . ?
C21 N2 1.453(5) . ?
C21 H21A 0.9600 . ?
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C22 N2 1.449(5) . ?
C22 H22A 0.9600 . ?
C22 H22B 0.9600 . ?
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C22 H22C 0.9600 . ?
N1 C12 1.433(12) 3_455 ?
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O2 Eu1 O4 141.4(3) . 7_566 ?
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O6 Eu1 C1 71.9(3) . . ?
O5 Eu1 C1 154.8(3) . . ?
O9 Eu1 C1 83.2(4) . . ?
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O7 Eu1 C1 87.4(4) . . ?
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O4 Eu1 C9 100.5(3) . . ?
O6 Eu1 C9 71.5(3) . . ?
O5 Eu1 C9 75.9(2) . . ?
O9 Eu1 C9 149.3(4) . . ?
O3 Eu1 C9 24.6(2) . . ?
O7 Eu1 C9 92.8(5) . . ?
O2 Eu1 C9 141.0(3) . . ?
O1 Eu1 C9 101.1(3) . . ?
O4 Eu1 C9 25.5(2) 7_566 . ?
C1 Eu1 C9 123.1(3) . . ?
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O4 Eu1 Eu1 34.59(13) 7_566 7_566 ?
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C14 C15 C10 119.7(8) . . ?
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C10 C15 H15 120.2 . . ?
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O6 C16 C14 116.8(8) 4_546 . ?
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C18 C17 H17A 108.1 . . ?
O7 C17 H17B 108.1 . . ?
C18 C17 H17B 108.1 . . ?
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O8 C18 C17 117(4) . . ?
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O8 C18 H18 111.7 . . ?
C17 C18 H18 111.7 . . ?
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S1 C19 H19A 104.8 . . ?
C18 C19 H19B 104.8 . . ?
S1 C19 H19B 104.8 . . ?
H19A C19 H19B 105.8 . . ?
O9 C20 N2 109.7(19) . . ?
N2 C21 H21A 109.5 . . ?
N2 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
N2 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
N2 C22 H22A 109.5 . . ?
N2 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
N2 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?
C8 N1 C12 117.7(11) . 3_455 ?
C22 N2 C20 116(2) . . ?
C22 N2 C21 104.9(5) . . ?
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C20 N2 C21 136(2) . . ?
C1 O1 Eu1 91.5(6) . . ?
C1 O2 Eu1 93.8(7) . . ?
C9 O3 Eu1 102.4(6) . . ?
C9 O4 Eu1 163.2(7) 7_566 . ?
C9 O4 Eu1 87.9(6) 7_566 7_566 ?
Eu1 O4 Eu1 104.5(2) . 7_566 ?
C16 O5 Eu1 136.2(7) 6_565 . ?
C16 O6 Eu1 135.6(6) 4_556 . ?
C17 O7 Eu1 143.4(18) . . ?
C18 O8 H8 109.4 . . ?
C20 O9 Eu1 136.4(15) . . ?

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 'C21 H12 Eu N3 O7'
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 _atom_type_scat_dispersion_imag
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 'Eu'  'Eu'  -8.9294  11.1857
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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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Diffraction)'
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Source'
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Atlas'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
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_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4562
_refine_ls_number_parameters      292
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d . . .
O3 O 0.29328(12) 0.0652(3) 0.4654(3) 0.0429(9) Uani 1 1 d . . .
O4 O 0.27073(12) 0.3464(3) 0.5396(3) 0.0383(8) Uani 1 1 d . . .
O5 O 0.30085(13) 0.2522(3) 0.3712(3) 0.0445(9) Uani 1 1 d . . .
O6 O 0.22879(14) 0.3205(3) 0.3186(3) 0.0470(10) Uani 1 1
d . . .
O7 O 0.3635(3) 0.2775(5) 0.7282(6) 0.0890(19) Uani 1 1 d DU . .
N1 N 0.40545(18) 0.4142(4) 0.1502(5) 0.0572(15) Uani 1 1
d . . .
N2 N 0.3590(2) 0.0858(6) 0.6809(6) 0.0862(18) Uani 1 1 d DU . .
N3 N 0.3683(5) -0.0281(9) 0.8239(9) 0.138(3) Uani 1 1 d DU . .
C1 C 0.4041(2) 0.2528(5) 0.4941(5) 0.0472(14) Uani 1 1 d . . .
C2 C 0.4479(2) 0.2756(5) 0.4512(6) 0.0469(15) Uani 1 1 d . . .
C3 C 0.4745(3) 0.2058(5) 0.4203(9) 0.071(3) Uani 1 1 d . . .
H3 H 0.4638 0.1446 0.4200 0.086 Uiso 1 1 calc R . .
C4 C 0.4836(3) 0.2243(5) 0.1100(9) 0.076(3) Uani 1 1 d . . .
H4 H 0.4654 0.1759 0.1283 0.091 Uiso 1 1 calc R . .
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C5 C 0.4683(2) 0.3162(6) 0.1133(6) 0.0573(17) Uani 1 1 d . . .
C6 C 0.4968(3) 0.3885(6) 0.0879(6) 0.065(2) Uani 1 1 d . . .
H6 H 0.4873 0.4501 0.0916 0.078 Uiso 1 1 calc R . .
C7 C 0.4617(2) 0.3684(6) 0.4422(7) 0.0636(19) Uani 1 1 d . . .
H7 H 0.4424 0.4164 0.4568 0.076 Uiso 1 1 calc R . .
C8 C 0.4217(2) 0.3338(5) 0.1420(6) 0.0568(17) Uani 1 1 d D . .
C9 C 0.24850(18) 0.0788(4) 0.4368(4) 0.0365(11) Uani 1 1
d . . .
C10 C 0.28256(18) 0.5045(4) 0.1233(4) 0.0362(11) Uani 1 1
d . . .
C11 C 0.32996(19) 0.4954(5) 0.1146(5) 0.0486(15) Uani 1 1
d . . .
H11 H 0.3429 0.5376 0.0740 0.058 Uiso 1 1 calc R . .
C12 C 0.35786(19) 0.4227(4) 0.1672(6) 0.0488(15) Uani 1 1
d . . .
C13 C 0.33942(19) 0.3645(4) 0.2338(5) 0.0456(14) Uani 1 1
d . . .
H13 H 0.3588 0.3186 0.2726 0.055 Uiso 1 1 calc R . .
C14 C 0.29245(18) 0.3736(4) 0.2436(4) 0.0367(11) Uani 1 1
d . . .
C15 C 0.26347(17) 0.4429(4) 0.1869(4) 0.0375(11) Uani 1 1
d . . .
H15 H 0.2316 0.4481 0.1913 0.045 Uiso 1 1 calc R . .
C16 C 0.27274(19) 0.3110(4) 0.3178(5) 0.0391(12) Uani 1 1
d . . .
C17 C 0.3739(6) 0.1154(7) 0.7845(7) 0.132(3) Uani 1 1 d DU . .
C18 C 0.3827(6) 0.0552(9) 0.8691(9) 0.142(3) Uani 1 1 d DU . .
C19 C 0.3539(5) -0.0006(8) 0.7202(9) 0.134(3) Uani 1 1 d DU . .
H19 H 0.3392 -0.0453 0.6712 0.160 Uiso 1 1 calc R . .
C20 C 0.3997(7) 0.0546(14) 0.9890(9) 0.170(4) Uani 1 1 d DU . .
H20A H 0.3991 -0.0079 1.0150 0.255 Uiso 1 1 calc R . .
H20B H 0.3790 0.0930 1.0200 0.255 Uiso 1 1 calc R . .
H20C H 0.4319 0.0784 1.0084 0.255 Uiso 1 1 calc R . .
C21 C 0.3758(7) 0.2198(7) 0.7981(10) 0.132(3) Uani 1 1 d DU . .
Eu1 Eu 0.318254(9) 0.21129(2) 0.55582(2) 0.03027(16) Uani 1 1
d . . .
H16 H 0.403(2) 0.280(3) 0.152(5) 0.036 Uiso 1 1 d D . .

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O2 0.034(2) 0.056(3) 0.086(3) -0.021(2) 0.037(2) -0.015(2)
O3 0.0190(16) 0.040(2) 0.074(2) -0.0018(19) 0.0187(16) -
0.0009(15)
O4 0.0263(16) 0.0322(19) 0.064(2) -0.0039(16) 0.0253(15)
0.0014(15)
O5 0.0258(19) 0.055(3) 0.059(2) 0.011(2) 0.0230(17) 0.0078(19)
O6 0.030(2) 0.065(3) 0.054(2) 0.019(2) 0.0258(17) 0.006(2)
O7 0.088(4) 0.099(3) 0.076(3) -0.001(2) 0.011(3) -0.027(3)
N1 0.030(2) 0.061(4) 0.093(4) 0.025(3) 0.038(2) 0.014(2)
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N2 0.052(3) 0.089(3) 0.114(3) 0.007(3) 0.011(3) 0.030(3)
N3 0.136(5) 0.137(4) 0.140(4) 0.026(3) 0.028(4) 0.000(4)
C1 0.028(3) 0.052(4) 0.067(4) 0.003(3) 0.021(3) 0.000(3)
C2 0.023(3) 0.054(4) 0.070(4) -0.010(3) 0.024(3) -0.005(2)
C3 0.054(5) 0.044(4) 0.133(8) -0.007(4) 0.055(5) -0.004(3)
C4 0.049(4) 0.058(4) 0.142(8) 0.019(5) 0.066(5) 0.003(3)
C5 0.031(3) 0.066(4) 0.084(5) 0.017(4) 0.032(3) 0.007(3)
C6 0.057(4) 0.058(4) 0.090(5) 0.019(4) 0.036(4) 0.025(4)
C7 0.040(3) 0.067(5) 0.097(5) -0.022(4) 0.042(3) -0.009(3)
C8 0.033(3) 0.054(4) 0.093(5) 0.015(4) 0.034(3) 0.009(3)
C9 0.024(2) 0.039(3) 0.053(3) 0.001(2) 0.023(2) -0.003(2)
C10 0.024(2) 0.033(3) 0.057(3) -0.001(2) 0.021(2) 0.000(2)
C11 0.025(3) 0.048(3) 0.081(4) 0.015(3) 0.029(3) 0.004(2)
C12 0.023(2) 0.048(4) 0.084(4) 0.013(3) 0.031(3) 0.006(2)
C13 0.030(3) 0.044(3) 0.069(4) 0.018(3) 0.023(2) 0.010(2)
C14 0.026(2) 0.038(3) 0.051(3) 0.003(2) 0.020(2) 0.001(2)
C15 0.023(2) 0.039(3) 0.054(3) -0.001(2) 0.017(2) -0.001(2)
C16 0.025(3) 0.045(3) 0.052(3) 0.003(3) 0.020(2) 0.001(2)
C17 0.138(6) 0.125(3) 0.131(4) 0.003(3) 0.023(4) 0.001(4)
C18 0.145(6) 0.140(4) 0.136(3) 0.016(3) 0.018(4) 0.003(5)
C19 0.143(6) 0.120(4) 0.137(4) 0.015(3) 0.028(4) -0.005(5)
C20 0.181(7) 0.174(6) 0.151(4) 0.011(4) 0.028(5) -0.008(5)
C21 0.142(6) 0.124(3) 0.125(5) 0.006(3) 0.019(5) -0.006(5)
Eu1 0.0142(2) 0.0326(2) 0.0490(2) 0.00204(11) 0.01756(14) -
0.00048(9)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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O4 Eu1 2.352(4) . ?
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O4 Eu1 2.693(4) 7_556 ?
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O5 Eu1 2.379(4) . ?
O6 C16 1.267(7) . ?
O6 Eu1 2.364(4) 7_556 ?
O7 C21 1.213(5) . ?
O7 Eu1 2.483(7) . ?
N1 C8 1.259(9) . ?
N1 C12 1.432(7) . ?
N2 C19 1.359(5) . ?
N2 C17 1.367(5) . ?
N2 Eu1 2.517(7) . ?
N3 C18 1.353(5) . ?
N3 C19 1.358(5) . ?
C1 C2 1.516(8) . ?
C1 Eu1 2.807(6) . ?
C2 C3 1.369(10) . ?
C2 C7 1.402(10) . ?
C3 C4 1.368(11) 2_655 ?
C3 H3 0.9300 . ?
C4 C3 1.368(11) 2_655 ?
C4 C5 1.395(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.404(10) . ?
C5 C8 1.480(8) . ?
C6 C7 1.359(9) 2_655 ?
C6 H6 0.9300 . ?
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C7 H7 0.9300 . ?
C8 H16 0.96(2) . ?
C9 O4 1.274(7) 7_556 ?
C9 C10 1.488(8) 4_545 ?
C9 Eu1 2.925(5) . ?
C10 C11 1.391(7) . ?
C10 C15 1.395(8) . ?
C10 C9 1.488(8) 4 ?
C11 C12 1.392(8) . ?
C11 H11 0.9300 . ?
C12 C13 1.382(8) . ?
C13 C14 1.383(7) . ?
C13 H13 0.9300 . ?
C14 C15 1.391(7) . ?
C14 C16 1.508(8) . ?
C15 H15 0.9300 . ?
C17 C18 1.365(5) . ?
C17 C21 1.511(5) . ?
C17 C19 1.889(16) . ?
C18 C20 1.503(5) . ?
C19 H19 0.9300 . ?
C20 H20A 0.9600 . ?
C20 H20B 0.9600 . ?
C20 H20C 0.9600 . ?
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Eu1 O6 2.364(4) 7_556 ?
Eu1 O4 2.693(4) 7_556 ?
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C1 O2 Eu1 92.4(4) . . ?
C9 O3 Eu1 100.0(3) . . ?
C9 O4 Eu1 161.3(4) 7_556 . ?
C9 O4 Eu1 87.3(3) 7_556 7_556 ?
Eu1 O4 Eu1 104.72(13) . 7_556 ?
C16 O5 Eu1 132.2(4) . . ?
C16 O6 Eu1 134.7(4) . 7_556 ?
C21 O7 Eu1 113.7(8) . . ?
C8 N1 C12 118.3(6) . . ?
C19 N2 C17 87.7(9) . . ?
C19 N2 Eu1 144.7(8) . . ?
C17 N2 Eu1 113.1(7) . . ?
C18 N3 C19 99.0(11) . . ?
O2 C1 O1 122.8(6) . . ?
O2 C1 C2 119.2(6) . . ?
O1 C1 C2 118.0(6) . . ?
O2 C1 Eu1 61.4(3) . . ?
O1 C1 Eu1 61.5(3) . . ?
C2 C1 Eu1 175.2(5) . . ?
C3 C2 C7 119.3(6) . . ?
C3 C2 C1 120.3(6) . . ?
C7 C2 C1 120.4(6) . . ?
C4 C3 C2 121.2(7) 2_655 . ?
C4 C3 H3 119.4 2_655 . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
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P=(Fo^2^+2Fc^2^)/3'
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C6 C 0.5023(4) 0.4064(8) 0.4024(8) 0.052(3) Uani 1 1 d . . .
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C7 C 0.4595(4) 0.3800(8) 0.4371(8) 0.055(3) Uani 1 1 d . . .
H7 H 0.4408 0.4246 0.4631 0.066 Uiso 1 1 calc R . .
C8 C 0.5765(4) 0.3709(9) 0.3340(9) 0.060(3) Uani 1 1 d D . .
H16 H 0.594(4) 0.316(6) 0.354(10) 0.072 Uiso 1 1 d D . .
C9 C 0.2439(3) 0.1029(6) 0.3922(6) 0.0319(19) Uani 1 1 d . . .
C10 C 0.2124(3) 0.0388(6) 0.3338(6) 0.034(2) Uani 1 1 d . . .
C11 C 0.1655(3) 0.0303(7) 0.3495(7) 0.039(2) Uani 1 1 d . . .
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d . . .
C15 C 0.2305(3) -0.0171(6) 0.2667(6) 0.034(2) Uani 1 1 d . . .
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C16 C 0.2219(3) -0.1450(7) 0.1454(7) 0.039(2) Uani 1 1 d . . .
C17 C 0.3442(12) 0.007(2) 0.6491(17) 0.183(7) Uani 1 1 d DU . .
C18 C 0.3660(13) -0.156(2) 0.572(2) 0.213(8) Uani 1 1 d DU . .
H18A H 0.3565 -0.1279 0.5128 0.320 Uiso 1 1 calc R . .
H18B H 0.3501 -0.2155 0.5770 0.320 Uiso 1 1 calc R . .
H18C H 0.3991 -0.1670 0.5773 0.320 Uiso 1 1 calc R . .
C19 C 0.3626(12) -0.124(2) 0.746(2) 0.196(8) Uani 1 1 d DU . .
H19A H 0.3690 -0.1901 0.7475 0.294 Uiso 1 1 calc R . .
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DU . .
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DU . .
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C22 C 0.2322(9) -0.1164(18) 0.551(2) 0.160(4) Uani 1 1 d DU . .
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DU . .
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DU . .
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DU . .
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DU . .
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O6 O 0.3042(2) 0.2899(4) 0.3879(5) 0.0373(15) Uani 1 1 d . . .
O7 O 0.3463(4) 0.0392(8) 0.5686(11) 0.110(4) Uani 1 1 d DU . .
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C14 0.026(4) 0.035(4) 0.042(5) -0.007(4) 0.009(4) 0.002(4)
C15 0.028(4) 0.035(5) 0.041(5) -0.004(4) 0.009(4) -0.003(4)
C16 0.039(5) 0.036(5) 0.046(6) -0.005(4) 0.014(4) -0.005(4)
C17 0.183(9) 0.185(8) 0.180(8) 0.008(4) 0.017(5) -0.002(5)
C18 0.217(10) 0.212(9) 0.211(9) -0.007(5) 0.021(5) 0.006(5)
C19 0.197(9) 0.197(9) 0.194(8) 0.009(5) 0.017(5) -0.001(5)
C20 0.161(5) 0.157(5) 0.156(5) 0.000(3) 0.012(3) 0.001(3)
C21 0.163(5) 0.158(5) 0.157(5) 0.001(3) 0.012(3) 0.000(3)
C22 0.163(5) 0.159(5) 0.158(5) 0.000(3) 0.014(3) -0.001(3)
C23 0.162(5) 0.158(5) 0.158(5) 0.000(3) 0.015(3) 0.001(3)
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N2 0.199(8) 0.187(7) 0.192(7) 0.010(4) 0.017(5) 0.003(5)
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O6 0.034(4) 0.036(3) 0.043(4) 0.009(3) 0.012(3) 0.005(3)
O7 0.074(7) 0.106(7) 0.158(10) -0.013(7) 0.058(7) 0.025(6)
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 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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O6 Eu1 O3 76.5(2) . . ?
O5 Eu1 O3 88.8(2) . . ?
O8 Eu1 O3 144.9(3) . . ?
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O7 C17 N2 109(2) . . ?
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N2 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
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H18A C18 H18C 109.5 . . ?
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N2 C19 H19B 109.5 . . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C4 C 0.9040(6) 0.8925(5) 0.4946(5) 0.0537(18) Uani 1 1 d . . .
H4 H 0.9771 0.9004 0.5139 0.064 Uiso 1 1 calc R . .
C5 C 0.8630(5) 0.8458(5) 0.5469(5) 0.0524(18) Uani 1 1 d . . .
C6 C 0.7545(5) 0.8348(6) 0.5173(6) 0.065(2) Uani 1 1 d . . .
H6 H 0.7256 0.8045 0.5521 0.078 Uiso 1 1 calc R . .
C7 C 0.6892(6) 0.8682(6) 0.4367(6) 0.063(2) Uani 1 1 d . . .
H7 H 0.6163 0.8574 0.4165 0.075 Uiso 1 1 calc R . .
C8 C 0.9309(6) 0.8140(5) 0.6376(6) 0.0529(18) Uani 1 1 d D . .
C9 C 0.3373(5) 0.8933(4) -0.0255(5) 0.0425(15) Uani 1 1 d . . .
C10 C 0.2374(5) 0.8376(4) -0.0858(5) 0.0406(14) Uani 1 1
d . . .
C11 C 1.1972(5) 0.7751(4) -0.0449(5) 0.0405(14) Uani 1 1
d . . .
H11 H 1.2333 0.7669 0.0178 0.049 Uiso 1 1 calc R . .
C12 C 1.1039(5) 0.7253(4) -0.0970(4) 0.0361(13) Uani 1 1
d . . .
C13 C 1.0474(5) 0.7415(4) -0.1894(5) 0.0399(14) Uani 1 1
d . . .
H13 H 0.9829 0.7100 -0.2235 0.048 Uiso 1 1 calc R . .
C14 C 0.0857(5) 0.8041(4) -0.2314(5) 0.0434(15) Uani 1 1
d . . .
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C15 C 0.1835(5) 0.8497(4) -0.1788(5) 0.0427(15) Uani 1 1
d . . .
H15 H 0.2127 0.8887 -0.2069 0.051 Uiso 1 1 calc R . .
C16 C 1.0622(5) 0.6550(5) -0.0564(5) 0.0423(15) Uani 1 1
d . . .
C17 C 0.2975(7) 1.1153(8) 0.1896(7) 0.0795(17) Uani 1 1 d U . .
H17 H 0.3189 1.1658 0.1688 0.095 Uiso 1 1 calc R . .
C18 C 0.2035(7) 1.1194(8) 0.2098(7) 0.0893(19) Uani 1 1 d U . .
H18 H 0.1638 1.1713 0.2018 0.107 Uiso 1 1 calc R . .
C19 C 0.1750(8) 1.0451(9) 0.2405(8) 0.0930(19) Uani 1 1 d U . .
H19 H 0.1139 1.0454 0.2530 0.112 Uiso 1 1 calc R . .
C20 C 0.2336(7) 0.9704(8) 0.2535(7) 0.0870(18) Uani 1 1 d U . .
H20 H 0.2156 0.9199 0.2767 0.104 Uiso 1 1 calc R . .
C21 C 0.3219(7) 0.9720(7) 0.2307(7) 0.0771(16) Uani 1 1 d U . .
H21 H 0.3614 0.9200 0.2375 0.093 Uiso 1 1 calc R . .
C22 C 0.8885(5) 0.5207(4) -0.3003(5) 0.0422(15) Uani 1 1
d . . .
C23 C 0.8866(5) 0.5599(5) -0.3852(5) 0.0457(16) Uani 1 1
d . . .
C24 C 0.7917(6) 0.5812(6) -0.4544(6) 0.059(2) Uani 1 1 d . . .
H24 H 0.7289 0.5755 -0.4452 0.071 Uiso 1 1 calc R . .
C25 C 0.7890(5) 0.6105(6) -0.5364(6) 0.059(2) Uani 1 1 d . . .
H25 H 0.7243 0.6221 -0.5829 0.071 Uiso 1 1 calc R . .
C26 C 0.8822(5) 0.6230(5) 0.4504(5) 0.0493(17) Uani 1 1 d . . .
C27 C 0.9784(6) 0.6067(5) -0.4779(5) 0.0552(18) Uani 1 1
d . . .
H27 H 1.0419 0.6176 -0.4846 0.066 Uiso 1 1 calc R . .
C28 C 0.9802(6) 0.5749(5) -0.3981(5) 0.0515(17) Uani 1 1
d . . .
H28 H 1.0449 0.5631 -0.3517 0.062 Uiso 1 1 calc R . .
C29 C 0.8784(6) 0.6517(5) 0.3610(5) 0.0517(17) Uani 1 1 d D . .
C30 C 0.8446(5) 0.5958(4) 0.0058(5) 0.0402(15) Uani 1 1 d . . .
C31 C 0.8065(4) 0.6584(4) 0.0672(5) 0.0378(14) Uani 1 1 d . . .
C32 C 0.8335(5) 0.6438(4) 0.1602(5) 0.0398(14) Uani 1 1 d . . .
H32 H 0.8841 0.6019 0.1877 0.048 Uiso 1 1 calc R . .
C33 C 0.7844(5) 0.6924(5) 0.2116(5) 0.0435(15) Uani 1 1 d . . .
C34 C 0.7148(5) 0.7587(4) 0.1714(5) 0.0420(15) Uani 1 1 d . . .
H34 H 0.6814 0.7907 0.2056 0.050 Uiso 1 1 calc R . .
C35 C 0.6938(5) 0.7784(4) 0.0805(5) 0.0388(14) Uani 1 1 d . . .
C36 C 0.7388(5) 0.7261(4) 0.0285(5) 0.0402(14) Uani 1 1 d . . .
H36 H 0.7233 0.7367 -0.0330 0.048 Uiso 1 1 calc R . .
C37 C 0.6217(5) 0.8548(5) 0.0424(5) 0.0449(16) Uani 1 1 d . . .
C38 C 0.6587(5) 0.3290(5) -0.1839(5) 0.0500(13) Uani 1 1 d
U . .
H38 H 0.7118 0.2872 -0.1654 0.060 Uiso 1 1 calc R . .
C39 C 0.5552(5) 0.2998(6) -0.2050(5) 0.0572(14) Uani 1 1 d
U . .
H39 H 0.5390 0.2399 -0.1994 0.069 Uiso 1 1 calc R . .
C40 C 0.4759(6) 0.3619(6) -0.2345(6) 0.0590(15) Uani 1 1 d
U . .
H40 H 0.4052 0.3443 -0.2502 0.071 Uiso 1 1 calc R . .
C41 C 0.5045(6) 0.4500(6) -0.2399(6) 0.0591(15) Uani 1 1 d
U . .
H41 H 0.4536 0.4937 -0.2585 0.071 Uiso 1 1 calc R . .
C42 C 0.6104(5) 0.4722(5) -0.2171(5) 0.0544(14) Uani 1 1 d
U . .
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H42 H 0.6291 0.5316 -0.2219 0.065 Uiso 1 1 calc R . .
C43 C 0.9823(6) 0.1566(6) 0.9153(7) 0.0661(15) Uani 1 1 d U . .
H43 H 0.9337 0.1864 0.9346 0.079 Uiso 1 1 calc R . .
C44 C 1.0477(7) 0.0961(6) 0.9713(7) 0.0733(16) Uani 1 1 d U . .
H44 H 1.0451 0.0872 1.0285 0.088 Uiso 1 1 calc R . .
C45 C 1.1157(7) 0.0498(6) 0.9414(7) 0.0735(16) Uani 1 1 d U . .
H45 H 1.1600 0.0078 0.9772 0.088 Uiso 1 1 calc R . .
C46 C 1.1178(6) 0.0662(5) 0.8570(7) 0.0694(15) Uani 1 1 d U . .
H46 H 1.1631 0.0349 0.8344 0.083 Uiso 1 1 calc R . .
C47 C 1.0529(6) 0.1286(5) 0.8074(7) 0.0639(15) Uani 1 1 d U . .
H47 H 1.0554 0.1403 0.7508 0.077 Uiso 1 1 calc R . .
C48 C 0.8447(8) 0.2035(9) 0.5708(9) 0.098(2) Uani 1 1 d U . .
H48 H 0.8815 0.1667 0.6172 0.118 Uiso 1 1 calc R . .
C49 C 0.8150(8) 0.1713(9) 0.4732(9) 0.106(2) Uani 1 1 d U . .
H49 H 0.8294 0.1123 0.4565 0.127 Uiso 1 1 calc R . .
C50 C 0.7676(8) 0.2256(10) 0.4080(9) 0.107(2) Uani 1 1 d U . .
H50 H 0.7550 0.2068 0.3461 0.129 Uiso 1 1 calc R . .
C51 C 0.7371(8) 0.3084(9) 0.4304(8) 0.103(2) Uani 1 1 d U . .
H51 H 0.6989 0.3449 0.3843 0.123 Uiso 1 1 calc R . .
C52 C 0.7638(8) 0.3373(9) 0.5230(8) 0.093(2) Uani 1 1 d U . .
H52 H 0.7431 0.3945 0.5379 0.112 Uiso 1 1 calc R . .
C53 C 0.7146(6) 0.3655(5) 0.1998(6) 0.0615(15) Uani 1 1 d U . .
H53 H 0.7697 0.3582 0.2565 0.074 Uiso 1 1 calc R . .
C54 C 0.7327(7) 0.4210(5) 0.1411(7) 0.0662(16) Uani 1 1 d U . .
H54 H 0.7986 0.4508 0.1586 0.079 Uiso 1 1 calc R . .
C55 C 0.6537(7) 0.4321(6) 0.0571(7) 0.0719(17) Uani 1 1 d U . .
H55 H 0.6644 0.4684 0.0157 0.086 Uiso 1 1 calc R . .
C56 C 0.5583(7) 0.3877(6) 0.0363(7) 0.0755(17) Uani 1 1 d U . .
H56 H 0.5023 0.3941 -0.0202 0.091 Uiso 1 1 calc R . .
C57 C 0.5439(7) 0.3331(6) 0.0986(6) 0.0666(16) Uani 1 1 d U . .
H57 H 0.4780 0.3040 0.0834 0.080 Uiso 1 1 calc R . .
N1 N 1.0295(4) 0.8316(4) 0.6770(4) 0.0487(14) Uani 1 1 d . . .
N2 N 0.3540(5) 1.0424(5) 0.1998(5) 0.0671(14) Uani 1 1 d U . .
N3 N 0.7931(4) 0.6720(4) 0.3006(4) 0.0502(14) Uani 1 1 d . . .
N4 N 0.6856(4) 0.4143(4) -0.1892(4) 0.0463(11) Uani 1 1 d U . .
N5 N 0.9861(5) 0.1736(4) 0.8363(5) 0.0631(13) Uani 1 1 d U . .
N6 N 0.8180(6) 0.2878(6) 0.5933(6) 0.0864(18) Uani 1 1 d U . .
N7 N 0.6219(5) 0.3215(4) 0.1793(5) 0.0589(13) Uani 1 1 d U . .
O1 O 0.5547(4) 0.9414(3) 0.2752(3) 0.0499(12) Uani 1 1 d . . .
O2 O 0.6899(3) 1.0069(3) 0.2588(3) 0.0499(12) Uani 1 1 d . . .
O3 O 0.3585(3) 0.9081(3) 0.0595(3) 0.0476(11) Uani 1 1 d . . .
O4 O 0.3907(3) 0.9271(3) -0.0651(4) 0.0535(13) Uani 1 1 d . . .
O5 O 0.9752(3) 0.6155(3) -0.1059(3) 0.0444(11) Uani 1 1 d . . .
O6 O 0.8808(3) 0.3605(3) -0.0273(3) 0.0401(10) Uani 1 1 d . . .
O7 O 0.5441(4) 1.1648(3) 0.2278(4) 0.0602(13) Uani 1 1 d . . .
O8 O 0.9709(3) 0.4884(3) -0.2473(3) 0.0464(11) Uani 1 1 d . . .
O9 O 0.8033(3) 0.5213(3) -0.2841(3) 0.0481(11) Uani 1 1 d . . .
O10 O 0.9292(3) 0.5540(3) 0.0434(3) 0.0403(10) Uani 1 1 d . . .
O11 O 0.7888(3) 0.5840(3) -0.0783(3) 0.0441(11) Uani 1 1
d . . .
O12 O 0.5763(3) 0.8880(3) 0.0936(3) 0.0466(11) Uani 1 1 d . . .
O13 O 0.6133(3) 0.8798(3) -0.0345(3) 0.0472(11) Uani 1 1
d . . .
O14 O 0.8721(4) 0.3247(3) -0.2187(3) 0.0512(12) Uani 1 1
d . . .
H16 H 0.894(5) 0.772(4) 0.664(5) 0.061 Uiso 1 1 d D . .
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H37 H 0.952(3) 0.661(5) 0.362(5) 0.061 Uiso 1 1 d D . .
Eu1 Eu 0.50368(2) 1.01880(2) 0.13457(2) 0.03709(12) Uani 1 1
d . . .
Eu2 Eu 0.89000(2) 0.47009(2) -0.12900(2) 0.03631(12) Uani 1 1
d . . .

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 _atom_site_aniso_U_12
C1 0.044(4) 0.047(4) 0.037(4) 0.007(3) 0.011(3) 0.004(3)
C2 0.048(4) 0.047(4) 0.046(4) 0.006(3) 0.016(3) -0.001(3)
C3 0.058(4) 0.053(4) 0.045(4) 0.012(4) 0.021(3) 0.002(3)
C4 0.050(4) 0.057(4) 0.052(5) 0.009(4) 0.016(3) -0.002(3)
C5 0.054(4) 0.045(4) 0.048(4) 0.008(3) 0.009(3) -0.006(3)
C6 0.048(4) 0.082(6) 0.062(5) 0.035(5) 0.014(4) -0.001(4)
C7 0.044(4) 0.073(5) 0.068(5) 0.025(5) 0.014(4) -0.001(4)
C8 0.056(4) 0.051(4) 0.053(5) 0.019(4) 0.020(4) 0.004(3)
C9 0.043(3) 0.041(3) 0.047(4) 0.017(3) 0.019(3) 0.005(3)
C10 0.038(3) 0.043(4) 0.039(4) 0.009(3) 0.013(3) 0.003(3)
C11 0.044(3) 0.041(3) 0.035(3) 0.011(3) 0.012(3) 0.004(3)
C12 0.039(3) 0.037(3) 0.034(3) 0.008(3) 0.015(3) 0.004(3)
C13 0.034(3) 0.035(3) 0.044(4) 0.003(3) 0.008(3) 0.006(3)
C14 0.052(4) 0.039(3) 0.039(4) 0.010(3) 0.018(3) 0.005(3)
C15 0.042(3) 0.041(3) 0.049(4) 0.009(3) 0.021(3) 0.000(3)
C16 0.043(4) 0.047(4) 0.041(4) 0.010(3) 0.020(3) 0.009(3)
C17 0.069(3) 0.104(4) 0.067(4) -0.006(3) 0.030(3) 0.015(3)
C18 0.069(3) 0.118(4) 0.080(4) -0.006(4) 0.033(3) 0.016(3)
C19 0.070(3) 0.126(5) 0.084(4) -0.006(4) 0.035(3) 0.002(3)
C20 0.071(3) 0.120(4) 0.076(4) 0.001(4) 0.038(3) -0.007(3)
C21 0.067(3) 0.106(4) 0.065(4) 0.001(3) 0.035(3) -0.006(3)
C22 0.051(4) 0.038(3) 0.037(4) 0.000(3) 0.017(3) -0.003(3)
C23 0.044(4) 0.047(4) 0.047(4) 0.010(3) 0.016(3) 0.005(3)
C24 0.049(4) 0.079(5) 0.055(5) 0.023(4) 0.023(4) 0.008(4)
C25 0.045(4) 0.078(5) 0.055(5) 0.029(4) 0.016(3) 0.013(4)
C26 0.054(4) 0.047(4) 0.047(4) 0.014(3) 0.018(3) 0.009(3)
C27 0.051(4) 0.066(5) 0.051(4) 0.009(4) 0.022(3) 0.001(4)
C28 0.053(4) 0.055(4) 0.049(4) 0.018(4) 0.019(3) 0.010(3)
C29 0.050(4) 0.053(4) 0.054(5) 0.015(4) 0.021(4) 0.006(3)
C30 0.045(4) 0.033(3) 0.047(4) 0.013(3) 0.021(3) 0.001(3)
C31 0.034(3) 0.037(3) 0.043(4) 0.009(3) 0.015(3) 0.002(3)
C32 0.037(3) 0.037(3) 0.045(4) 0.011(3) 0.014(3) 0.008(3)
C33 0.042(3) 0.047(4) 0.042(4) 0.011(3) 0.016(3) 0.001(3)
C34 0.045(3) 0.042(3) 0.043(4) 0.006(3) 0.022(3) 0.008(3)
C35 0.038(3) 0.035(3) 0.041(4) 0.009(3) 0.011(3) 0.006(3)
C36 0.039(3) 0.037(3) 0.043(4) 0.006(3) 0.013(3) 0.000(3)
C37 0.042(4) 0.047(4) 0.046(4) 0.005(3) 0.017(3) 0.003(3)
C38 0.047(2) 0.053(3) 0.047(3) 0.014(3) 0.014(2) -0.001(2)
C39 0.052(3) 0.061(3) 0.052(3) 0.017(3) 0.012(3) -0.006(2)
C40 0.046(3) 0.072(3) 0.055(3) 0.012(3) 0.014(2) -0.004(2)
C41 0.048(2) 0.065(3) 0.057(3) 0.012(3) 0.011(3) 0.003(2)
C42 0.046(2) 0.053(3) 0.055(3) 0.010(3) 0.009(2) 0.003(2)
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C43 0.067(3) 0.055(3) 0.082(4) 0.011(3) 0.035(3) 0.002(3)
C44 0.077(3) 0.059(3) 0.088(4) 0.016(3) 0.035(3) 0.002(3)
C45 0.074(3) 0.052(3) 0.095(4) 0.018(3) 0.031(3) 0.005(3)
C46 0.068(3) 0.049(3) 0.096(4) 0.010(3) 0.037(3) 0.005(2)
C47 0.068(3) 0.046(3) 0.084(4) 0.008(3) 0.036(3) 0.003(2)
C48 0.082(4) 0.113(5) 0.089(4) -0.013(4) 0.026(4) 0.003(4)
C49 0.087(4) 0.122(5) 0.095(4) -0.022(4) 0.029(4) 0.002(4)
C50 0.088(4) 0.138(5) 0.084(4) -0.014(4) 0.026(4) -0.008(4)
C51 0.088(4) 0.131(5) 0.077(4) -0.001(4) 0.021(4) -0.008(4)
C52 0.081(4) 0.117(5) 0.073(4) 0.002(4) 0.023(3) -0.007(4)
C53 0.061(3) 0.051(3) 0.070(3) 0.001(3) 0.024(3) 0.000(3)
C54 0.069(3) 0.054(3) 0.080(4) 0.003(3) 0.035(3) 0.000(3)
C55 0.082(3) 0.059(3) 0.078(4) 0.011(3) 0.034(3) 0.002(3)
C56 0.079(3) 0.063(3) 0.075(4) 0.009(3) 0.020(3) 0.004(3)
C57 0.064(3) 0.061(3) 0.070(4) 0.002(3) 0.021(3) -0.002(3)
N1 0.051(3) 0.049(3) 0.045(3) 0.015(3) 0.014(3) 0.002(3)
N2 0.059(3) 0.093(4) 0.055(3) 0.001(3) 0.030(2) 0.007(3)
N3 0.052(3) 0.054(3) 0.046(3) 0.014(3) 0.018(3) 0.010(3)
N4 0.043(2) 0.049(2) 0.045(3) 0.012(2) 0.015(2) 0.0028(19)
N5 0.066(3) 0.048(3) 0.080(3) 0.008(3) 0.034(3) 0.004(2)
N6 0.075(4) 0.105(4) 0.073(4) -0.006(3) 0.026(3) 0.000(3)
N7 0.060(3) 0.053(3) 0.063(3) -0.002(3) 0.025(2) -0.001(2)
O1 0.049(3) 0.055(3) 0.044(3) 0.013(2) 0.015(2) 0.002(2)
O2 0.050(3) 0.046(3) 0.049(3) 0.015(2) 0.013(2) -0.004(2)
O3 0.045(2) 0.051(3) 0.044(3) 0.007(2) 0.014(2) -0.002(2)
O4 0.043(2) 0.061(3) 0.055(3) 0.033(3) 0.011(2) 0.004(2)
O5 0.043(2) 0.043(2) 0.042(3) 0.008(2) 0.011(2) 0.000(2)
O6 0.041(2) 0.039(2) 0.038(3) 0.008(2) 0.0122(19) -0.0033(19)
O7 0.083(3) 0.047(3) 0.045(3) 0.002(2) 0.019(3) -0.005(3)
O8 0.043(2) 0.052(3) 0.044(3) 0.012(2) 0.015(2) 0.008(2)
O9 0.048(3) 0.055(3) 0.040(3) 0.014(2) 0.013(2) 0.002(2)
O10 0.041(2) 0.039(2) 0.046(3) 0.015(2) 0.019(2) 0.0081(19)
O11 0.039(2) 0.048(3) 0.041(3) 0.005(2) 0.011(2) 0.006(2)
O12 0.047(2) 0.047(3) 0.048(3) 0.011(2) 0.019(2) 0.012(2)
O13 0.055(3) 0.046(3) 0.043(3) 0.013(2) 0.020(2) 0.013(2)
O14 0.062(3) 0.046(3) 0.049(3) 0.006(2) 0.025(2) 0.008(2)
Eu1 0.03884(19) 0.03599(19) 0.0360(2) 0.00805(15) 0.01326(14)
0.00315(14)
Eu2 0.03759(19) 0.03638(19) 0.0349(2) 0.00905(15) 0.01297(14)
0.00316(14)

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;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;
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C1 O1 1.265(7) . ?
C1 C2 1.477(9) . ?
C1 Eu1 2.851(7) . ?
C2 C7 1.366(10) . ?
C2 C3 1.402(9) . ?
C3 C4 1.391(10) . ?
C3 H3 0.9300 . ?
C4 C5 1.383(10) . ?
C4 H4 0.9300 . ?
C5 C6 1.376(10) . ?
C5 C8 1.482(10) . ?
C6 C7 1.368(10) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 N1 1.261(9) . ?
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C9 O3 1.244(8) . ?
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 'Eu'  'Eu'  -8.9294  11.1857
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 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    29.7931(10)
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Source'
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Atlas'
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_computing_publication_material    'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C3 C 0.0267(4) 0.6748(11) 0.0755(10) 0.057(3) Uani 1 1 d . . .
H3 H 0.0354 0.6067 0.0631 0.068 Uiso 1 1 calc R . .
C4 C -0.0165(4) 0.6957(10) 0.1016(10) 0.057(3) Uani 1 1 d . . .
H4 H -0.0363 0.6407 0.1086 0.069 Uiso 1 1 calc R . .
C5 C -0.0301(4) 0.7962(9) 0.1170(9) 0.050(3) Uani 1 1 d . . .
C6 C -0.0005(3) 0.8773(10) 0.1123(9) 0.058(3) Uani 1 1 d . . .
H6 H -0.0094 0.9449 0.1262 0.069 Uiso 1 1 calc R . .
C7 C 0.0433(4) 0.8586(11) 0.0864(9) 0.055(3) Uani 1 1 d . . .
H7 H 0.0632 0.9140 0.0815 0.066 Uiso 1 1 calc R . .
C8 C 0.4221(3) 0.3113(9) 0.1373(9) 0.048(3) Uani 1 1 d D . .
H16 H 0.405(4) 0.247(6) 0.154(9) 0.057 Uiso 1 1 d D . .
C9 C 0.2556(3) 0.5573(7) 0.0522(6) 0.0323(17) Uani 1 1 d . . .
C10 C 0.2853(3) 0.4864(7) 0.1120(6) 0.0317(17) Uani 1 1 d . . .
C11 C 0.3317(3) 0.4810(8) 0.1028(7) 0.038(2) Uani 1 1 d . . .
H11 H 0.3446 0.5251 0.0597 0.046 Uiso 1 1 calc R . .
C12 C 0.3584(3) 0.4097(8) 0.1581(7) 0.040(2) Uani 1 1 d . . .
C13 C 0.3398(3) 0.3481(8) 0.2264(7) 0.0349(19) Uani 1 1 d . . .
H13 H 0.3580 0.3018 0.2642 0.042 Uiso 1 1 calc R . .
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C14 C 0.2937(3) 0.3546(7) 0.2392(6) 0.0329(18) Uani 1 1 d . . .
C15 C 0.2663(3) 0.4215(8) 0.1789(7) 0.0361(19) Uani 1 1 d . . .
H15 H 0.2354 0.4227 0.1834 0.043 Uiso 1 1 calc R . .
C16 C 0.2737(3) 0.7082(7) -0.1836(7) 0.0331(19) Uani 1 1
d . . .
C17 C 0.1124(4) 0.5299(10) -0.1807(9) 0.056(3) Uani 1 1 d . . .
H17 H 0.0869 0.5634 -0.1622 0.067 Uiso 1 1 calc R . .
C18 C 0.1128(4) 0.4550(11) -0.2526(10) 0.066(3) Uani 1 1
d . . .
H18 H 0.0881 0.4320 -0.2930 0.079 Uiso 1 1 calc R . .
C19 C 0.1801(3) 0.4764(8) -0.1862(8) 0.046(2) Uani 1 1 d . . .
H19 H 0.2110 0.4676 -0.1717 0.056 Uiso 1 1 calc R . .
C20 C 0.6879(8) 0.642(2) 0.1302(17) 0.116(4) Uani 1 1 d U . .
H20 H 0.6898 0.5779 0.1622 0.140 Uiso 1 1 calc R . .
C21 C 0.6642(10) 0.7938(17) 0.0662(19) 0.111(4) Uani 1 1 d
U . .
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N2 N 0.1547(3) 0.5469(7) -0.1415(6) 0.0388(17) Uani 1 1 d . . .
N3 N 0.1552(3) 0.4218(8) -0.2532(7) 0.051(2) Uani 1 1 d . . .
N4 N 0.6516(8) 0.7149(14) 0.1266(15) 0.114(4) Uani 1 1 d U . .
N5 N 0.7216(8) 0.6893(14) 0.0727(16) 0.116(4) Uani 1 1 d U . .
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O1 O 0.11637(19) 0.6465(6) 0.0298(5) 0.0396(14) Uani 1 1
d . . .
O2 O 0.1271(2) 0.8154(6) 0.0173(5) 0.0411(15) Uani 1 1 d . . .
O3 O 0.2149(2) 0.5360(5) 0.0348(4) 0.0359(13) Uani 1 1 d . . .
O4 O 0.27173(19) 0.6426(5) 0.0223(4) 0.0315(12) Uani 1 1
d . . .
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d . . .
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O8 O 0.0638(3) 0.8902(9) -0.1693(11) 0.098(4) Uani 1 1 d . . .
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d . . .

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C3 0.023(5) 0.071(7) 0.079(8) 0.012(6) 0.022(5) 0.005(5)
C4 0.028(6) 0.072(8) 0.076(8) 0.014(6) 0.026(6) 0.006(5)
C5 0.024(5) 0.078(8) 0.050(6) 0.010(5) 0.014(4) 0.007(4)
C6 0.024(5) 0.068(7) 0.084(8) -0.009(6) 0.025(5) 0.012(5)
C7 0.028(5) 0.072(7) 0.068(7) -0.006(6) 0.023(5) 0.005(5)
C8 0.023(5) 0.059(6) 0.064(7) 0.015(5) 0.018(5) 0.006(4)
C9 0.018(4) 0.045(4) 0.037(4) 0.001(4) 0.019(3) 0.005(3)
C10 0.017(4) 0.045(5) 0.036(4) -0.002(4) 0.014(3) -0.002(3)
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C12 0.018(4) 0.057(6) 0.048(5) 0.003(4) 0.021(4) 0.005(4)
C13 0.018(4) 0.047(5) 0.041(4) 0.008(4) 0.012(3) 0.007(3)
C14 0.019(4) 0.045(5) 0.036(4) -0.006(4) 0.012(3) 0.000(3)
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C16 0.023(4) 0.048(5) 0.029(4) 0.006(3) 0.009(3) 0.005(3)
C17 0.035(5) 0.065(7) 0.068(7) -0.024(6) 0.014(5) -0.010(5)
C18 0.050(7) 0.072(8) 0.075(8) -0.026(7) -0.002(6) -0.004(6)
C19 0.033(5) 0.049(5) 0.059(6) 0.000(5) 0.015(4) 0.000(4)
C20 0.117(6) 0.122(5) 0.111(6) -0.001(4) 0.014(4) 0.000(4)
C21 0.112(5) 0.114(5) 0.108(6) -0.005(4) 0.010(4) -0.010(4)
N1 0.016(3) 0.063(5) 0.049(4) 0.010(4) 0.015(3) 0.005(3)
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N4 0.115(5) 0.117(5) 0.111(6) 0.002(4) 0.014(4) -0.005(4)
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N7 0.120(6) 0.119(5) 0.116(6) 0.004(4) 0.009(5) -0.007(4)
O1 0.015(3) 0.054(4) 0.052(4) -0.006(3) 0.013(2) 0.000(3)
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O3 0.021(3) 0.048(3) 0.041(3) 0.001(3) 0.012(2) -0.003(3)
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O5 0.018(3) 0.057(3) 0.021(2) -0.007(3) 0.009(2) -0.008(3)
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Eu1 0.0101(3) 0.0396(4) 0.0313(4) -0.00060(17) 0.0115(2)
0.00061(15)

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l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C2 C7 1.376(18) . ?
C2 C3 1.404(17) . ?
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C5 C8 1.486(14) 3_455 ?
C6 C7 1.405(13) . ?
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C16 O6 1.269(11) . ?
C16 C14 1.501(12) 6_565 ?
C17 N2 1.342(13) . ?
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C18 N3 1.335(16) . ?
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C20 N5 1.47(3) . ?
C20 H20 0.9300 . ?
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C21 N7 1.38(3) . ?
C21 N4 1.38(3) . ?
N2 Eu1 2.551(9) . ?
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O4 Eu1 2.371(6) 7_565 ?
O4 Eu1 2.697(6) . ?
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C10 C11 H11 119.9 . . ?
C13 C12 C11 120.1(8) . . ?
C13 C12 N1 121.5(9) . . ?
C11 C12 N1 118.4(8) . . ?
C12 C13 C14 120.6(8) . . ?
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C13 C14 C15 119.1(8) . . ?
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O6 C16 C14 115.9(8) . 6_565 ?
N2 C17 C18 109.6(10) . . ?
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C18 C17 H17 125.2 . . ?
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C17 C18 H18 126.5 . . ?
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N3 C19 H19 124.3 . . ?
N2 C19 H19 124.3 . . ?
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N5 C20 H20 127.3 . . ?
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N6 C21 N4 108(2) . . ?
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N5 N6 C21 114(2) . . ?
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C16 O6 Eu1 135.9(6) . . ?
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O6 Eu1 O2 138.4(2) . . ?
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 'x+1/2, y+1/2, z'
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 '-x, -y, -z'
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 'x+1/2, -y+1/2, z-1/2'

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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_refine_ls_extinction_method      none
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C2 C 0.4644(4) 0.1695(8) 0.0423(11) 0.0233(19) Uani 0.50 1 d
PU A 1
C2A C 0.4586(5) 0.2055(9) -0.0094(15) 0.039(2) Uani 0.50 1 d
PU A 2
C3 C 0.4783(4) 0.1997(7) -0.0622(11) 0.0250(19) Uani 0.50 1 d
PU A 1
H3 H 0.4594 0.2428 -0.1155 0.030 Uiso 0.50 1 calc PR A 1
C3A C 0.4837(6) 0.2655(9) -0.0587(14) 0.045(3) Uani 0.50 1 d
PU A 2
H3A H 0.4727 0.3193 -0.0673 0.054 Uiso 0.50 1 calc PR A 2
C4 C 0.5193(5) 0.1650(8) -0.0838(13) 0.028(2) Uani 0.50 1 d PU
A 1
H4 H 0.5282 0.1848 -0.1524 0.034 Uiso 0.50 1 calc PR A 1
C4A C 0.5251(5) 0.2414(8) -0.0936(14) 0.043(2) Uani 0.50 1 d
PU A 2
H4A H 0.5424 0.2787 -0.1261 0.052 Uiso 0.50 1 calc PR A 2
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C5 C 0.5495(4) 0.0977(6) -0.0014(10) 0.0218(18) Uani 0.50 1 d
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C5A C 0.5401(6) 0.1596(9) -0.0787(15) 0.041(3) Uani 0.50 1 d
PU A 2
C6 C 0.5349(4) 0.0686(7) 0.0990(11) 0.029(2) Uani 0.50 1 d PU
A 1
H6 H 0.5537 0.0254 0.1523 0.035 Uiso 0.50 1 calc PR A 1
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H6A H 0.5292 0.0502 -0.0258 0.058 Uiso 0.50 1 calc PR A 2
C7 C 0.4922(4) 0.1031(7) 0.1215(12) 0.031(2) Uani 0.50 1 d PU
A 1
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C7A C 0.4750(5) 0.1286(10) 0.0112(15) 0.050(3) Uani 0.50 1 d
PU A 2
H7A H 0.4602 0.0918 0.0510 0.060 Uiso 0.50 1 calc PR A 2
C8 C 0.5943(4) 0.0615(6) -0.0270(10) 0.024(2) Uani 0.50 1 d PU
A 1
C8A C 0.5868(5) 0.1367(9) -0.1203(14) 0.045(3) Uani 0.50 1 d
PU A 2
C9 C 0.26532(19) 0.1683(3) -0.2019(5) 0.0255(11) Uani 1 1
d . . .
C10 C 0.28519(19) 0.1055(3) -0.2705(5) 0.0230(11) Uani 1 1
d . . .
C11 C 0.24398(19) 0.5350(3) -0.1788(5) 0.0236(11) Uani 1 1
d . . .
H11 H 0.2770 0.5275 -0.1830 0.028 Uiso 1 1 calc R . .
C12 C 0.22342(19) 0.4761(3) -0.1218(5) 0.0228(11) Uani 1 1 d .
A .
C13 C 0.17515(18) 0.4874(3) -0.1090(5) 0.0240(11) Uani 1 1
d . . .
H13 H 0.1613 0.4466 -0.0733 0.029 Uiso 1 1 calc R . .
C14 C 0.64774(19) 0.0609(3) -0.1505(5) 0.0258(11) Uani 1 1
d . . .
C15 C 0.33303(19) 0.1169(3) -0.2823(5) 0.0269(11) Uani 1 1
d . . .
H15 H 0.3532 0.1629 -0.2445 0.032 Uiso 1 1 calc R . .
C16 C 0.25560(19) 0.3996(3) -0.0694(5) 0.0220(10) Uani 1 1
d . . .
C17 C 0.3900(5) 0.4538(7) 0.2767(13) 0.038(3) Uani 0.50 1 d PU
A 1
H17 H 0.3574 0.4767 0.2210 0.045 Uiso 0.50 1 calc PR A 1
C17A C 0.3952(5) 0.4045(9) 0.3690(15) 0.056(3) Uani 0.50 1 d
PU A 2
H17A H 0.3647 0.3920 0.3830 0.067 Uiso 0.50 1 calc PR A 2
C18 C 0.4281(5) 0.5015(7) 0.3726(13) 0.041(3) Uani 0.50 1 d PU
A 1
H18 H 0.4190 0.5544 0.3845 0.050 Uiso 0.50 1 calc PR A 1
C18A C 0.4337(6) 0.4531(10) 0.4644(16) 0.059(4) Uani 0.50 1 d
PU A 2
H18A H 0.4282 0.4711 0.5391 0.071 Uiso 0.50 1 calc PR A 2
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C20A C 0.4868(4) 0.3926(7) 0.4361(13) 0.035(2) Uani 0.50 1 d
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C21 C 0.4468(7) 0.3847(12) 0.2636(19) 0.078(4) Uani 0.50 1 d
PU A 1
H21 H 0.4549 0.3551 0.2014 0.094 Uiso 0.50 1 calc PR A 1
C21A C 0.4468(4) 0.3471(7) 0.3414(13) 0.034(2) Uani 0.50 1 d
PU A 2
H21A H 0.4539 0.2928 0.3327 0.041 Uiso 0.50 1 calc PR A 2
N1 N 0.60159(19) 0.0785(4) -0.1284(5) 0.0426(13) Uani 1 1
d . . .
N2 N 0.39885(17) 0.3753(3) 0.2620(5) 0.0306(10) Uani 1 1
d . . .
O1 O 0.39895(16) 0.1781(3) 0.1197(5) 0.0513(13) Uani 1 1 d .
A .
O2 O 0.40200(17) 0.2912(4) 0.0149(5) 0.0519(14) Uani 1 1 d .
A .
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d . . .
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O5 O 0.23178(13) 0.3343(2) -0.0635(3) 0.0224(7) Uani 1 1
d . . .
O6 O 0.30527(13) 0.4031(2) -0.0291(4) 0.0272(8) Uani 1 1 d .
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C3A 0.044(4) 0.048(4) 0.049(5) -0.005(4) 0.026(4) 0.000(3)
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C5 0.016(3) 0.025(3) 0.027(3) 0.000(3) 0.011(3) -0.001(2)
C5A 0.038(5) 0.043(4) 0.041(5) -0.003(4) 0.015(4) 0.001(3)
C6 0.031(4) 0.030(4) 0.036(4) 0.004(3) 0.023(3) 0.005(3)
C6A 0.053(5) 0.046(4) 0.050(5) 0.004(4) 0.026(4) 0.006(3)
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C7A 0.043(4) 0.050(4) 0.059(5) 0.001(4) 0.024(4) -0.001(4)
C8 0.022(3) 0.026(4) 0.030(4) -0.002(3) 0.017(3) 0.000(3)
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C9 0.023(3) 0.029(3) 0.027(2) 0.000(2) 0.013(2) 0.002(2)
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C15 0.024(2) 0.033(3) 0.028(3) -0.005(2) 0.014(2) -0.004(2)
C16 0.023(2) 0.023(3) 0.027(2) -0.001(2) 0.017(2) 0.001(2)
C17 0.035(4) 0.022(5) 0.046(5) -0.011(4) 0.005(4) -0.008(4)
C17A 0.037(4) 0.070(7) 0.065(6) -0.025(5) 0.025(5) -0.006(5)
C18 0.032(5) 0.023(5) 0.051(6) -0.007(4) -0.002(4) -0.003(4)
C18A 0.050(6) 0.069(7) 0.067(7) -0.027(5) 0.034(5) -0.008(5)
C19 0.023(3) 0.030(3) 0.040(3) -0.009(3) 0.015(2) -0.003(2)
C20 0.053(5) 0.096(8) 0.083(7) -0.024(6) 0.043(5) -0.016(5)
C20A 0.027(4) 0.025(5) 0.044(5) -0.005(4) 0.005(4) 0.002(4)
C21 0.078(7) 0.086(8) 0.080(7) -0.039(6) 0.041(6) -0.005(5)
C21A 0.027(4) 0.022(5) 0.043(5) -0.002(4) 0.003(4) 0.003(4)
N1 0.033(3) 0.059(4) 0.048(3) 0.002(3) 0.029(2) 0.012(3)
N2 0.025(2) 0.034(3) 0.037(2) -0.009(2) 0.017(2) -0.009(2)
O1 0.024(2) 0.055(3) 0.079(3) -0.025(3) 0.024(2) 0.008(2)
O2 0.022(2) 0.100(4) 0.044(3) -0.022(3) 0.024(2) -0.019(3)
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0.0091(15)
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0.0006(15)
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0.0035(14)
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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O5 2.647(3) . ?
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C9 O3 1.267(6) . ?
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O6 Eu1 O5 51.42(10) . . ?
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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G\"ottingen, Germany.

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Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0795P)^2^+16.3756P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4462
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_refine_ls_number_restraints      16
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_refine_ls_wR_factor_ref          0.1278
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1 d . . .
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d . . .
O2 O 0.88876(17) 0.6662(3) 0.2022(5) 0.0455(12) Uani 1 1
d . . .
O3 O 0.77843(14) 0.8327(3) -0.1237(4) 0.0299(9) Uani 1 1
d . . .
O4 O 0.79892(17) 0.7233(3) 0.2241(4) 0.0342(11) Uani 1 1
d . . .
O5 O 0.80551(14) 0.9153(3) 0.1424(4) 0.0301(9) Uani 1 1 d . . .
O6 O 0.73653(14) 0.8411(2) 0.0197(4) 0.0267(9) Uani 1 1 d . . .
O7 O 0.8472(2) 0.6823(4) -0.0517(6) 0.0595(13) Uani 1 1 d U . .
O8 O 0.8588(4) 0.7408(6) -0.1929(9) 0.106(2) Uani 1 1 d U . .
N1 N 1.1127(2) 0.6057(4) 0.8369(5) 0.0552(18) Uani 1 1 d . . .
N2 N 0.8536(3) 0.6716(6) -0.1414(8) 0.0795(19) Uani 1 1 d U . .
N3 N 0.88477(19) 0.8659(4) 0.0693(5) 0.0383(13) Uani 1 1
d . . .
C1 C 0.9125(3) 0.7133(5) 0.3013(7) 0.0430(17) Uani 1 1 d . . .
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C2 C 0.9607(3) 0.6768(6) 0.4099(7) 0.0530(19) Uani 1 1 d . . .
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H3 H 0.9759 0.5923 0.3073 0.068 Uiso 1 1 calc R . .
C4 C 1.0332(3) 0.5827(6) 0.4874(7) 0.060(2) Uani 1 1 d . . .
H4 H 1.0514 0.5429 0.4716 0.072 Uiso 1 1 calc R . .
C5 C 1.0516(3) 0.6101(6) 0.6093(7) 0.057(2) Uani 1 1 d . . .
C6 C 1.0243(3) 0.6689(7) 0.6329(9) 0.073(3) Uani 1 1 d . . .
H6 H 1.0351 0.6839 0.7159 0.088 Uiso 1 1 calc R . .
C7 C 0.9795(4) 0.7066(7) 0.5292(8) 0.071(3) Uani 1 1 d . . .
H7 H 0.9633 0.7514 0.5437 0.085 Uiso 1 1 calc R . .
C8 C 1.1021(3) 0.5745(7) 0.7180(8) 0.066(2) Uani 1 1 d D . .
C9 C 0.7338(2) 0.8269(4) -0.2170(5) 0.0272(12) Uani 1 1 d . . .
C10 C 0.7178(2) 0.8852(4) -0.3293(5) 0.0291(13) Uani 1 1
d . . .
C11 C 0.6727(2) 0.8686(4) -0.4406(6) 0.0358(15) Uani 1 1
d . . .
H11 H 0.6530 0.8221 -0.4439 0.043 Uiso 1 1 calc R . .
C12 C 0.6562(2) 0.9203(4) -0.5483(6) 0.0397(15) Uani 1 1
d . . .
C13 C 0.6839(2) 0.9952(4) -0.5377(6) 0.0323(13) Uani 1 1
d . . .
H13 H 0.6719 1.0338 -0.6059 0.039 Uiso 1 1 calc R . .
C14 C 0.7290(2) 1.0118(4) -0.4260(5) 0.0276(12) Uani 1 1
d . . .
C15 C 0.7470(2) 0.9549(4) -0.3230(5) 0.0250(12) Uani 1 1
d . . .
H15 H 0.7784 0.9637 -0.2504 0.030 Uiso 1 1 calc R . .
C17 C 0.8554(4) 0.5810(7) -0.1878(11) 0.086(3) Uani 1 1 d . . .
H17A H 0.8233 0.5675 -0.2640 0.103 Uiso 1 1 calc R . .
H17B H 0.8617 0.5376 -0.1238 0.103 Uiso 1 1 calc R . .
C16 C 0.7595(2) 0.9110(4) 0.0817(5) 0.0261(12) Uani 1 1 d . . .
C18 C 0.8719(3) 0.9461(5) 0.0142(8) 0.054(2) Uani 1 1 d . . .
H18 H 0.8414 0.9696 -0.0067 0.065 Uiso 1 1 calc R . .
C19 C 0.9010(3) 0.9949(6) -0.0128(10) 0.071(3) Uani 1 1 d . . .
H19 H 0.8902 1.0497 -0.0520 0.085 Uiso 1 1 calc R . .
C20 C 0.9472(3) 0.9615(6) 0.0192(10) 0.066(2) Uani 1 1 d . . .
C21 C 0.9608(3) 0.8784(6) 0.0758(9) 0.062(2) Uani 1 1 d . . .
H21 H 0.9914 0.8540 0.0994 0.075 Uiso 1 1 calc R . .
C22 C 0.9287(3) 0.8332(6) 0.0964(8) 0.0529(19) Uani 1 1 d . . .
H22 H 0.9378 0.7768 0.1310 0.063 Uiso 1 1 calc R . .
C23 C 0.9784(4) 1.0147(7) -0.0127(12) 0.089(3) Uani 1 1 d . . .
H16 H 1.101(4) 0.5103(16) 0.717(10) 0.106 Uiso 1 1 d D . .

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0.00024(10)
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O2 0.026(2) 0.046(3) 0.041(3) 0.005(2) 0.002(2) 0.010(2)
O3 0.021(2) 0.039(2) 0.023(2) 0.0074(18) 0.0080(18) -0.0016(17)
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O4 0.027(2) 0.045(3) 0.022(2) 0.0060(18) 0.0079(19) -0.0126(19)
O5 0.022(2) 0.028(2) 0.030(2) -0.0038(17) 0.0075(18) -
0.0004(17)
O6 0.028(2) 0.022(2) 0.024(2) -0.0007(16) 0.0098(18) -
0.0002(16)
O7 0.044(3) 0.065(4) 0.074(3) -0.008(3) 0.035(3) 0.005(3)
O8 0.113(3) 0.110(3) 0.104(3) 0.0123(18) 0.065(2) -0.0083(19)
N1 0.048(4) 0.064(4) 0.023(3) -0.004(3) -0.001(3) 0.024(3)
N2 0.084(3) 0.085(3) 0.077(2) -0.0028(17) 0.048(2) 0.0013(18)
N3 0.027(3) 0.043(3) 0.042(3) 0.001(3) 0.017(3) -0.006(2)
C1 0.025(4) 0.043(4) 0.047(5) 0.013(3) 0.010(3) -0.001(3)
C2 0.040(4) 0.060(5) 0.041(4) 0.010(4) 0.010(3) -0.002(4)
C3 0.041(4) 0.071(6) 0.043(4) 0.001(4) 0.013(4) 0.010(4)
C4 0.045(5) 0.069(6) 0.041(4) 0.009(4) 0.007(4) 0.010(4)
C5 0.049(5) 0.063(5) 0.044(5) 0.009(4) 0.015(4) -0.001(4)
C6 0.058(5) 0.091(7) 0.052(5) 0.008(5) 0.018(4) 0.022(5)
C7 0.057(6) 0.088(7) 0.041(5) 0.008(5) 0.010(4) 0.022(5)
C8 0.053(5) 0.075(6) 0.040(4) 0.013(4) 0.006(4) -0.002(5)
C9 0.027(3) 0.028(3) 0.023(3) 0.001(2) 0.011(3) -0.001(2)
C10 0.027(3) 0.034(3) 0.020(3) 0.001(2) 0.009(3) -0.003(3)
C11 0.034(3) 0.034(3) 0.028(3) 0.005(3) 0.009(3) -0.014(3)
C12 0.032(3) 0.042(4) 0.026(3) 0.002(3) 0.004(3) -0.010(3)
C13 0.029(3) 0.031(3) 0.023(3) 0.007(3) 0.005(3) -0.003(3)
C14 0.027(3) 0.025(3) 0.026(3) 0.002(2) 0.012(3) 0.000(2)
C15 0.024(3) 0.024(3) 0.020(3) 0.002(2) 0.007(2) -0.002(2)
C17 0.112(9) 0.078(7) 0.082(7) -0.010(6) 0.062(7) -0.005(6)
C16 0.028(3) 0.024(3) 0.018(3) -0.001(2) 0.008(2) 0.001(2)
C18 0.040(4) 0.044(4) 0.087(6) 0.011(4) 0.040(4) -0.001(3)
C19 0.062(5) 0.054(5) 0.114(8) 0.021(5) 0.058(6) 0.001(4)
C20 0.057(5) 0.054(5) 0.106(7) 0.018(5) 0.056(5) -0.004(4)
C21 0.042(4) 0.072(6) 0.083(6) 0.012(5) 0.041(5) 0.001(4)
C22 0.035(4) 0.060(5) 0.062(5) 0.018(4) 0.025(4) 0.002(3)
C23 0.066(6) 0.074(7) 0.153(10) 0.017(7) 0.076(7) -0.005(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O2 2.424(4) . ?
Eu1 O1 2.518(4) . ?
Eu1 N3 2.547(5) . ?
Eu1 O6 2.604(4) . ?
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Eu1 C16 2.879(6) . ?
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O2 C1 1.267(9) . ?
O3 C9 1.264(7) . ?
O4 C9 1.256(7) 7_665 ?
O5 C16 1.237(7) . ?
O6 C16 1.282(7) . ?
O6 Eu1 2.351(4) 7_665 ?
O7 N2 1.259(9) . ?
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N1 C12 1.410(8) 8_567 ?
N1 C8 1.420(11) . ?
N2 C17 1.504(13) . ?
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N3 C18 1.347(9) . ?
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C4 C5 1.371(11) . ?
C4 H4 0.9300 . ?
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C7 H7 0.9300 . ?
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C8 H16 0.97(2) . ?
C9 O4 1.256(7) 7_665 ?
C9 C10 1.497(8) . ?
C10 C15 1.382(8) . ?
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C11 C12 1.393(9) . ?
C11 H11 0.9300 . ?
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C13 C14 1.383(8) . ?
C13 H13 0.9300 . ?
C14 C15 1.391(8) . ?
C14 C16 1.491(8) 6_575 ?
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C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C16 C14 1.491(8) 6_576 ?
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C18 H18 0.9300 . ?
C19 C20 1.396(12) . ?
C19 H19 0.9300 . ?
C20 C21 1.393(12) . ?
C20 C23 1.494(11) . ?
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O4 Eu1 C1 76.14(19) . . ?
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O6 Eu1 C1 113.30(18) 7_665 . ?
O3 Eu1 C1 149.11(18) . . ?
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O1 Eu1 C1 26.19(19) . . ?
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O6 Eu1 C1 141.49(19) . . ?
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O2 Eu1 C16 150.24(16) . . ?
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N3 Eu1 C16 99.37(17) . . ?
O6 Eu1 C16 26.43(14) . . ?
O7 Eu1 C16 144.93(17) . . ?
C1 Eu1 C16 126.0(2) . . ?
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C9 O4 Eu1 136.4(4) 7_665 . ?
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O7 N2 C17 121.5(8) . . ?
O8 N2 C17 120.3(9) . . ?
C22 N3 C18 116.6(6) . . ?
C22 N3 Eu1 122.2(5) . . ?
C18 N3 Eu1 120.5(4) . . ?
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O1 C1 C2 120.9(7) . . ?
O2 C1 C2 117.2(7) . . ?
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C7 C2 C1 120.2(8) . . ?
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C4 C3 C2 120.8(8) . . ?
C4 C3 H3 119.6 . . ?
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C7 C6 H6 120.1 . . ?
C2 C7 C6 119.9(9) . . ?
C2 C7 H7 120.1 . . ?
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C5 C8 C17 112.7(8) . 2_755 ?
N1 C8 H16 109(7) . . ?
C5 C8 H16 109(7) . . ?
C17 C8 H16 95(7) 2_755 . ?
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C15 C10 C9 121.3(5) . . ?
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C13 C12 N1 123.0(6) . 8_464 ?
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C14 C13 H13 120.0 . . ?
C12 C13 H13 120.0 . . ?
C13 C14 C15 120.5(5) . . ?
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C15 C14 C16 119.9(5) . 6_575 ?
C10 C15 C14 119.6(5) . . ?
C10 C15 H15 120.2 . . ?
C14 C15 H15 120.2 . . ?
N2 C17 C8 111.3(9) . 2_755 ?
N2 C17 H17A 109.4 . . ?
C8 C17 H17A 109.4 2_755 . ?
N2 C17 H17B 109.4 . . ?
C8 C17 H17B 109.4 2_755 . ?
H17A C17 H17B 108.0 . . ?
O5 C16 O6 121.0(5) . . ?
O5 C16 C14 120.9(5) . 6_576 ?
O6 C16 C14 118.0(5) . 6_576 ?
O5 C16 Eu1 56.4(3) . . ?
O6 C16 Eu1 64.7(3) . . ?
C14 C16 Eu1 174.5(4) 6_576 . ?
N3 C18 C19 123.7(7) . . ?
N3 C18 H18 118.2 . . ?
C19 C18 H18 118.2 . . ?
C18 C19 C20 119.2(8) . . ?
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C18 C19 H19 120.4 . . ?
C20 C19 H19 120.4 . . ?
C21 C20 C19 117.6(7) . . ?
C21 C20 C23 123.6(8) . . ?
C19 C20 C23 118.7(8) . . ?
C22 C21 C20 119.2(8) . . ?
C22 C21 H21 120.4 . . ?
C20 C21 H21 120.4 . . ?
N3 C22 C21 123.6(7) . . ?
N3 C22 H22 118.2 . . ?
C21 C22 H22 118.2 . . ?
C23 C23 C20 121.2(12) 5_775 . ?

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 '-x, -y, -z'
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 MERCURY (Bruno et al. 2002)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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_refine_ls_extinction_coef        ?
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d . . .
O2 O 0.88876(17) 0.6662(3) 0.2022(5) 0.0455(12) Uani 1 1
d . . .
O3 O 0.77843(14) 0.8327(3) -0.1237(4) 0.0299(9) Uani 1 1
d . . .
O4 O 0.79892(17) 0.7233(3) 0.2241(4) 0.0342(11) Uani 1 1
d . . .
O5 O 0.80551(14) 0.9153(3) 0.1424(4) 0.0301(9) Uani 1 1 d . . .
O6 O 0.73653(14) 0.8411(2) 0.0197(4) 0.0267(9) Uani 1 1 d . . .
O7 O 0.8472(2) 0.6823(4) -0.0517(6) 0.0595(13) Uani 1 1 d U . .
O8 O 0.8588(4) 0.7408(6) -0.1929(9) 0.106(2) Uani 1 1 d U . .
N1 N 1.1127(2) 0.6057(4) 0.8369(5) 0.0552(18) Uani 1 1 d . . .
N2 N 0.8536(3) 0.6716(6) -0.1414(8) 0.0795(19) Uani 1 1 d U . .
N3 N 0.88477(19) 0.8659(4) 0.0693(5) 0.0383(13) Uani 1 1
d . . .
C1 C 0.9125(3) 0.7133(5) 0.3013(7) 0.0430(17) Uani 1 1 d . . .
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C2 C 0.9607(3) 0.6768(6) 0.4099(7) 0.0530(19) Uani 1 1 d . . .
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C4 C 1.0332(3) 0.5827(6) 0.4874(7) 0.060(2) Uani 1 1 d . . .
H4 H 1.0514 0.5429 0.4716 0.072 Uiso 1 1 calc R . .
C5 C 1.0516(3) 0.6101(6) 0.6093(7) 0.057(2) Uani 1 1 d . . .
C6 C 1.0243(3) 0.6689(7) 0.6329(9) 0.073(3) Uani 1 1 d . . .
H6 H 1.0351 0.6839 0.7159 0.088 Uiso 1 1 calc R . .
C7 C 0.9795(4) 0.7066(7) 0.5292(8) 0.071(3) Uani 1 1 d . . .
H7 H 0.9633 0.7514 0.5437 0.085 Uiso 1 1 calc R . .
C8 C 1.1021(3) 0.5745(7) 0.7180(8) 0.066(2) Uani 1 1 d D . .
C9 C 0.7338(2) 0.8269(4) -0.2170(5) 0.0272(12) Uani 1 1 d . . .
C10 C 0.7178(2) 0.8852(4) -0.3293(5) 0.0291(13) Uani 1 1
d . . .
C11 C 0.6727(2) 0.8686(4) -0.4406(6) 0.0358(15) Uani 1 1
d . . .
H11 H 0.6530 0.8221 -0.4439 0.043 Uiso 1 1 calc R . .
C12 C 0.6562(2) 0.9203(4) -0.5483(6) 0.0397(15) Uani 1 1
d . . .
C13 C 0.6839(2) 0.9952(4) -0.5377(6) 0.0323(13) Uani 1 1
d . . .
H13 H 0.6719 1.0338 -0.6059 0.039 Uiso 1 1 calc R . .
C14 C 0.7290(2) 1.0118(4) -0.4260(5) 0.0276(12) Uani 1 1
d . . .
C15 C 0.7470(2) 0.9549(4) -0.3230(5) 0.0250(12) Uani 1 1
d . . .
H15 H 0.7784 0.9637 -0.2504 0.030 Uiso 1 1 calc R . .
C17 C 0.8554(4) 0.5810(7) -0.1878(11) 0.086(3) Uani 1 1 d . . .
H17A H 0.8233 0.5675 -0.2640 0.103 Uiso 1 1 calc R . .
H17B H 0.8617 0.5376 -0.1238 0.103 Uiso 1 1 calc R . .
C16 C 0.7595(2) 0.9110(4) 0.0817(5) 0.0261(12) Uani 1 1 d . . .
C18 C 0.8719(3) 0.9461(5) 0.0142(8) 0.054(2) Uani 1 1 d . . .
H18 H 0.8414 0.9696 -0.0067 0.065 Uiso 1 1 calc R . .
C19 C 0.9010(3) 0.9949(6) -0.0128(10) 0.071(3) Uani 1 1 d . . .
H19 H 0.8902 1.0497 -0.0520 0.085 Uiso 1 1 calc R . .
C20 C 0.9472(3) 0.9615(6) 0.0192(10) 0.066(2) Uani 1 1 d . . .
C21 C 0.9608(3) 0.8784(6) 0.0758(9) 0.062(2) Uani 1 1 d . . .
H21 H 0.9914 0.8540 0.0994 0.075 Uiso 1 1 calc R . .
C22 C 0.9287(3) 0.8332(6) 0.0964(8) 0.0529(19) Uani 1 1 d . . .
H22 H 0.9378 0.7768 0.1310 0.063 Uiso 1 1 calc R . .
C23 C 0.9784(4) 1.0147(7) -0.0127(12) 0.089(3) Uani 1 1 d . . .
H16 H 1.101(4) 0.5103(16) 0.717(10) 0.106 Uiso 1 1 d D . .

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0.00024(10)
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O2 0.026(2) 0.046(3) 0.041(3) 0.005(2) 0.002(2) 0.010(2)
O3 0.021(2) 0.039(2) 0.023(2) 0.0074(18) 0.0080(18) -0.0016(17)
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O4 0.027(2) 0.045(3) 0.022(2) 0.0060(18) 0.0079(19) -0.0126(19)
O5 0.022(2) 0.028(2) 0.030(2) -0.0038(17) 0.0075(18) -
0.0004(17)
O6 0.028(2) 0.022(2) 0.024(2) -0.0007(16) 0.0098(18) -
0.0002(16)
O7 0.044(3) 0.065(4) 0.074(3) -0.008(3) 0.035(3) 0.005(3)
O8 0.113(3) 0.110(3) 0.104(3) 0.0123(18) 0.065(2) -0.0083(19)
N1 0.048(4) 0.064(4) 0.023(3) -0.004(3) -0.001(3) 0.024(3)
N2 0.084(3) 0.085(3) 0.077(2) -0.0028(17) 0.048(2) 0.0013(18)
N3 0.027(3) 0.043(3) 0.042(3) 0.001(3) 0.017(3) -0.006(2)
C1 0.025(4) 0.043(4) 0.047(5) 0.013(3) 0.010(3) -0.001(3)
C2 0.040(4) 0.060(5) 0.041(4) 0.010(4) 0.010(3) -0.002(4)
C3 0.041(4) 0.071(6) 0.043(4) 0.001(4) 0.013(4) 0.010(4)
C4 0.045(5) 0.069(6) 0.041(4) 0.009(4) 0.007(4) 0.010(4)
C5 0.049(5) 0.063(5) 0.044(5) 0.009(4) 0.015(4) -0.001(4)
C6 0.058(5) 0.091(7) 0.052(5) 0.008(5) 0.018(4) 0.022(5)
C7 0.057(6) 0.088(7) 0.041(5) 0.008(5) 0.010(4) 0.022(5)
C8 0.053(5) 0.075(6) 0.040(4) 0.013(4) 0.006(4) -0.002(5)
C9 0.027(3) 0.028(3) 0.023(3) 0.001(2) 0.011(3) -0.001(2)
C10 0.027(3) 0.034(3) 0.020(3) 0.001(2) 0.009(3) -0.003(3)
C11 0.034(3) 0.034(3) 0.028(3) 0.005(3) 0.009(3) -0.014(3)
C12 0.032(3) 0.042(4) 0.026(3) 0.002(3) 0.004(3) -0.010(3)
C13 0.029(3) 0.031(3) 0.023(3) 0.007(3) 0.005(3) -0.003(3)
C14 0.027(3) 0.025(3) 0.026(3) 0.002(2) 0.012(3) 0.000(2)
C15 0.024(3) 0.024(3) 0.020(3) 0.002(2) 0.007(2) -0.002(2)
C17 0.112(9) 0.078(7) 0.082(7) -0.010(6) 0.062(7) -0.005(6)
C16 0.028(3) 0.024(3) 0.018(3) -0.001(2) 0.008(2) 0.001(2)
C18 0.040(4) 0.044(4) 0.087(6) 0.011(4) 0.040(4) -0.001(3)
C19 0.062(5) 0.054(5) 0.114(8) 0.021(5) 0.058(6) 0.001(4)
C20 0.057(5) 0.054(5) 0.106(7) 0.018(5) 0.056(5) -0.004(4)
C21 0.042(4) 0.072(6) 0.083(6) 0.012(5) 0.041(5) 0.001(4)
C22 0.035(4) 0.060(5) 0.062(5) 0.018(4) 0.025(4) 0.002(3)
C23 0.066(6) 0.074(7) 0.153(10) 0.017(7) 0.076(7) -0.005(5)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O2 2.424(4) . ?
Eu1 O1 2.518(4) . ?
Eu1 N3 2.547(5) . ?
Eu1 O6 2.604(4) . ?
Eu1 O7 2.639(5) . ?
Eu1 C1 2.825(7) . ?
Eu1 C16 2.879(6) . ?
O1 C1 1.247(8) . ?
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O4 C9 1.256(7) 7_665 ?
O5 C16 1.237(7) . ?
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O6 Eu1 2.351(4) 7_665 ?
O7 N2 1.259(9) . ?
O8 N2 1.288(11) . ?
N1 C12 1.410(8) 8_567 ?
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N2 C17 1.504(13) . ?
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C4 C5 1.371(11) . ?
C4 H4 0.9300 . ?
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C7 H7 0.9300 . ?
C8 C17 1.599(14) 2_755 ?
C8 H16 0.97(2) . ?
C9 O4 1.256(7) 7_665 ?
C9 C10 1.497(8) . ?
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C10 C11 1.380(8) . ?
C11 C12 1.393(9) . ?
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C13 C14 1.383(8) . ?
C13 H13 0.9300 . ?
C14 C15 1.391(8) . ?
C14 C16 1.491(8) 6_575 ?
C15 H15 0.9300 . ?
C17 C8 1.599(14) 2_755 ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C16 C14 1.491(8) 6_576 ?
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C18 H18 0.9300 . ?
C19 C20 1.396(12) . ?
C19 H19 0.9300 . ?
C20 C21 1.393(12) . ?
C20 C23 1.494(11) . ?
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C21 H21 0.9300 . ?
C22 H22 0.9300 . ?
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O4 Eu1 O3 134.72(14) . . ?
O6 Eu1 O3 81.25(13) 7_665 . ?
O4 Eu1 O5 81.89(15) . . ?
O6 Eu1 O5 125.66(13) 7_665 . ?
O3 Eu1 O5 83.78(14) . . ?
O4 Eu1 O2 82.52(17) . . ?
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 '-x, -y, -z'

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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C6 C 0.1141(8) 0.4773(8) 0.4639(7) 0.0425(19) Uani 1 1 d . . .
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H19B H 0.4919 0.8212 0.0282 0.292 Uiso 1 1 calc R . .
H19C H 0.5528 0.7216 -0.0447 0.292 Uiso 1 1 calc R . .
C20 C 0.888(3) 0.8301(18) 0.5319(14) 0.080(4) Uani 0.50 1 d
PDU . .
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C22 C 1.106(2) 0.907(2) 0.578(2) 0.095(5) Uani 0.50 1 d PDU . .
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C23 C 1.133(2) 0.838(2) 0.4795(17) 0.094(4) Uani 0.50 1 d
PDU . .
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PDU . .
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PU . .
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C5 0.037(4) 0.028(4) 0.055(5) 0.005(4) 0.021(4) 0.011(3)
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C7 0.055(5) 0.047(5) 0.039(4) 0.000(4) 0.018(4) 0.024(4)
C8 0.045(5) 0.049(6) 0.051(5) 0.005(4) 0.018(4) 0.020(4)
C9 0.064(5) 0.027(4) 0.046(5) 0.010(4) 0.029(4) 0.022(4)
C10 0.076(6) 0.022(4) 0.043(5) 0.007(3) 0.024(4) 0.019(4)
C11 0.085(6) 0.024(4) 0.039(4) 0.004(3) 0.015(4) 0.022(4)
C12 0.094(7) 0.028(5) 0.045(5) 0.014(4) 0.021(5) 0.026(4)
C13 0.080(4) 0.072(5) 0.069(4) 0.026(4) 0.032(3) 0.015(4)
C14 0.075(4) 0.071(5) 0.067(4) 0.018(3) 0.030(3) 0.025(3)
C15 0.110(5) 0.099(6) 0.090(5) 0.045(4) 0.023(4) 0.029(4)
C16 0.111(5) 0.098(5) 0.094(5) 0.048(4) 0.019(4) 0.036(4)
C17 0.095(5) 0.094(5) 0.087(5) 0.036(4) 0.015(4) 0.029(4)
C18 0.081(4) 0.070(5) 0.067(4) 0.023(4) 0.019(3) 0.021(4)
C19 0.203(8) 0.190(8) 0.196(8) 0.094(6) 0.048(5) 0.025(4)
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O2 0.060(4) 0.030(3) 0.044(3) -0.005(3) 0.020(3) 0.017(3)
O3 0.061(4) 0.041(4) 0.047(3) 0.005(3) 0.024(3) 0.022(3)
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
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approximate (isotropic)
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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<b>30</b>, 565.

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Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C2 C -0.4074(9) 0.1079(9) -0.4192(8) 0.051(2) Uani 1 1 d . . .
C3 C -0.3938(13) 0.0620(12) -0.5200(10) 0.084(4) Uani 1 1
d . . .
H3 H -0.3211 0.1033 -0.5348 0.101 Uiso 1 1 calc R . .
C4 C -0.5111(14) 0.0482(13) -0.3968(11) 0.092(5) Uani 1 1 d
D . .
C5 C 0.1989(9) 0.4798(8) -0.0747(9) 0.046(2) Uani 1 1 d . . .
C6 C 0.3568(9) 0.4909(9) -0.0371(8) 0.049(2) Uani 1 1 d . . .
C7 C 0.4087(10) 0.4285(13) -0.1098(10) 0.082(4) Uani 1 1 d
D . .
C8 C 0.4456(10) 0.5603(12) 0.0704(10) 0.075(4) Uani 1 1 d . . .
H8 H 0.4094 0.6018 0.1197 0.090 Uiso 1 1 calc R . .
C9 C 0.0092(11) 0.7462(8) 0.0002(9) 0.056(3) Uani 1 1 d . . .
C10 C 0.0046(13) 0.8769(9) 0.0000(9) 0.067(3) Uani 1 1 d . . .
C11 C -0.0401(19) 0.9103(9) -0.1013(10) 0.103(6) Uani 1 1
d . . .
H11 H -0.0687 0.8491 -0.1713 0.123 Uiso 1 1 calc R . .
C12 C 0.0448(18) 0.9691(10) 0.1046(9) 0.097(5) Uani 1 1 d D . .
C13 C -0.362(3) 0.610(2) -0.224(2) 0.204(7) Uani 1 1 d DU . .
C14 C -0.602(3) 0.534(3) -0.366(3) 0.248(8) Uani 1 1 d DU . .
H14A H -0.6743 0.5546 -0.4269 0.372 Uiso 1 1 calc R . .
H14B H -0.6351 0.5232 -0.3069 0.372 Uiso 1 1 calc R . .
H14C H -0.5811 0.4590 -0.3983 0.372 Uiso 1 1 calc R . .
C15 C -0.517(3) 0.707(3) -0.231(3) 0.250(8) Uani 1 1 d DU . .
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H15A H -0.4426 0.7799 -0.1833 0.374 Uiso 1 1 calc R . .
H15B H -0.5355 0.6575 -0.1832 0.374 Uiso 1 1 calc R . .
H15C H -0.6014 0.7322 -0.2715 0.374 Uiso 1 1 calc R . .
C16 C 0.0210(14) 0.6171(15) -0.3349(18) 0.143(5) Uani 1 1 d
DU . .
C17 C -0.0557(17) 0.6917(14) -0.4108(13) 0.140(4) Uani 1 1 d
DU . .
C18 C -0.1753(17) 0.7302(15) -0.4068(16) 0.146(4) Uani 1 1 d
DU . .
H18 H -0.2154 0.7058 -0.3579 0.175 Uiso 1 1 calc R . .
C19 C -0.235(2) 0.8050(16) -0.4756(15) 0.156(5) Uani 1 1 d
DU . .
H19 H -0.3146 0.8308 -0.4731 0.187 Uiso 1 1 calc R . .
C20 C -0.174(2) 0.8407(18) -0.5484(17) 0.163(5) Uani 1 1 d
DU . .
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DU . .
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d . . .
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DU . .
O8 O -0.0904(9) 0.5232(7) -0.3359(7) 0.077(2) Uani 1 1 d D . .
O9 O 0.1254(15) 0.6916(14) -0.4846(13) 0.151(4) Uani 1 1 d
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PDU . .
N2 N 0.323(3) 0.366(3) -0.2318(12) 0.142(11) Uani 0.50 1 d
PDU . .
N3 N 0.063(4) 0.946(3) 0.2159(18) 0.151(12) Uani 0.50 1 d
PDU . .
N4 N -0.476(3) 0.635(2) -0.3157(19) 0.211(7) Uani 1 1 d DU . .
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O6 0.073(4) 0.024(3) 0.042(4) 0.006(3) 0.008(3) 0.007(3)
O7 0.071(5) 0.120(8) 0.082(6) 0.027(5) 0.006(5) 0.030(5)
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 are estimated using the full covariance matrix.  The cell
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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O6 C9 1.255(11) 2_565 ?
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 '-x, -y, -z'

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_cell_measurement_temperature     100(2)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

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<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C3 C 1.3628(12) 0.4453(12) 0.5035(12) 0.099(4) Uani 1 1 d . . .
H3 H 1.2703 0.4092 0.5075 0.119 Uiso 1 1 calc R . .
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C6 C 0.6431(9) 0.0052(9) 0.0403(8) 0.065(2) Uani 1 1 d . . .
C7 C 0.5991(11) 0.0840(12) 0.1058(10) 0.087(3) Uani 1 1 d D . .
C8 C 0.5459(11) -0.0741(11) -0.0653(10) 0.084(3) Uani 1 1
d . . .
H8 H 0.5777 -0.1224 -0.1109 0.101 Uiso 1 1 calc R . .
C9 C 0.9631(11) -0.2553(9) -0.0023(9) 0.072(2) Uani 1 1 d . . .
C10 C 0.9797(11) -0.3815(8) -0.0021(9) 0.074(2) Uani 1 1
d . . .
C11 C 0.9933(14) -0.4370(10) 0.0991(10) 0.088(3) Uani 1 1
d . . .
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C12 C 0.9849(14) -0.4490(9) -0.1035(9) 0.086(3) Uani 1 1 d
D . .
C13 C 1.274(2) -0.1697(16) 0.230(2) 0.201(6) Uani 1 1 d DU A .
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H15B H 1.4329 -0.1715 0.1175 0.356 Uiso 1 1 calc R A 1
H15C H 1.3269 -0.3111 0.1067 0.356 Uiso 1 1 calc R A 1
C14 C 1.372(4) -0.314(3) 0.333(3) 0.225(8) Uani 1 1 d DU A 2
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H14B H 1.3369 -0.3929 0.2764 0.338 Uiso 1 1 calc R A 2
H14C H 1.3016 -0.3126 0.3696 0.338 Uiso 1 1 calc R A 2
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C19 C 0.817(2) -0.215(2) 0.2995(19) 0.156(4) Uani 1 1 d U . .
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H19B H 0.7520 -0.1823 0.3240 0.234 Uiso 1 1 calc R . .
H19C H 0.7922 -0.3043 0.3031 0.234 Uiso 1 1 calc R . .
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N2 N 0.687(3) 0.171(2) 0.206(2) 0.113(7) Uani 0.50 1 d PDU . .
N3 N 0.987(3) -0.398(2) -0.212(2) 0.110(6) Uani 0.50 1 d
PDU . .
N4 N 1.399(2) -0.207(2) 0.2703(19) 0.201(5) Uani 1 1 d DU . .
N5 N 1.0760(16) -0.0665(13) 0.3547(12) 0.122(3) Uani 1 1 d
U . .
N6 N 1.161(2) -0.0687(19) 0.5586(16) 0.162(4) Uani 1 1 d U . .
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O3 O 0.8707(7) 0.0417(7) 0.1883(6) 0.0788(17) Uani 1 1 d . . .
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O5 O 0.9945(9) -0.1862(6) 0.1002(6) 0.0799(18) Uani 1 1 d . . .
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O7 O 1.2931(13) -0.0529(14) 0.2409(12) 0.141(3) Uani 1 1 d
DU . .
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d . . .

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C3 0.067(6) 0.090(7) 0.116(9) -0.021(7) 0.029(6) 0.006(5)
C4 0.091(8) 0.106(9) 0.110(9) -0.026(8) 0.031(7) 0.020(7)
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C6 0.053(4) 0.066(5) 0.070(5) 0.001(4) 0.013(4) 0.022(4)
C7 0.065(5) 0.109(8) 0.073(6) -0.016(6) 0.015(5) 0.029(5)
C8 0.063(5) 0.099(7) 0.086(7) -0.011(6) 0.021(5) 0.034(5)
C9 0.076(6) 0.054(5) 0.076(6) 0.003(4) 0.019(5) 0.017(4)
C10 0.082(6) 0.054(4) 0.075(6) 0.008(4) 0.013(5) 0.024(4)
C11 0.119(9) 0.073(6) 0.073(6) 0.000(5) 0.030(6) 0.043(6)
C12 0.125(9) 0.061(5) 0.067(6) 0.007(4) 0.018(6) 0.040(6)
C13 0.203(7) 0.183(6) 0.212(8) 0.035(5) 0.058(4) 0.074(6)
C15 0.236(9) 0.244(10) 0.240(9) 0.033(5) 0.089(6) 0.088(6)
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C16 0.142(5) 0.146(6) 0.143(5) 0.029(5) 0.045(4) 0.049(4)
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N2 0.110(8) 0.114(8) 0.115(8) 0.012(5) 0.036(5) 0.042(5)
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N4 0.205(7) 0.189(7) 0.215(7) 0.041(5) 0.059(5) 0.085(5)
N5 0.134(4) 0.117(5) 0.125(4) 0.016(4) 0.050(3) 0.055(4)
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O4 0.059(3) 0.067(3) 0.082(4) 0.004(3) 0.023(3) 0.024(3)
O5 0.104(5) 0.062(3) 0.072(4) 0.007(3) 0.024(4) 0.032(3)
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0.0210(2)

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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C2 C4 1.423(18) . ?
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C3 H3 0.9300 . ?
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C4 N1 1.45(3) . ?
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C9 O5 1.285(12) . ?
C9 C10 1.473(13) . ?
C10 C11 1.382(15) . ?
C10 C12 1.396(14) . ?
C11 C12 1.363(14) 2_745 ?
C11 H11 0.9300 . ?
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C19 H19C 0.9600 . ?
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O4 Eu01 2.684(6) . ?
O5 Eu01 2.348(7) . ?
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O4 C5 C6 119.0(9) . . ?
O3 C5 C6 120.0(8) . . ?
O4 C5 Eu01 66.3(5) . . ?
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H15B C15 H15C 109.5 . . ?
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N4 C14 H14B 109.5 . . ?
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H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
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N5 C16 H16 122.2 . . ?
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C9 O6 Eu01 141.0(6) 2_755 . ?
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 '-x, -y, -z'

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Source'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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DU . .
N6 N 0.5274(19) 0.6528(17) 0.5147(17) 0.150(4) Uani 1 1 d
DU . .
C1 C 0.1948(15) 0.2399(13) 0.6502(13) 0.063(3) Uani 1 1 d . . .
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C4 C -0.0400(18) 0.0579(17) 0.5816(16) 0.094(6) Uani 1 1 d
D . .
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C6 C 0.8566(13) 0.4988(12) 0.9605(11) 0.053(3) Uani 1 1 d . . .
C7 C 0.8985(15) 0.4242(14) 0.8930(13) 0.070(4) Uani 1 1 d D . .
C8 C 0.9574(14) 0.5751(14) 1.0657(12) 0.069(4) Uani 1 1 d . . .
H8 H 0.9309 0.6275 1.1110 0.083 Uiso 1 1 calc R . .
C9 C 0.5253(16) 0.7501(11) 0.9998(12) 0.062(4) Uani 1 1 d . . .
C10 C 0.5131(17) 0.8793(11) 1.0041(12) 0.065(4) Uani 1 1
d . . .
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C11 C 0.4908(18) 0.9314(16) 0.8957(15) 0.085(5) Uani 1 1 d
U . .
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C12 C 0.5278(17) 0.9482(15) 1.1080(14) 0.076(4) Uani 1 1 d
DU . .
C13 C 0.171(4) 0.635(3) 0.791(3) 0.199(6) Uani 1 1 d DU . .
C14 C 0.053(4) 0.772(3) 0.767(3) 0.201(6) Uani 1 1 d DU . .
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H14B H -0.0108 0.7640 0.8111 0.302 Uiso 1 1 calc R . .
H14C H 0.0291 0.8212 0.7045 0.302 Uiso 1 1 calc R . .
C15 C -0.086(3) 0.579(3) 0.603(3) 0.202(6) Uani 1 1 d DU . .
H15A H -0.0734 0.5028 0.5738 0.302 Uiso 1 1 calc R . .
H15B H -0.0948 0.6308 0.5407 0.302 Uiso 1 1 calc R . .
H15C H -0.1724 0.5570 0.6211 0.302 Uiso 1 1 calc R . .
C16 C 0.380(2) 0.6684(17) 0.5938(17) 0.146(4) Uani 1 1 d DU . .
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C17 C 0.437(2) 0.7185(18) 0.5129(17) 0.149(4) Uani 1 1 d DU . .
C18 C 0.5210(19) 0.5698(18) 0.5931(16) 0.146(4) Uani 1 1 d
DU . .
H18 H 0.5745 0.5151 0.6084 0.175 Uiso 1 1 calc R . .
C19 C 0.425(3) 0.820(2) 0.437(2) 0.152(4) Uani 1 1 d DU . .
H19A H 0.4803 0.8212 0.3859 0.228 Uiso 1 1 calc R . .
H19B H 0.4621 0.9010 0.4894 0.228 Uiso 1 1 calc R . .
H19C H 0.3258 0.8042 0.3867 0.228 Uiso 1 1 calc R . .
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O2 O 0.3061(11) 0.2941(8) 0.6381(8) 0.069(3) Uani 1 1 d . . .
O3 O 0.6261(9) 0.4672(9) 0.8120(8) 0.065(2) Uani 1 1 d . . .
O4 O 0.3421(9) 0.4755(8) 0.9957(8) 0.058(2) Uani 1 1 d . . .
O5 O 0.4916(12) 0.6844(8) 0.8984(9) 0.075(3) Uani 1 1 d . . .
O6 O 0.4317(11) 0.2829(7) 0.8991(8) 0.066(2) Uani 1 1 d . . .
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DU . .

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N2 0.141(13) 0.142(13) 0.142(13) 0.024(3) 0.052(5) 0.047(5)
N3 0.141(13) 0.141(13) 0.141(13) 0.024(3) 0.052(5) 0.047(5)
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C2 0.064(9) 0.060(8) 0.047(7) -0.005(6) 0.002(7) 0.011(7)
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C5 0.048(8) 0.052(7) 0.069(9) 0.016(6) 0.017(7) 0.020(6)
C6 0.042(7) 0.068(8) 0.054(7) 0.005(6) 0.020(6) 0.024(6)
C7 0.043(8) 0.095(10) 0.066(9) -0.017(7) 0.019(7) 0.022(7)
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C9 0.086(11) 0.037(7) 0.056(8) 0.017(6) 0.011(7) 0.026(7)
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O1 0.051(6) 0.070(7) 0.121(9) -0.022(6) 0.021(6) 0.014(5)
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O7 0.150(11) 0.142(11) 0.103(10) 0.048(7) 0.034(9) 0.019(8)

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 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu01 C1 2.861(14) . ?
Eu01 C5 2.958(13) . ?
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N2 C7 1.447(5) . ?
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N5 C16 1.350(2) . ?
N6 C17 1.353(5) . ?
N6 C18 1.354(5) . ?
C1 O2 1.201(15) . ?
C1 O1 1.288(17) . ?
C1 C2 1.484(18) . ?
C2 C4 1.37(2) . ?
C2 C3 1.38(2) . ?
C3 C4 1.40(2) 2_556 ?
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C4 C3 1.40(2) 2_556 ?
C5 O3 1.230(15) . ?
C5 O4 1.291(15) 2_667 ?
C5 C6 1.491(17) . ?
C6 C8 1.362(17) . ?
C6 C7 1.376(17) . ?
C7 C8 1.411(18) 2_767 ?
C8 C7 1.411(18) 2_767 ?
C8 H8 0.9300 . ?
C9 O6 1.245(14) 2_667 ?
C9 O5 1.251(15) . ?
C9 C10 1.491(17) . ?
C10 C12 1.349(19) . ?
C10 C11 1.415(19) . ?
C11 C12 1.42(2) 2_677 ?
C11 H11 0.9300 . ?
C12 C11 1.42(2) 2_677 ?
C13 O7 1.250(5) . ?
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H15A C15 H15B 109.5 . . ?
N4 C15 H15C 109.5 . . ?
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H15B C15 H15C 109.5 . . ?
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N6 C18 H18 124.6 . . ?
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H19A C19 H19B 109.5 . . ?
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H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
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C5 O4 Eu01 162.8(8) 2_667 . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.3099(6) 0.2792(5) 0.6507(5) 0.0435(14) Uani 1 1 d . . .
O3 O 0.6202(6) 0.4346(7) 0.8159(5) 0.0550(18) Uani 1 1 d . . .
O4 O 0.3493(5) 0.4830(5) 1.0016(5) 0.0403(14) Uani 1 1 d . . .
O5 O 0.4365(7) 0.2788(5) 0.9037(5) 0.0452(15) Uani 1 1 d . . .
O6 O 0.4798(9) 0.6751(6) 0.8988(6) 0.066(2) Uani 1 1 d . . .
O7 O 0.1925(15) 0.5293(15) 0.7379(12) 0.146(4) Uani 1 1 d
DU . .
C1 C 0.1953(9) 0.2307(8) 0.6648(8) 0.043(2) Uani 1 1 d . . .
C2 C 0.0959(9) 0.1100(8) 0.5800(8) 0.048(2) Uani 1 1 d . . .
C3 C 0.1269(12) 0.0516(12) 0.4916(11) 0.087(5) Uani 1 1 d . . .
H3 H 0.2129 0.0862 0.4846 0.105 Uiso 1 1 calc R . .
C4 C -0.0335(12) 0.0587(12) 0.5889(12) 0.088(5) Uani 1 1 d
D . .
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C7 C 0.9060(9) 0.4207(12) 0.8905(9) 0.065(3) Uani 1 1 d . . .
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C10 C 0.4900(14) 0.1210(8) 0.9974(8) 0.062(3) Uani 1 1 d . . .
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H11 H 0.5466 0.1385 1.1732 0.111 Uiso 1 1 calc R . .
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C14 C 0.541(2) 0.664(2) 0.5783(19) 0.204(5) Uani 1 1 d DU . .
C15 C 0.152(3) 0.625(2) 0.746(2) 0.204(6) Uani 1 1 d DU . .
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H16B H 0.1394 0.7294 0.5918 0.348 Uiso 1 1 calc R . .
H16C H 0.1099 0.8058 0.6933 0.348 Uiso 1 1 calc R . .
C17 C -0.129(2) 0.561(3) 0.633(3) 0.220(7) Uani 1 1 d DU . .
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H17C H -0.1445 0.4722 0.6195 0.330 Uiso 1 1 calc R . .
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N3 N 0.442(3) 0.069(2) 0.7806(13) 0.087(6) Uani 0.50 1 d
PDU . .
N2 N 0.825(2) 0.341(3) 0.789(2) 0.133(13) Uani 0.50 1 d P . .
N4 N 0.4295(14) 0.5408(11) 0.6649(11) 0.109(3) Uani 1 1 d
DU . .
N5 N 0.5026(18) 0.6583(14) 0.6723(18) 0.171(4) Uani 1 1 d
DU . .
N6 N 0.500(2) 0.5550(19) 0.497(2) 0.193(5) Uani 1 1 d DU . .
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C2 0.031(4) 0.042(5) 0.046(5) -0.019(4) 0.000(4) 0.005(4)
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C6 0.025(4) 0.057(5) 0.041(5) -0.007(4) 0.009(4) 0.005(4)
C7 0.023(4) 0.096(8) 0.050(6) -0.027(6) 0.006(4) 0.010(5)
C8 0.036(5) 0.074(7) 0.060(6) -0.031(6) 0.020(5) 0.011(5)
C9 0.084(7) 0.025(4) 0.033(5) 0.007(4) 0.012(5) 0.016(4)
C10 0.115(9) 0.021(4) 0.032(5) -0.002(4) 0.011(5) 0.016(5)
C11 0.194(16) 0.028(5) 0.034(5) 0.003(4) 0.019(8) 0.032(7)
C12 0.161(13) 0.038(6) 0.034(5) 0.012(4) 0.016(7) 0.035(7)
C13 0.178(7) 0.182(5) 0.150(6) 0.017(4) 0.085(6) 0.050(4)
C14 0.208(7) 0.201(5) 0.206(7) 0.052(4) 0.094(6) 0.040(4)
C15 0.205(7) 0.202(7) 0.206(7) 0.048(3) 0.075(3) 0.063(3)
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C16 0.236(10) 0.227(9) 0.232(10) 0.077(7) 0.081(5) 0.065(5)
C17 0.207(7) 0.228(9) 0.219(10) 0.051(6) 0.076(6) 0.063(5)
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N3 0.100(9) 0.079(8) 0.082(8) 0.018(6) 0.030(6) 0.035(6)
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N8 0.204(7) 0.196(8) 0.220(9) 0.052(5) 0.077(4) 0.073(5)

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 All esds (except the esd in the dihedral angle between two
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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu01 O7 2.408(17) . ?
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Eu01 O1 2.477(6) . ?
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C1 C2 1.502(11) . ?
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N8 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
N8 C17 H17C 109.5 . . ?
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H17B C17 H17C 109.5 . . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C13 C 0.4359(16) 0.479(2) 0.819(3) 0.140(6) Uani 0.50 1 d
PDU . .
C13A C 0.329(5) 0.373(4) 0.726(4) 0.143(6) Uani 0.50 1 d PU . .
C14 C 0.633(2) 0.420(2) 0.873(2) 0.170(5) Uani 1 1 d DU . .
H14A H 0.6734 0.3561 0.8650 0.254 Uiso 1 1 calc R . .
H14B H 0.6413 0.4370 0.9563 0.254 Uiso 1 1 calc R . .
H14C H 0.6853 0.4970 0.8494 0.254 Uiso 1 1 calc R . .
C15 C 0.460(3) 0.265(2) 0.714(2) 0.171(6) Uani 1 1 d DU . .
H15A H 0.5253 0.2233 0.7535 0.257 Uiso 1 1 calc R . .
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H15B H 0.4822 0.2947 0.6439 0.257 Uiso 1 1 calc R . .
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DU . .
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C17 C 0.0474(15) 0.2905(15) 1.0035(13) 0.159(5) Uani 1 1 d
DU . .
C18 C 0.1013(13) 0.3225(9) 0.9095(12) 0.139(4) Uani 1 1 d
DU . .
C19 C 0.1869(16) 0.2559(16) 0.8917(18) 0.159(5) Uani 1 1 d
DU . .
H19 H 0.2273 0.2722 0.8310 0.191 Uiso 1 1 calc R . .
C20 C 0.212(2) 0.1653(18) 0.9640(18) 0.175(6) Uani 1 1 d DU . .
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DU . .
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O7 O 0.3059(9) 0.4613(8) 0.7592(9) 0.089(3) Uani 1 1 d D . .
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C15 0.175(7) 0.169(7) 0.174(7) 0.018(4) 0.061(5) 0.069(5)
C16 0.149(7) 0.151(7) 0.148(7) 0.023(4) 0.058(5) 0.060(5)
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 and torsion angles; correlations between esds in cell
parameters are only
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approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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_exptl_crystal_density_diffrn     1.598
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              573
_exptl_absorpt_coefficient_mu     2.626
_exptl_absorpt_correction_type    'multi-scan'
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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_diffrn_ambient_temperature       100(2)
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_diffrn_radiation_source          'SuperNova (Mo) X-ray
Source'
_diffrn_radiation_monochromator   'mirror'
_diffrn_measurement_device_type   'SuperNova, Dual, Cu at zero,
Atlas'
_diffrn_measurement_method        '\w scans'
_diffrn_detector_area_resol_mean  10.4223
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
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_diffrn_reflns_number             8005
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_diffrn_reflns_av_sigmaI/netI     0.0562
_diffrn_reflns_limit_h_min        -12
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_diffrn_reflns_limit_k_max        13
_diffrn_reflns_limit_l_min        -13
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_diffrn_reflns_theta_min          3.23
_diffrn_reflns_theta_max          25.00
_reflns_number_total              4280
_reflns_number_gt                 3699
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        ?
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_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick,
1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick,
1997)'
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_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1111P)^2^+1.1972P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4280
_refine_ls_number_parameters      307
_refine_ls_number_restraints      118
_refine_ls_R_factor_all           0.0658
_refine_ls_R_factor_gt            0.0581
_refine_ls_wR_factor_ref          0.1713
_refine_ls_wR_factor_gt           0.1622
_refine_ls_goodness_of_fit_ref    1.091
_refine_ls_restrained_S_all       1.113
_refine_ls_shift/su_max           0.001
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d . . .
O1 O 0.1912(7) 0.7072(6) 0.8616(6) 0.0580(17) Uani 1 1 d . . .
O2 O 0.3407(7) 0.7062(7) 0.7694(7) 0.068(2) Uani 1 1 d . . .
O3 O 0.1551(6) 0.5189(6) 0.5028(6) 0.0532(16) Uani 1 1 d . . .
O4 O 0.1244(7) 0.4596(7) 0.3100(6) 0.0577(17) Uani 1 1 d . . .
O5 O 0.0079(9) 0.3155(6) 0.6021(6) 0.066(2) Uani 1 1 d . . .
O6 O 0.0738(8) 0.7170(6) 0.6021(6) 0.0614(17) Uani 1 1 d . . .
O7 O 0.021(3) 0.178(3) 1.149(2) 0.262(7) Uani 1 1 d DU . .
H7 H 0.0746 0.2428 1.1974 0.394 Uiso 1 1 calc R . .
O8 O 0.3025(14) 0.4503(14) 0.7631(12) 0.133(4) Uani 1 1 d
DU . .
C1 C 0.3100(10) 0.7576(9) 0.8494(9) 0.053(2) Uani 1 1 d . . .
C2 C 0.4098(10) 0.8838(9) 0.9271(9) 0.057(2) Uani 1 1 d . . .
C3 C 0.3702(12) 0.9434(12) 1.0068(12) 0.083(4) Uani 1 1 d . . .
H3 H 0.2812 0.9050 1.0117 0.099 Uiso 1 1 calc R . .
C4 C 0.5414(13) 0.9387(12) 0.9174(13) 0.087(4) Uani 1 1 d . . .
C5 C 0.2031(9) 0.4905(9) 0.4201(9) 0.047(2) Uani 1 1 d . . .
C6 C 0.3554(9) 0.4959(9) 0.4605(8) 0.050(2) Uani 1 1 d . . .
C7 C 0.3981(10) 0.4225(12) 0.3902(10) 0.068(3) Uani 1 1 d . . .
C8 C 0.4548(10) 0.5697(12) 0.5672(10) 0.068(3) Uani 1 1 d . . .
H8 H 0.4253 0.6175 0.6146 0.081 Uiso 1 1 calc R . .
C9 C -0.0286(12) 0.2492(8) 0.5003(9) 0.054(2) Uani 1 1 d . . .
C10 C -0.0150(13) 0.1213(9) 0.4966(10) 0.062(3) Uani 1 1
d . . .
C11 C 0.0095(17) 0.0691(11) 0.6035(10) 0.086(4) Uani 1 1
d . . .
H11 H 0.0151 0.1157 0.6744 0.104 Uiso 1 1 calc R . .
C12 C -0.0257(18) 0.0493(10) 0.3909(10) 0.085(4) Uani 1 1
d . . .
C13 C -0.027(2) 0.421(3) 0.906(2) 0.170(4) Uani 1 1 d DU . .
H13 H -0.0941 0.4631 0.8812 0.204 Uiso 1 1 calc R . .
C14 C 0.071(4) 0.286(3) 0.988(3) 0.214(5) Uani 1 1 d DU . .
C15 C 0.132(3) 0.337(2) 0.907(3) 0.179(5) Uani 1 1 d DU . .
H15 H 0.2028 0.3145 0.8881 0.215 Uiso 1 1 calc R . .
C16 C 0.063(4) 0.168(3) 1.044(3) 0.224(6) Uani 1 1 d DU . .
H16A H -0.0064 0.0953 0.9825 0.269 Uiso 1 1 calc R . .
H16B H 0.1564 0.1550 1.0701 0.269 Uiso 1 1 calc R . .
C17 C 0.335(3) 0.362(2) 0.722(2) 0.182(6) Uani 1 1 d DU . .
C18 C 0.456(3) 0.233(2) 0.711(3) 0.195(6) Uani 1 1 d DU . .
H18A H 0.5400 0.2072 0.7440 0.292 Uiso 1 1 calc R . .
H18B H 0.4492 0.2559 0.6317 0.292 Uiso 1 1 calc R . .
H18C H 0.3717 0.1644 0.7013 0.292 Uiso 1 1 calc R . .
C19 C 0.624(2) 0.397(3) 0.837(3) 0.198(5) Uani 1 1 d DU . .
H19A H 0.6689 0.3368 0.8726 0.296 Uiso 1 1 calc R . .
H19B H 0.6557 0.4711 0.8973 0.296 Uiso 1 1 calc R . .
H19C H 0.6513 0.4192 0.7684 0.296 Uiso 1 1 calc R . .
N1 N 0.585(4) 0.876(4) 0.849(4) 0.164(13) Uani 0.50 1 d PU . .
N2 N 0.304(2) 0.341(4) 0.288(2) 0.158(17) Uani 0.50 1 d P . .
N3 N -0.034(3) 0.096(3) 0.277(3) 0.109(8) Uani 0.50 1 d PU . .
N4 N 0.0745(14) 0.4252(14) 0.8579(10) 0.116(3) Uani 1 1 d
DU . .
N5 N -0.021(3) 0.347(3) 0.994(2) 0.205(5) Uani 1 1 d DU . .
N6 N 0.469(2) 0.341(2) 0.794(2) 0.188(5) Uani 1 1 d DU . .
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0.01100(19)
O1 0.056(4) 0.049(4) 0.048(4) -0.016(3) 0.011(3) 0.000(3)
O2 0.036(3) 0.063(4) 0.079(5) -0.044(4) 0.010(3) 0.002(3)
O3 0.036(3) 0.058(4) 0.057(4) -0.015(3) 0.013(3) 0.014(3)
O4 0.039(3) 0.074(5) 0.046(4) -0.002(3) 0.002(3) 0.016(3)
O5 0.105(6) 0.027(3) 0.052(4) -0.005(3) 0.017(4) 0.016(4)
O6 0.075(5) 0.034(3) 0.055(4) -0.005(3) 0.000(4) 0.020(3)
O7 0.271(9) 0.272(9) 0.249(7) 0.066(5) 0.116(6) 0.070(5)
O8 0.127(5) 0.132(5) 0.125(6) 0.036(4) 0.034(4) 0.032(4)
C1 0.035(5) 0.053(6) 0.049(5) -0.015(4) -0.001(4) 0.007(4)
C2 0.040(5) 0.053(6) 0.054(6) -0.022(4) 0.003(4) 0.004(4)
C3 0.047(6) 0.074(8) 0.093(9) -0.042(7) 0.023(6) -0.015(5)
C4 0.064(7) 0.070(8) 0.099(9) -0.044(7) 0.033(7) -0.009(6)
C5 0.035(4) 0.046(5) 0.058(6) 0.000(4) 0.012(4) 0.018(4)
C6 0.034(4) 0.064(6) 0.040(5) -0.007(4) 0.009(4) 0.011(4)
C7 0.031(4) 0.095(8) 0.060(6) -0.031(6) 0.003(4) 0.022(5)
C8 0.036(5) 0.095(9) 0.059(6) -0.026(6) 0.014(5) 0.014(5)
C9 0.071(6) 0.028(4) 0.047(5) -0.008(4) 0.012(5) 0.005(4)
C10 0.090(8) 0.030(5) 0.054(6) -0.002(4) 0.015(6) 0.020(5)
C11 0.152(13) 0.047(6) 0.048(6) -0.003(5) 0.016(7) 0.044(7)
C12 0.156(13) 0.035(6) 0.051(6) 0.003(5) 0.020(7) 0.034(7)
C13 0.165(6) 0.188(7) 0.177(7) 0.017(4) 0.086(4) 0.060(5)
C14 0.214(7) 0.211(7) 0.216(7) 0.046(4) 0.072(4) 0.075(4)
C15 0.180(6) 0.169(7) 0.189(7) 0.026(4) 0.051(5) 0.082(4)
C16 0.228(8) 0.217(6) 0.223(7) 0.054(5) 0.080(5) 0.071(5)
C17 0.188(6) 0.180(7) 0.184(8) 0.029(4) 0.062(4) 0.077(5)
C18 0.197(7) 0.191(7) 0.205(8) 0.021(4) 0.070(5) 0.083(4)
C19 0.186(5) 0.199(7) 0.201(7) 0.039(5) 0.059(4) 0.069(5)
N1 0.162(14) 0.164(14) 0.164(14) 0.025(6) 0.065(7) 0.048(6)
N2 0.049(12) 0.28(4) 0.099(18) -0.11(2) -0.014(12) 0.063(18)
N3 0.111(8) 0.109(8) 0.108(8) 0.017(4) 0.041(5) 0.038(4)
N4 0.109(8) 0.150(9) 0.059(6) -0.059(4) -0.008(5) 0.060(7)
N5 0.207(7) 0.209(7) 0.203(7) 0.042(4) 0.086(5) 0.062(4)
N6 0.184(5) 0.188(7) 0.206(7) 0.028(4) 0.072(4) 0.085(4)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
```

```
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
;

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Eu01 O5 2.368(6) . ?
Eu01 O6 2.372(7) . ?
Eu01 O8 2.408(15) . ?
Eu01 O2 2.464(6) . ?
Eu01 O4 2.465(6) 2_566 ?
Eu01 O1 2.482(6) . ?
Eu01 N4 2.518(16) . ?
Eu01 O3 2.731(6) 2_566 ?
Eu01 C1 2.845(9) . ?
Eu01 C5 2.967(8) 2_566 ?
Eu01 Eu01 4.0257(10) 2_566 ?
O1 C1 1.269(11) . ?
O2 C1 1.250(11) . ?
O3 C5 1.296(10) . ?
O3 Eu01 2.731(6) 2_566 ?
O4 C5 1.234(11) . ?
O4 Eu01 2.465(6) 2_566 ?
O5 C9 1.242(11) . ?
O6 C9 1.257(12) 2_566 ?
O7 C16 1.453(5) . ?
O7 H7 0.8200 . ?
O8 C17 1.248(5) . ?
C1 C2 1.508(13) . ?
C2 C3 1.355(14) . ?
C2 C4 1.383(15) . ?
C3 C4 1.411(15) 2_677 ?
C3 H3 0.9300 . ?
C4 N1 1.31(4) . ?
C4 C3 1.411(15) 2_677 ?
C5 C6 1.477(12) . ?
C5 Eu01 2.967(8) 2_566 ?
C6 C8 1.351(13) . ?
C6 C7 1.391(13) . ?
C7 N2 1.34(2) . ?
C7 C8 1.416(13) 2_666 ?
C8 C7 1.416(13) 2_666 ?
C8 H8 0.9300 . ?
C9 O6 1.257(12) 2_566 ?
C9 C10 1.478(13) . ?
C10 C11 1.391(15) . ?
C10 C12 1.390(14) . ?
C11 C12 1.386(15) 2_556 ?
C11 H11 0.9300 . ?
```

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C12 C11 1.386(15) 2_556 ?
C12 N3 1.45(3) . ?
C13 N4 1.353(5) . ?
C13 N5 1.354(5) . ?
C13 H13 0.9300 . ?
C14 N5 1.353(5) . ?
C14 C15 1.392(5) . ?
C14 C16 1.501(5) . ?
C15 N4 1.352(5) . ?
C15 H15 0.9300 . ?
C16 H16A 0.9700 . ?
C16 H16B 0.9700 . ?
C17 N6 1.452(5) . ?
C18 N6 1.454(5) . ?
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C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
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C19 H19B 0.9600 . ?
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O5 Eu01 O8 74.4(4) . . ?
O6 Eu01 O8 137.3(4) . . ?
O3 Eu01 O2 85.5(2) . . ?
O5 Eu01 O2 141.0(3) . . ?
O6 Eu01 O2 72.0(3) . . ?
O8 Eu01 O2 69.4(4) . . ?
O3 Eu01 O4 124.4(2) . 2_566 ?
O5 Eu01 O4 91.3(3) . 2_566 ?
O6 Eu01 O4 74.9(3) . 2_566 ?
O8 Eu01 O4 145.3(3) . 2_566 ?
O2 Eu01 O4 127.1(2) . 2_566 ?
O3 Eu01 O1 133.5(2) . . ?
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O6 Eu01 O1 73.0(2) . . ?
O8 Eu01 O1 96.8(4) . . ?
O2 Eu01 O1 52.4(2) . . ?
O4 Eu01 O1 79.0(2) 2_566 . ?
O3 Eu01 N4 145.5(3) . . ?
O5 Eu01 N4 73.9(3) . . ?
O6 Eu01 N4 138.2(3) . . ?
O8 Eu01 N4 72.3(4) . . ?
O2 Eu01 N4 107.4(3) . . ?
```

```
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O5 Eu01 O3 69.2(3) . 2_566 ?
O6 Eu01 O3 68.0(2) . 2_566 ?
O8 Eu01 O3 141.2(4) . 2_566 ?
O2 Eu01 O3 138.7(3) . 2_566 ?
O4 Eu01 O3 49.91(19) 2_566 2_566 ?
O1 Eu01 O3 121.3(2) . 2_566 ?
N4 Eu01 O3 108.9(3) . 2_566 ?
O3 Eu01 C1 109.3(3) . . ?
O5 Eu01 C1 156.2(3) . . ?
O6 Eu01 C1 69.5(3) . . ?
O8 Eu01 C1 83.1(4) . . ?
O2 Eu01 C1 26.0(2) . . ?
O4 Eu01 C1 103.2(2) 2_566 . ?
O1 Eu01 C1 26.5(2) . . ?
N4 Eu01 C1 92.0(3) . . ?
O3 Eu01 C1 134.4(2) 2_566 . ?
O3 Eu01 C5 100.7(2) . 2_566 ?
O5 Eu01 C5 80.2(3) . 2_566 ?
O6 Eu01 C5 69.2(3) . 2_566 ?
O8 Eu01 C5 152.6(4) . 2_566 ?
O2 Eu01 C5 137.7(2) . 2_566 ?
O4 Eu01 C5 24.1(2) 2_566 2_566 ?
O1 Eu01 C5 99.5(2) . 2_566 ?
N4 Eu01 C5 90.9(3) . 2_566 ?
O3 Eu01 C5 25.9(2) 2_566 2_566 ?
C1 Eu01 C5 119.9(3) . 2_566 ?
O3 Eu01 Eu01 41.03(15) . 2_566 ?
O5 Eu01 Eu01 67.69(18) . 2_566 ?
O6 Eu01 Eu01 66.64(16) . 2_566 ?
O8 Eu01 Eu01 117.5(3) . 2_566 ?
O2 Eu01 Eu01 117.7(2) . 2_566 ?
O4 Eu01 Eu01 83.82(15) 2_566 2_566 ?
O1 Eu01 Eu01 138.98(18) . 2_566 ?
N4 Eu01 Eu01 134.5(3) . 2_566 ?
O3 Eu01 Eu01 34.37(12) 2_566 2_566 ?
C1 Eu01 Eu01 131.9(2) . 2_566 ?
C5 Eu01 Eu01 59.88(18) 2_566 2_566 ?
C1 O1 Eu01 92.9(5) . . ?
C1 O2 Eu01 94.3(5) . . ?
C5 O3 Eu01 163.2(6) . . ?
C5 O3 Eu01 87.3(5) . 2_566 ?
Eu01 O3 Eu01 104.6(2) . 2_566 ?
C5 O4 Eu01 101.4(5) . 2_566 ?
C9 O5 Eu01 135.8(6) . . ?
C9 O6 Eu01 139.7(6) 2_566 . ?
C16 O7 H7 109.5 . . ?
C17 O8 Eu01 134.1(14) . . ?
O2 C1 O1 120.3(8) . . ?
O2 C1 C2 120.1(8) . . ?
O1 C1 C2 119.5(8) . . ?
O2 C1 Eu01 59.7(5) . . ?
O1 C1 Eu01 60.6(4) . . ?
C2 C1 Eu01 173.7(8) . . ?
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N1 C4 C2 120(2) . . ?
N1 C4 C3 123(2) . 2_677 ?
C2 C4 C3 117.3(10) . 2_677 ?
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O4 C5 C6 120.2(8) . . ?
O3 C5 C6 118.5(8) . . ?
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O3 C5 Eu01 66.8(4) . 2_566 ?
C6 C5 Eu01 174.5(6) . 2_566 ?
C8 C6 C7 118.9(8) . . ?
C8 C6 C5 120.8(8) . . ?
C7 C6 C5 120.2(8) . . ?
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C6 C8 C7 122.8(9) . 2_666 ?
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O5 C9 C10 118.8(9) . . ?
O6 C9 C10 116.0(8) 2_566 . ?
C11 C10 C12 117.7(9) . . ?
C11 C10 C9 119.0(9) . . ?
C12 C10 C9 123.3(10) . . ?
C10 C11 C12 123.0(10) . 2_556 ?
C10 C11 H11 118.5 . . ?
C12 C11 H11 118.5 2_556 . ?
C11 C12 C10 119.3(10) 2_556 . ?
C11 C12 N3 116.2(14) 2_556 . ?
C10 C12 N3 123.9(14) . . ?
N4 C13 N5 113(2) . . ?
N4 C13 H13 123.6 . . ?
N5 C13 H13 123.6 . . ?
N5 C14 C15 107(2) . . ?
N5 C14 C16 117(3) . . ?
C15 C14 C16 134(2) . . ?
N4 C15 C14 111(2) . . ?
N4 C15 H15 124.7 . . ?
C14 C15 H15 124.7 . . ?
O7 C16 C14 110(2) . . ?
O7 C16 H16A 109.6 . . ?
C14 C16 H16A 109.6 . . ?
O7 C16 H16B 109.6 . . ?
C14 C16 H16B 109.6 . . ?
H16A C16 H16B 108.1 . . ?
O8 C17 N6 120(2) . . ?
N6 C18 H18A 109.5 . . ?
N6 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N6 C18 H18C 109.5 . . ?
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H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
N6 C19 H19A 109.5 . . ?
N6 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
N6 C19 H19C 109.5 . . ?
H19A C19 H19C 109.5 . . ?
H19B C19 H19C 109.5 . . ?
C15 N4 C13 103.4(19) . . ?
C15 N4 Eu01 127.9(14) . . ?
C13 N4 Eu01 127.4(14) . . ?
C14 N5 C13 106(2) . . ?
C17 N6 C19 142(3) . . ?
C17 N6 C18 98.6(18) . . ?
C19 N6 C18 96(2) . . ?

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   2  0.257  0.134  0.859        9         1 ' '
   3  0.439  0.366  0.043       15         2 ' '
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 '-x, -y, -z'

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Diffraction)'

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Source'
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Atlas'
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 MERCURY (Bruno et al. 2002)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0794P)^2^+0.9385P] where
P=(Fo^2^+2Fc^2^)/3'
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C2 C 0.4104(9) 0.6192(8) 0.5734(8) 0.048(2) Uani 1 1 d . . .
C3 C 0.3551(12) 0.5544(10) 0.5179(11) 0.075(3) Uani 1 1 d . . .
H3 H 0.2552 0.5904 0.5287 0.090 Uiso 1 1 calc R . .
C4 C 0.5585(14) 0.5638(11) 0.5547(12) 0.085(4) Uani 1 1 d . . .
C5 C -0.0393(10) 1.2549(8) 1.0020(8) 0.045(2) Uani 1 1 d . . .
C6 C -0.0204(10) 1.3823(7) 1.0013(7) 0.044(2) Uani 1 1 d . . .
C7 C -0.0259(12) 1.4422(8) 1.1072(8) 0.051(2) Uani 1 1 d . . .
C8 C 0.0023(12) 1.4421(8) 0.8955(8) 0.055(2) Uani 1 1 d . . .
C9 C -0.2038(8) 0.9976(8) 0.9205(7) 0.0367(18) Uani 1 1 d . . .
C10 C -0.3556(8) 0.9989(8) 0.9616(7) 0.0374(18) Uani 1 1
d . . .
C11 C -0.4658(9) 1.0785(9) 1.0631(8) 0.047(2) Uani 1 1 d . . .
H11 H -0.4426 1.1331 1.1053 0.057 Uiso 1 1 calc R . .
C12 C -0.3894(9) 0.9183(10) 0.8937(8) 0.048(2) Uani 1 1 d . . .
C13 C -0.0305(13) 1.1070(13) 0.5955(11) 0.095(4) Uani 1 1 d
DU . .
H13 H -0.0985 1.0663 0.6229 0.114 Uiso 1 1 calc R . .
C14 C -0.0261(14) 1.1809(11) 0.5039(10) 0.085(3) Uani 1 1 d
DU . .
H14 H -0.0862 1.1981 0.4580 0.101 Uiso 1 1 calc R . .
C15 C 0.1344(17) 1.1793(14) 0.5822(13) 0.111(4) Uani 1 1 d
DU . .
H15 H 0.2045 1.2020 0.5997 0.133 Uiso 1 1 calc R . .
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C16 C 0.3304(13) 1.1543(10) 0.7927(11) 0.099(4) Uani 1 1 d
DU . .
H16 H 0.2600 1.2046 0.8654 0.119 Uiso 1 1 calc R . .
C17 C 0.4516(12) 1.0118(15) 0.6513(14) 0.139(5) Uani 1 1 d
DU . .
H17 H 0.4830 0.9357 0.6005 0.167 Uiso 1 1 calc R . .
C18 C 0.5428(17) 1.0776(16) 0.6365(15) 0.152(6) Uani 1 1 d
DU . .
H18 H 0.6370 1.0617 0.5782 0.182 Uiso 1 1 calc R . .
N1 N 0.628(3) 0.640(3) 0.598(3) 0.132(10) Uani 0.50 1 d PU . .
N2 N -0.034(3) 1.393(2) 1.216(2) 0.036(6) Uani 0.25 1 d PU . .
N2A N -0.005(4) 1.392(4) 0.790(3) 0.071(10) Uani 0.25 1 d
PU . .
N3 N -0.288(2) 0.827(2) 0.8008(18) 0.074(5) Uani 0.50 1 d
PU . .
N4 N 0.0727(9) 1.0977(7) 0.6435(7) 0.054(2) Uani 1 1 d D . .
N5 N 0.0840(15) 1.2247(15) 0.4927(13) 0.128(4) Uani 1 1 d
DU . .
N6 N 0.3147(10) 1.0564(7) 0.7399(7) 0.062(2) Uani 1 1 d DU . .
N7 N 0.4580(13) 1.1730(12) 0.7305(12) 0.103(3) Uani 1 1 d
DU . .
O1 O 0.1908(7) 0.8078(6) 0.6405(5) 0.0506(15) Uani 1 1 d . . .
O2 O 0.3553(6) 0.7911(6) 0.7226(6) 0.0550(17) Uani 1 1 d . . .
O3 O 0.1570(5) 0.9770(5) 0.9991(5) 0.0367(12) Uani 1 1 d . . .
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O5 O 0.0867(7) 0.7824(5) 0.8973(5) 0.0456(14) Uani 1 1 d . . .
O6 O -0.0008(7) 1.1930(5) 0.8983(5) 0.0474(15) Uani 1 1 d . . .
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d . . .

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C2 0.039(5) 0.038(5) 0.048(5) -0.011(4) -0.007(4) -0.002(4)
C3 0.045(6) 0.060(7) 0.095(8) -0.038(6) -0.022(6) 0.005(5)
C4 0.073(8) 0.052(7) 0.110(10) -0.045(6) -0.035(7) 0.002(6)
C5 0.048(5) 0.026(4) 0.048(5) -0.005(4) -0.007(4) -0.008(4)
C6 0.063(6) 0.025(4) 0.036(4) -0.004(3) -0.008(4) -0.018(4)
C7 0.082(7) 0.027(4) 0.038(5) 0.002(3) -0.010(4) -0.024(4)
C8 0.085(7) 0.036(5) 0.037(5) 0.000(4) -0.009(5) -0.029(5)
C9 0.030(4) 0.041(5) 0.039(5) -0.007(3) -0.013(3) -0.012(3)
C10 0.033(4) 0.047(5) 0.030(4) -0.004(3) -0.009(3) -0.015(4)
C11 0.034(4) 0.055(6) 0.050(5) -0.017(4) -0.013(4) -0.013(4)
C12 0.029(4) 0.074(6) 0.041(5) -0.015(4) -0.008(4) -0.025(4)
C13 0.105(6) 0.097(5) 0.084(5) 0.021(4) -0.040(4) -0.033(4)
C14 0.094(5) 0.081(5) 0.073(5) 0.014(4) -0.038(4) -0.019(4)
C15 0.111(6) 0.120(7) 0.115(6) 0.019(4) -0.051(5) -0.047(4)
C16 0.096(5) 0.095(6) 0.102(6) 0.023(4) -0.025(4) -0.042(4)
C17 0.139(5) 0.139(5) 0.140(5) 0.0180(13) -0.051(2) -0.052(2)
C18 0.138(6) 0.156(7) 0.160(8) 0.031(5) -0.038(4) -0.068(5)
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N2 0.040(7) 0.032(7) 0.035(7) 0.003(5) -0.010(5) -0.017(5)
N2A 0.074(11) 0.070(11) 0.071(11) 0.008(5) -0.027(6) -0.028(6)
N3 0.068(6) 0.079(7) 0.077(7) -0.003(5) -0.026(5) -0.031(5)
N4 0.076(5) 0.054(5) 0.041(4) 0.017(3) -0.023(4) -0.031(4)
N5 0.129(6) 0.135(6) 0.129(6) 0.042(4) -0.051(4) -0.057(4)
N6 0.107(6) 0.041(4) 0.064(5) 0.020(4) -0.048(4) -0.042(4)
N7 0.101(5) 0.108(5) 0.110(5) 0.023(4) -0.034(4) -0.056(4)
O1 0.049(4) 0.042(3) 0.043(3) -0.013(3) -0.014(3) 0.000(3)
O2 0.037(3) 0.045(4) 0.064(4) -0.031(3) -0.011(3) -0.001(3)
O3 0.026(3) 0.045(3) 0.043(3) -0.002(2) -0.013(2) -0.017(2)
O4 0.028(3) 0.063(4) 0.036(3) 0.004(3) -0.009(2) -0.020(3)
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O6 0.072(4) 0.024(3) 0.037(3) -0.005(2) -0.011(3) -0.017(3)
Eu01 0.0249(2) 0.0239(2) 0.0304(2) -0.00524(15) -0.00394(16) -
0.01084(16)

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l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C2 C3 1.354(13) . ?
C2 C4 1.374(14) . ?
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C3 H3 0.9300 . ?
C4 C3 1.391(14) 2_666 ?
C4 N1 1.48(3) . ?
C5 O5 1.244(10) 2_577 ?
C5 O6 1.268(10) . ?
C5 C6 1.500(11) . ?
C6 C8 1.393(12) . ?
C6 C7 1.394(12) . ?
C7 N2 1.37(3) . ?
C7 C8 1.393(12) 2_587 ?
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C9 O4 1.260(9) . ?
C9 O3 1.277(9) 2_577 ?
C9 C10 1.466(11) . ?
C9 Eu01 2.965(8) . ?
C10 C11 1.370(11) . ?
C10 C12 1.413(11) . ?
C11 C12 1.390(11) 2_477 ?
C11 H11 0.9300 . ?
C12 N3 1.35(2) . ?
C12 C11 1.390(11) 2_477 ?
C13 N4 1.347(5) . ?
C13 C14 1.351(5) . ?
C13 H13 0.9300 . ?
C14 N5 1.353(5) . ?
C14 H14 0.9300 . ?
C15 N4 1.352(5) . ?
C15 N5 1.353(5) . ?
C15 H15 0.9300 . ?
C16 N6 1.347(5) . ?
C16 N7 1.353(5) . ?
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C16 H16 0.9300 . ?
C17 N6 1.3503(11) . ?
C17 C18 1.3504(11) . ?
C17 H17 0.9300 . ?
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C18 H18 0.9300 . ?
N4 Eu01 2.531(7) . ?
N6 Eu01 2.473(7) . ?
O1 Eu01 2.487(6) . ?
O2 Eu01 2.496(6) . ?
O3 C9 1.277(9) 2_577 ?
O3 Eu01 2.358(5) . ?
O3 Eu01 2.729(5) 2_577 ?
O4 Eu01 2.446(5) . ?
O5 C5 1.244(10) 2_577 ?
O5 Eu01 2.378(5) . ?
O6 Eu01 2.365(5) . ?
Eu01 O3 2.729(5) 2_577 ?
Eu01 Eu01 4.0509(7) 2_577 ?

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O1 C1 C2 117.8(8) . . ?
O2 C1 Eu01 60.4(4) . . ?
O1 C1 Eu01 60.2(4) . . ?
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C2 C1 Eu01 172.9(6) . . ?
C3 C2 C4 117.2(9) . . ?
C3 C2 C1 122.0(8) . . ?
C4 C2 C1 120.8(9) . . ?
C2 C3 C4 122.7(10) . 2_666 ?
C2 C3 H3 118.6 . . ?
C4 C3 H3 118.6 2_666 . ?
C2 C4 C3 120.1(10) . 2_666 ?
C2 C4 N1 118.8(15) . . ?
C3 C4 N1 120.5(16) 2_666 . ?
O5 C5 O6 125.8(8) 2_577 . ?
O5 C5 C6 117.9(7) 2_577 . ?
O6 C5 C6 116.3(8) . . ?
C8 C6 C7 119.3(7) . . ?
C8 C6 C5 120.7(8) . . ?
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 '-x, -y, -z'

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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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PDU . .
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C2 0.067(5) 0.051(5) 0.075(5) -0.016(4) 0.028(4) -0.003(4)
C3 0.081(7) 0.083(7) 0.117(8) -0.049(6) 0.044(6) -0.030(6)
C4 0.084(7) 0.084(7) 0.111(8) -0.043(6) 0.046(6) -0.022(6)
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C6 0.042(4) 0.069(5) 0.058(4) -0.001(3) 0.019(3) 0.018(4)
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C8 0.053(6) 0.212(15) 0.075(6) -0.023(7) 0.027(5) 0.042(7)
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esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
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approximate (isotropic)
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
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P=(Fo^2^+2Fc^2^)/3'
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O3 O 0.7768(7) 0.0845(7) 0.6662(5) 0.0650(18) Uani 1 1 d . . .
O4 O 0.3523(7) -0.0055(6) 0.5046(5) 0.0565(15) Uani 1 1 d . . .
O5 O 0.5354(8) 0.2312(6) 0.5922(5) 0.0638(18) Uani 1 1 d . . .
O6 O 0.5579(8) -0.1576(6) 0.5878(5) 0.0664(19) Uani 1 1 d . . .
O7 O 0.3720(19) -0.0638(19) 0.7043(15) 0.197(5) Uani 1 1 d
DU . .
C1 C 0.5233(10) 0.2809(8) 0.8243(6) 0.049(2) Uani 1 1 d . . .
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C3 C 0.3850(11) 0.4302(11) 0.9160(8) 0.068(3) Uani 1 1 d . . .
H3 H 0.3069 0.3840 0.8601 0.082 Uiso 1 1 calc R . .
C4 C 0.6222(11) 0.4651(10) 0.9978(8) 0.068(3) Uani 1 1 d D . .
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C6 C 0.8852(10) 0.0198(9) 0.5347(7) 0.060(2) Uani 1 1 d . . .
C7 C 1.0171(10) 0.0682(12) 0.6075(8) 0.070(3) Uani 1 1 d D . .
C8 C 0.8734(10) -0.0522(11) 0.4261(8) 0.070(3) Uani 1 1 d . . .
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C16 C 0.420(2) -0.100(3) 0.781(2) 0.199(6) Uani 1 1 d DU . .
C17 C 0.529(3) -0.188(3) 0.965(2) 0.209(6) Uani 1 1 d DU . .
H17A H 0.5776 -0.1737 1.0394 0.313 Uiso 1 1 calc R . .
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N2 N 1.039(3) 0.134(3) 0.7154(19) 0.108(7) Uani 0.50 1 d
PDU . .
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PDU . .
N4 N 0.658(2) 0.000(2) 0.8196(15) 0.189(5) Uani 1 1 d DU . .
N5 N 0.718(2) -0.051(2) 0.9557(19) 0.199(4) Uani 1 1 d DU . .
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C9 0.065(4) 0.047(4) 0.057(4) 0.017(3) 0.030(3) 0.013(3)
C10 0.072(4) 0.043(4) 0.052(4) 0.015(3) 0.026(3) 0.011(3)
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C12 0.090(5) 0.056(4) 0.058(4) 0.019(3) 0.026(3) 0.011(4)
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C15 0.198(5) 0.192(6) 0.194(5) 0.070(4) 0.066(3) 0.029(3)
C16 0.201(6) 0.198(7) 0.196(7) 0.069(5) 0.067(4) 0.031(5)
C17 0.213(7) 0.210(7) 0.208(7) 0.082(4) 0.070(4) 0.025(3)
N1 0.188(16) 0.187(16) 0.188(15) 0.068(7) 0.062(6) 0.026(4)
N2 0.106(8) 0.109(8) 0.108(8) 0.037(4) 0.037(4) 0.015(4)
N3 0.092(7) 0.086(7) 0.087(6) 0.032(4) 0.028(4) 0.011(4)
N4 0.191(6) 0.183(6) 0.189(5) 0.066(4) 0.062(3) 0.028(3)
N5 0.202(5) 0.200(5) 0.198(5) 0.076(3) 0.064(3) 0.029(3)
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0.0121(2)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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O3 C5 1.241(12) . ?
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O5 C9 1.225(11) . ?
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O6 Eu01 2.371(6) . ?
O7 C16 1.249(5) . ?
O7 Eu01 2.63(2) . ?
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C1 Eu01 2.802(8) . ?
C2 C4 1.344(14) . ?
C2 C3 1.384(14) . ?
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C3 H3 0.9300 . ?
C4 N1 1.35(3) . ?
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C7 N2 1.37(2) . ?
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C10 C11 1.428(14) . ?
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C11 N3 1.42(2) . ?
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C13 C15 2.018(17) . ?
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C14 N5 1.353(5) . ?
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C15 N4 1.356(5) . ?
C15 C16 1.493(5) . ?
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C17 H17B 0.9600 . ?
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O1 C1 C2 119.4(8) . . ?
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C3 C2 C1 119.8(9) . . ?
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C4 C3 H3 120.9 2_667 . ?
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O5 Eu01 O4 69.4(2) . 2_656 ?
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O2 Eu01 O4 120.0(2) . 2_656 ?
N4 Eu01 O4 118.8(5) . 2_656 ?
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O4 Eu01 C1 138.0(2) 2_656 . ?
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O6 Eu01 C5 73.7(3) . . ?
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RESPONSE: This is due to the severe disorder of this
atom, which could not eliminated although
we have applied several restaints to limit it.
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 '-x, -y, -z'

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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


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 Refinement of F^2^ against ALL reflections.  The weighted R-
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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PDU . .
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N4 N 0.9194(16) 0.5610(11) 0.1623(13) 0.136(3) Uani 1 1 d
DU . .
N5 N 0.569(3) 0.716(3) 0.273(2) 0.207(6) Uani 0.70 1 d PDU . .
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DU . .
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DU . .
H14 H 0.7750 0.5264 -0.1223 0.227 Uiso 1 1 calc R . .
C15 C 0.957(2) 0.6670(17) -0.0216(19) 0.192(4) Uani 1 1 d
DU . .
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C16 C 1.053(2) 0.717(2) 0.0951(18) 0.190(4) Uani 1 1 d DU . .
H16 H 1.1310 0.7877 0.1125 0.228 Uiso 1 1 calc R . .
C17 C 1.0360(18) 0.6652(14) 0.1873(18) 0.187(4) Uani 1 1 d
DU . .
H17 H 1.1024 0.7004 0.2644 0.224 Uiso 1 1 calc R . .
C18 C 0.664(4) 0.638(3) 0.290(3) 0.204(6) Uani 0.70 1 d PDU A .
C19 C 0.471(4) 0.621(3) 0.167(3) 0.205(6) Uani 0.70 1 d PDU A
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H19C H 0.5178 0.6136 0.1137 0.308 Uiso 0.70 1 calc PR A 1
C20 C 0.582(4) 0.749(3) 0.167(3) 0.206(6) Uani 0.70 1 d PDU A
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O3 0.036(3) 0.086(4) 0.046(3) 0.011(3) 0.011(3) 0.019(3)
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O5 0.100(5) 0.032(3) 0.052(3) 0.008(2) 0.021(3) 0.024(3)
O6 0.144(7) 0.032(3) 0.059(4) 0.007(3) 0.036(4) 0.028(3)
O7 0.158(9) 0.181(10) 0.142(9) 0.048(6) 0.067(7) 0.026(7)
O7A 0.169(12) 0.180(8) 0.159(13) 0.056(7) 0.072(8) 0.031(7)
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C2 0.083(8) 0.113(9) 0.091(8) -0.060(7) 0.036(7) -0.026(7)
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0.069(11)
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0.064(10)
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 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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 DIAMOND (Brandenburg, 2006)
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

Farrugia, L. J. (1999). <i>J. Appl. Cryst.</i> <b>32</b>, 837-
-838.

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RED</i>. Oxford
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G\"ottingen, Germany.

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Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1049P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
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C2 C 0.5140(12) 0.3912(9) 0.4229(8) 0.089(2) Uani 1 1 d U . .
C3 C 0.3896(13) 0.4217(11) 0.4211(10) 0.117(4) Uani 1 1 d U . .
H3 H 0.3132 0.3699 0.3662 0.141 Uiso 1 1 calc R . .
C4 C 0.6230(13) 0.4725(12) 0.5009(11) 0.123(4) Uani 1 1 d
DU . .
C5 C 0.7616(10) 0.0338(8) 0.0650(9) 0.079(2) Uani 1 1 d . . .
C6 C 0.8857(9) 0.0176(8) 0.0331(8) 0.079(2) Uani 1 1 d . . .
C7 C 1.0156(10) 0.0625(10) 0.1119(8) 0.093(3) Uani 1 1 d D . .
C8 C 0.8748(11) -0.0460(9) -0.0783(8) 0.091(3) Uani 1 1 d . . .
H8 H 0.7899 -0.0785 -0.1319 0.109 Uiso 1 1 calc R . .
C9 C 0.4943(10) 0.2441(7) 0.0003(8) 0.074(2) Uani 1 1 d . . .
C10 C 0.4963(10) 0.3759(7) 0.0003(7) 0.080(2) Uani 1 1 d . . .
C11 C 0.4569(11) 0.4034(7) -0.1006(8) 0.086(3) Uani 1 1 d . . .
H11 H 0.4276 0.3379 -0.1695 0.103 Uiso 1 1 calc R . .
C12 C 0.5404(11) 0.4765(8) 0.1025(8) 0.086(3) Uani 1 1 d D . .
C13 C 0.503(2) -0.092(2) 0.3531(19) 0.162(3) Uani 0.50 1 d
PDU . .
C14 C 0.528(2) -0.143(2) 0.441(2) 0.162(3) Uani 0.50 1 d PDU
C .
H14 H 0.4609 -0.1936 0.4482 0.195 Uiso 0.50 1 calc PR . .
C15 C 0.658(3) -0.115(2) 0.5180(18) 0.162(3) Uani 0.50 1 d
PDU . .
H15 H 0.6781 -0.1481 0.5780 0.195 Uiso 0.50 1 calc PR C .
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C16 C 0.759(2) -0.040(2) 0.5084(19) 0.162(3) Uani 0.50 1 d PDU
B .
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PDU . .
N2 N 1.043(2) 0.121(2) 0.2332(9) 0.124(6) Uani 0.50 1 d PDU . .
N3 N 0.601(3) 0.463(3) 0.2139(13) 0.143(8) Uani 0.50 1 d
PDU . .
N4 N 0.600(3) -0.016(2) 0.3397(17) 0.162(3) Uani 0.50 1 d PDU
B .
O1 O 0.4222(7) 0.1975(6) 0.2720(5) 0.0881(17) Uani 1 1 d . B .
O2 O 0.6416(7) 0.2473(6) 0.3372(5) 0.0881(17) Uani 1 1 d . B .
O3 O 0.7732(7) 0.0751(6) 0.1719(6) 0.0931(18) Uani 1 1 d . . .
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O5 O 0.5375(7) 0.2253(5) 0.0952(5) 0.0805(16) Uani 1 1 d . . .
O6 O 0.4492(7) 0.1589(5) -0.0964(5) 0.0838(16) Uani 1 1 d . . .
C17 C 0.728(2) 0.008(2) 0.419(2) 0.162(3) Uani 0.50 1 d PDU B
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H17 H 0.7954 0.0588 0.4115 0.195 Uiso 0.50 1 calc PR B 1
O8 O 0.6898(14) 0.0047(12) 0.3342(10) 0.086(3) Uani 0.50 1 d
PU B 2
C18 C 0.355(4) -0.158(4) 0.254(3) 0.161(3) Uani 0.50 1 d PU C
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H18A H 0.3421 -0.1256 0.1914 0.242 Uiso 0.50 1 calc PR C 1
H18B H 0.2844 -0.1382 0.2868 0.242 Uiso 0.50 1 calc PR C 1
H18C H 0.3520 -0.2466 0.2274 0.242 Uiso 0.50 1 calc PR C 1
O7 O 0.3923(13) -0.0583(12) 0.2348(9) 0.161(3) Uani 1 1 d U B
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d . . .

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C3 0.113(5) 0.097(7) 0.113(8) -0.013(6) 0.041(6) 0.021(6)
C4 0.120(5) 0.099(7) 0.112(8) -0.019(5) 0.034(6) 0.028(6)
C5 0.081(7) 0.057(4) 0.102(7) 0.017(4) 0.042(5) 0.009(4)
C6 0.083(6) 0.059(4) 0.096(6) 0.015(4) 0.041(5) 0.008(4)
C7 0.076(6) 0.096(7) 0.089(6) -0.003(5) 0.034(5) 0.010(5)
C8 0.084(7) 0.088(6) 0.090(6) 0.009(5) 0.031(5) 0.011(5)
C9 0.091(6) 0.053(4) 0.088(6) 0.021(4) 0.044(5) 0.018(4)
C10 0.105(7) 0.056(4) 0.081(5) 0.018(4) 0.038(5) 0.014(4)
C11 0.115(8) 0.049(4) 0.081(5) 0.003(4) 0.031(5) 0.009(4)
C12 0.113(8) 0.067(5) 0.084(5) 0.028(4) 0.038(5) 0.015(5)
C13 0.162(3) 0.163(3) 0.163(3) 0.0522(19) 0.0553(19) 0.0252(19)
C14 0.163(3) 0.163(3) 0.163(3) 0.0523(19) 0.0552(19) 0.0250(19)
C15 0.163(3) 0.163(3) 0.163(3) 0.0524(19) 0.0550(19) 0.0249(19)
C16 0.163(3) 0.163(3) 0.163(3) 0.0524(19) 0.0549(19) 0.0250(19)
N1 0.128(5) 0.151(8) 0.158(7) 0.038(5) 0.047(5) 0.025(5)
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N2 0.122(8) 0.128(8) 0.121(7) 0.036(5) 0.045(5) 0.017(5)
N3 0.147(9) 0.141(9) 0.142(9) 0.047(5) 0.047(5) 0.020(5)
N4 0.162(3) 0.162(3) 0.162(3) 0.0523(19) 0.0551(19) 0.0252(19)
O1 0.086(4) 0.076(4) 0.087(4) -0.002(3) 0.037(3) 0.004(3)
O2 0.096(5) 0.074(4) 0.087(4) 0.006(3) 0.039(3) 0.019(3)
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O4 0.075(4) 0.066(3) 0.105(4) 0.023(3) 0.035(3) 0.013(3)
O5 0.113(5) 0.057(3) 0.081(4) 0.023(3) 0.044(3) 0.022(3)
O6 0.111(5) 0.061(3) 0.086(4) 0.022(3) 0.042(3) 0.019(3)
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O7 0.161(3) 0.163(4) 0.162(3) 0.052(2) 0.057(2) 0.028(2)
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0.0177(2)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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C2 C4 1.357(16) . ?
C2 C3 1.367(16) . ?
C3 C4 1.361(14) 2_666 ?
C3 H3 0.9300 . ?
C4 C3 1.361(14) 2_666 ?
C4 N1 1.447(5) . ?
C5 O4 1.230(11) 2_655 ?
C5 O3 1.289(11) . ?
C5 C6 1.488(13) . ?
C5 Eu01 2.963(9) . ?
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C6 C7 1.402(13) . ?
C7 C8 1.353(14) 2_755 ?
C7 N2 1.446(5) . ?
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C8 C7 1.353(14) 2_755 ?
C8 H8 0.9300 . ?
C9 O5 1.261(10) . ?
C9 O6 1.270(10) . ?
C9 C10 1.489(11) . ?
C10 C11 1.378(13) . ?
C10 C12 1.398(12) . ?
C11 C12 1.363(12) 2_665 ?
C11 H11 0.9300 . ?
C12 C11 1.363(12) 2_665 ?
C12 N3 1.449(5) . ?
C13 C14 1.387(5) . ?
C13 N4 1.389(5) . ?
C13 C18 1.66(4) . ?
C13 O7 1.78(2) . ?
C14 C15 1.388(5) . ?
C14 H14 0.9300 . ?
C15 C16 1.387(5) . ?
C15 H15 0.9300 . ?
C16 C17 1.384(5) . ?
C16 H16 0.9300 . ?
N4 O8 0.99(3) . ?
N4 C17 1.384(5) . ?
N4 Eu01 2.497(19) . ?
O1 Eu01 2.437(6) . ?
O2 Eu01 2.461(6) . ?
O3 Eu01 2.388(7) . ?
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O4 Eu01 2.349(7) . ?
O4 Eu01 2.756(6) 2_655 ?
O5 Eu01 2.357(6) . ?
O6 Eu01 2.362(6) 2_655 ?
C17 H17 0.9300 . ?
O8 Eu01 2.470(12) . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
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Eu01 O6 2.362(6) 2_655 ?
Eu01 O4 2.756(6) 2_655 ?

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O2 C1 Eu01 61.1(4) . . ?
C2 C1 Eu01 175.5(7) . . ?
C4 C2 C3 117.8(9) . . ?
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C3 C2 C1 119.8(10) . . ?
C4 C3 C2 120.4(11) 2_666 . ?
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C2 C3 H3 119.8 . . ?
C2 C4 C3 121.7(12) . 2_666 ?
C2 C4 N1 123.8(13) . . ?
C3 C4 N1 114.5(14) 2_666 . ?
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O4 C5 C6 121.5(9) 2_655 . ?
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O4 C5 Eu01 68.3(5) 2_655 . ?
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C8 C6 C7 117.3(9) . . ?
C8 C6 C5 119.5(9) . . ?
C7 C6 C5 123.2(8) . . ?
C8 C7 C6 120.9(8) 2_755 . ?
C8 C7 N2 115.7(13) 2_755 . ?
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C14 C15 H15 118.9 . . ?
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H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
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O4 Eu01 O5 76.0(2) . . ?
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O3 Eu01 C1 107.0(3) . . ?
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 'O'  'O'   0.0106   0.0060
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 '-x, -y, -z'

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_cell_length_b                    11.1657(8)
_cell_length_c                    11.9254(8)
_cell_angle_alpha                 90.062(6)
_cell_angle_beta                  110.667(7)
_cell_angle_gamma                 109.830(7)
_cell_volume                      1209.66(18)
_cell_formula_units_Z             1
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used   2487
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_cell_measurement_theta_max     29.2915

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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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Source'
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Atlas'
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_diffrn_reflns_number             7650
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_diffrn_reflns_limit_k_max        12
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_diffrn_reflns_theta_min          3.34
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1997)'
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 MERCURY (Bruno et al. 2002)
;

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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1120P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
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_refine_ls_number_restraints      124
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O2 O 0.6916(9) 0.6957(7) 0.3581(7) 0.069(2) Uani 1 1 d . . .
O3 O 0.6599(7) 0.5242(6) 0.0052(6) 0.0504(16) Uani 1 1 d . . .
O4 O 0.3771(8) 0.5254(8) 0.1863(6) 0.0602(19) Uani 1 1 d . . .
O5 O 0.5843(9) 0.7173(6) 0.1007(7) 0.0602(19) Uani 1 1 d . . .
O6 O 0.4977(9) 0.3075(6) 0.0981(6) 0.061(2) Uani 1 1 d . . .
C1 C 0.8149(13) 0.7561(10) 0.3502(11) 0.062(3) Uani 1 1 d . . .
C2 C 0.9129(14) 0.8816(10) 0.4251(10) 0.065(3) Uani 1 1 d . . .
C3 C 0.8548(15) 0.9457(12) 0.4811(15) 0.092(5) Uani 1 1 d . . .
H3 H 0.7556 0.9103 0.4691 0.111 Uiso 1 1 calc R . .
C4 C 1.0565(16) 0.9357(14) 0.4437(15) 0.095(5) Uani 1 1 d D . .
C5 C 0.2938(11) 0.5039(10) 0.0727(10) 0.051(2) Uani 1 1 d . . .
C6 C 0.1447(11) 0.5013(9) 0.0377(9) 0.048(2) Uani 1 1 d . . .
C7 C 0.1077(12) 0.5790(12) 0.1029(10) 0.063(3) Uani 1 1 d D . .
C8 C 0.0356(12) 0.4247(12) -0.0646(11) 0.065(3) Uani 1 1
d . . .
H8 H 0.0584 0.3732 -0.1101 0.078 Uiso 1 1 calc R . .
C9 C 0.5374(12) 0.7535(8) 0.0002(9) 0.049(2) Uani 1 1 d . . .
C10 C 0.5193(12) 0.8813(8) 0.0008(9) 0.051(2) Uani 1 1 d . . .
C11 C 0.5002(15) 0.9418(10) -0.1013(10) 0.065(3) Uani 1 1
d . . .
H11 H 0.5017 0.9035 -0.1699 0.079 Uiso 1 1 calc R . .
C12 C 0.5215(15) 0.9408(9) 0.1048(10) 0.062(3) Uani 1 1 d D . .
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C13 C 0.473(2) 0.4055(19) 0.4059(17) 0.127(3) Uani 1 1 d DU . .
H13 H 0.4172 0.4574 0.3835 0.153 Uiso 1 1 calc R . .
C14 C 0.462(2) 0.3275(18) 0.4912(17) 0.130(3) Uani 1 1 d DU . .
H14 H 0.3983 0.3115 0.5327 0.156 Uiso 1 1 calc R . .
C15 C 0.630(2) 0.3238(19) 0.4198(17) 0.129(3) Uani 1 1 d DU . .
H15 H 0.7044 0.3025 0.4102 0.155 Uiso 1 1 calc R . .
C16 C 0.831(2) 0.345(2) 0.215(2) 0.203(5) Uani 1 1 d DU . .
H16 H 0.7601 0.2966 0.1418 0.244 Uiso 1 1 calc R . .
C17 C 1.021(2) 0.409(3) 0.357(2) 0.207(5) Uani 1 1 d DU . .
N1 N 1.123(5) 0.861(4) 0.400(4) 0.174(15) Uani 0.50 1 d PDU . .
N2 N 0.224(2) 0.6757(19) 0.1997(17) 0.093(7) Uani 0.50 1 d
PDU . .
N3 N 0.526(4) 0.891(3) 0.2177(18) 0.128(10) Uani 0.50 1 d
PDU . .
N4 N 0.5697(15) 0.4041(12) 0.3549(12) 0.102(3) Uani 1 1 d
DU . .
N5 N 0.5668(19) 0.2786(17) 0.5005(16) 0.135(3) Uani 1 1 d
DU . .
N6 N 0.802(2) 0.4402(15) 0.2588(14) 0.147(4) Uani 1 1 d DU . .
N7 N 0.942(2) 0.4869(19) 0.340(2) 0.205(5) Uani 1 1 d DU . .
N8 N 0.951(2) 0.3122(19) 0.264(2) 0.205(5) Uani 1 1 d DU . .
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0.01324(19)
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O2 0.068(5) 0.056(4) 0.058(5) -0.013(3) 0.017(4) -0.002(4)
O3 0.035(4) 0.057(4) 0.064(4) 0.008(3) 0.021(3) 0.020(3)
O4 0.046(4) 0.090(5) 0.048(4) 0.008(4) 0.014(4) 0.034(4)
O5 0.075(5) 0.040(4) 0.058(5) 0.007(3) 0.012(4) 0.026(3)
O6 0.088(6) 0.031(3) 0.049(4) -0.008(3) 0.012(4) 0.020(3)
C1 0.049(7) 0.048(6) 0.060(7) 0.004(5) 0.004(5) 0.000(5)
C2 0.070(8) 0.043(6) 0.059(7) -0.016(5) 0.009(6) 0.009(5)
C3 0.051(8) 0.065(8) 0.130(13) -0.035(8) 0.026(8) -0.008(6)
C4 0.063(9) 0.075(8) 0.126(13) -0.052(8) 0.032(8) 0.002(7)
C5 0.037(5) 0.057(6) 0.063(7) -0.004(5) 0.022(5) 0.018(4)
C6 0.036(5) 0.060(6) 0.047(6) -0.008(4) 0.010(4) 0.022(4)
C7 0.040(6) 0.087(8) 0.053(6) -0.020(5) 0.004(5) 0.029(5)
C8 0.051(7) 0.076(7) 0.076(8) -0.016(6) 0.032(6) 0.027(6)
C9 0.057(6) 0.028(4) 0.049(6) 0.003(4) 0.007(5) 0.012(4)
C10 0.067(7) 0.032(5) 0.051(6) -0.006(4) 0.016(5) 0.020(4)
C11 0.098(10) 0.043(6) 0.044(6) -0.004(4) 0.012(6) 0.028(6)
C12 0.094(9) 0.039(5) 0.052(6) 0.009(5) 0.017(6) 0.032(5)
C13 0.128(4) 0.129(4) 0.127(4) 0.018(2) 0.050(2) 0.046(2)
C14 0.132(4) 0.130(4) 0.128(4) 0.0190(19) 0.050(2) 0.045(2)
C15 0.130(4) 0.129(4) 0.130(4) 0.021(2) 0.047(2) 0.049(2)
C16 0.205(5) 0.203(5) 0.205(5) 0.0261(19) 0.079(2) 0.076(2)
C17 0.207(5) 0.207(5) 0.208(5) 0.0286(19) 0.077(2) 0.076(2)
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N1 0.174(15) 0.174(15) 0.174(15) 0.023(3) 0.065(6) 0.064(6)
N2 0.093(7) 0.094(7) 0.093(7) 0.011(2) 0.035(3) 0.034(3)
N3 0.128(10) 0.128(10) 0.128(10) 0.018(2) 0.048(4) 0.047(4)
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N5 0.136(4) 0.135(4) 0.134(4) 0.024(2) 0.051(2) 0.049(2)
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N7 0.204(5) 0.205(5) 0.204(5) 0.0268(19) 0.075(3) 0.073(3)
N8 0.205(5) 0.205(5) 0.206(5) 0.0303(19) 0.077(2) 0.076(2)
N9 0.208(5) 0.212(5) 0.212(5) 0.028(2) 0.076(2) 0.078(3)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu01 O3 2.786(7) 2_665 ?
Eu01 C1 2.878(11) . ?
Eu01 C5 3.009(10) . ?
Eu01 Eu01 4.0881(9) 2_665 ?
O1 C1 1.268(15) . ?
O2 C1 1.269(14) . ?
O3 C5 1.270(12) 2_665 ?
O3 Eu01 2.786(7) 2_665 ?
O4 C5 1.294(12) . ?
O5 C9 1.249(11) . ?
O6 C9 1.224(12) 2_665 ?
C1 C2 1.479(15) . ?
C2 C4 1.344(18) . ?
C2 C3 1.380(19) . ?
C3 C4 1.412(17) 2_776 ?
C3 H3 0.9300 . ?
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C4 C3 1.412(17) 2_776 ?
C4 N1 1.449(5) . ?
C5 O3 1.270(12) 2_665 ?
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C7 N2 1.445(5) . ?
C8 C7 1.384(16) 2_565 ?
C8 H8 0.9300 . ?
C9 O6 1.224(12) 2_665 ?
C9 C10 1.502(13) . ?
C10 C11 1.378(14) . ?
C10 C12 1.395(15) . ?
C11 C12 1.402(15) 2_675 ?
C11 H11 0.9300 . ?
C12 C11 1.402(15) 2_675 ?
C12 N3 1.449(5) . ?
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C14 N5 1.352(5) . ?
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C15 N5 1.353(5) . ?
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C16 N7 1.90(3) . ?
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O6 Eu01 O5 131.5(2) . . ?
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N6 Eu01 O4 145.2(4) . . ?
O6 Eu01 O4 89.8(3) . . ?
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O3 Eu01 O1 88.0(3) . . ?
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O5 Eu01 O1 72.4(3) . . ?
O4 Eu01 O1 125.9(3) . . ?
O3 Eu01 O2 134.7(2) . . ?
N6 Eu01 O2 99.6(5) . . ?
O6 Eu01 O2 148.7(3) . . ?
O5 Eu01 O2 73.2(3) . . ?
O4 Eu01 O2 77.6(3) . . ?
O1 Eu01 O2 52.0(3) . . ?
O3 Eu01 N4 145.6(3) . . ?
N6 Eu01 N4 72.5(5) . . ?
O6 Eu01 N4 74.4(3) . . ?
O5 Eu01 N4 138.9(4) . . ?
O4 Eu01 N4 73.3(4) . . ?
O1 Eu01 N4 106.0(4) . . ?
O2 Eu01 N4 74.6(3) . . ?
O3 Eu01 O3 74.9(2) . 2_665 ?
N6 Eu01 O3 140.0(5) . 2_665 ?
O6 Eu01 O3 67.8(2) . 2_665 ?
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O4 Eu01 O3 49.6(2) . 2_665 ?
O1 Eu01 O3 139.4(3) . 2_665 ?
O2 Eu01 O3 119.7(3) . 2_665 ?
N4 Eu01 O3 108.7(3) . 2_665 ?
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O6 Eu01 C1 159.1(3) . . ?
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O4 Eu01 C1 101.3(3) . . ?
O1 Eu01 C1 26.1(3) . . ?
O2 Eu01 C1 26.1(3) . . ?
N4 Eu01 C1 91.8(4) . . ?
O3 Eu01 C1 132.6(3) 2_665 . ?
O3 Eu01 C5 99.1(3) . . ?
N6 Eu01 C5 152.7(4) . . ?
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O1 Eu01 C5 136.1(3) . . ?
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N4 Eu01 C5 92.3(4) . . ?
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C1 Eu01 C5 117.3(3) . . ?
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N4 Eu01 Eu01 134.0(3) . 2_665 ?
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C1 O2 Eu01 93.9(7) . . ?
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O1 C1 C2 120.4(11) . . ?
O2 C1 C2 120.6(13) . . ?
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O2 C1 Eu01 60.0(6) . . ?
C2 C1 Eu01 173.4(8) . . ?
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C3 C4 N1 120(2) 2_776 . ?
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O4 C5 Eu01 52.2(5) . . ?
C6 C5 Eu01 171.1(7) . . ?
C8 C6 C7 117.5(9) . . ?
C8 C6 C5 120.4(9) . . ?
C7 C6 C5 122.1(9) . . ?
C8 C7 C6 120.1(9) 2_565 . ?
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C6 C7 N2 118.9(14) . . ?
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C12 C10 C9 120.5(9) . . ?
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C11 C12 N3 111.8(17) 2_675 . ?
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N4 C15 H15 124.4 . . ?
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N6 C16 N7 45.1(9) . . ?
N8 C16 N7 83.0(9) . . ?
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N7 C16 C17 40.7(4) . . ?
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N9 C17 C16 150.5(15) . . ?
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C15 N4 Eu01 133.7(11) . . ?
C14 N5 C15 109.6(16) . . ?
N7 N6 C16 89.7(17) . . ?
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C17 N8 C16 94.9(11) . . ?

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 'Eu'  'Eu'  -0.1578   3.6682
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 'x, y, z'
 '-x, -y, -z'

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Source'
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 MERCURY (Bruno et al. 2002)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
Cryst</i>.
<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.5846(7) 0.2760(6) 0.2549(6) 0.069(2) Uani 1 1 d . . .
O3 O 0.2289(6) 0.3881(6) 0.3486(5) 0.0469(14) Uani 1 1 d . . .
O4 O 0.3520(5) 0.4929(5) 0.5156(5) 0.0401(13) Uani 1 1 d . . .
O5 O 0.4569(6) 0.2685(5) 0.4136(4) 0.0423(14) Uani 1 1 d . . .
O6 O 0.4486(7) 0.6491(5) 0.4104(5) 0.0491(16) Uani 1 1 d . . .
O7 O 0.5798(9) 0.5279(8) 0.2580(7) 0.083(2) Uani 1 1 d U . .
N1 N 0.731(3) 0.133(4) 0.176(2) 0.199(17) Uani 0.50 1 d PDU . .
N2 N -0.032(3) 0.358(2) 0.2855(9) 0.102(7) Uani 0.50 1 d
PDU . .
N3 N 0.611(2) 0.976(2) 0.6960(12) 0.103(7) Uani 0.50 1 d
PDU . .
N4 N 0.2749(9) 0.4630(8) 0.1907(7) 0.070(2) Uani 1 1 d DU . .
C1 C 0.4797(10) 0.2057(9) 0.1820(8) 0.052(2) Uani 1 1 d . . .
C2 C 0.4919(10) 0.1003(9) 0.0878(8) 0.055(2) Uani 1 1 d . . .
C3 C 0.3808(12) 0.0329(12) 0.0021(9) 0.091(5) Uani 1 1 d . . .
H3 H 0.2975 0.0526 0.0030 0.109 Uiso 1 1 calc R . .
C4 C 0.6104(11) 0.0651(13) 0.0869(9) 0.098(5) Uani 1 1 d D . .
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C6 C 0.1149(8) 0.4725(8) 0.4730(7) 0.0390(18) Uani 1 1 d . . .
C7 C -0.0119(10) 0.4252(11) 0.3971(8) 0.064(3) Uani 1 1 d D . .
C8 C 0.1252(9) 0.5477(10) 0.5737(8) 0.059(3) Uani 1 1 d . . .
H8 H 0.2099 0.5820 0.6246 0.071 Uiso 1 1 calc R . .
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C9 C 0.5001(9) 0.7441(8) 0.5000(8) 0.049(2) Uani 1 1 d . . .
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C12 C 0.5511(12) 0.9833(9) 0.5945(8) 0.064(3) Uani 1 1 d DU . .
C13 C 0.2117(10) 0.5619(10) 0.2132(10) 0.103(4) Uani 1 1 d
DU . .
H13 H 0.2426 0.6230 0.2824 0.124 Uiso 1 1 calc R . .
C14 C 0.1047(11) 0.5815(11) 0.1427(8) 0.105(4) Uani 1 1 d
DU . .
H14 H 0.0665 0.6527 0.1650 0.126 Uiso 1 1 calc R . .
C15 C 0.0556(11) 0.4934(9) 0.0387(8) 0.080(3) Uani 1 1 d DU . .
C16 C 0.1184(13) 0.3900(12) 0.0133(13) 0.128(4) Uani 1 1 d
DU . .
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C17 C 0.2253(13) 0.3784(12) 0.0893(8) 0.126(4) Uani 1 1 d
DU . .
H17 H 0.2649 0.3078 0.0688 0.152 Uiso 1 1 calc R . .

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0.01337(16)
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O2 0.045(4) 0.060(4) 0.066(5) -0.019(3) 0.021(4) 0.014(3)
O3 0.036(3) 0.063(4) 0.034(4) 0.008(3) 0.013(3) 0.013(3)
O4 0.025(3) 0.040(3) 0.048(4) 0.013(3) 0.007(3) 0.006(2)
O5 0.059(4) 0.032(3) 0.029(3) 0.009(2) 0.005(3) 0.015(3)
O6 0.076(5) 0.023(3) 0.038(3) 0.010(2) 0.005(3) 0.012(3)
O7 0.084(4) 0.098(4) 0.085(4) 0.047(3) 0.043(3) 0.009(3)
N1 0.196(17) 0.200(17) 0.198(17) 0.071(8) 0.064(7) 0.047(6)
N2 0.095(9) 0.106(8) 0.100(9) 0.029(5) 0.033(5) 0.027(5)
N3 0.111(9) 0.095(8) 0.101(8) 0.041(5) 0.027(5) 0.019(5)
N4 0.081(7) 0.064(5) 0.069(5) 0.030(4) 0.021(5) 0.030(5)
C1 0.042(5) 0.053(5) 0.045(6) -0.004(4) 0.015(5) 0.017(4)
C2 0.050(6) 0.050(5) 0.045(6) -0.007(4) 0.016(5) 0.020(4)
C3 0.054(7) 0.098(9) 0.062(8) -0.033(6) 0.007(6) 0.028(6)
C4 0.046(6) 0.114(10) 0.056(7) -0.048(7) -0.003(5) 0.032(6)
C5 0.030(4) 0.030(4) 0.057(6) 0.014(4) 0.012(4) 0.009(3)
C6 0.020(4) 0.047(5) 0.041(5) 0.009(4) 0.007(3) 0.006(3)
C7 0.032(5) 0.098(8) 0.037(6) -0.001(5) 0.011(4) 0.013(5)
C8 0.031(5) 0.088(7) 0.042(6) 0.004(5) 0.011(4) 0.018(5)
C9 0.052(6) 0.029(4) 0.054(6) 0.010(4) 0.005(5) 0.011(4)
C10 0.062(6) 0.025(4) 0.041(5) 0.008(4) 0.001(4) 0.004(4)
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C12 0.083(5) 0.047(4) 0.058(4) 0.026(3) 0.008(4) 0.017(3)
C13 0.100(6) 0.095(5) 0.101(5) 0.035(4) 0.008(4) 0.037(4)
C14 0.105(6) 0.099(5) 0.102(5) 0.037(4) 0.011(4) 0.044(4)
C15 0.106(9) 0.058(6) 0.063(6) 0.032(5) 0.000(6) 0.009(5)
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C17 0.126(5) 0.125(5) 0.125(5) 0.046(2) 0.036(2) 0.034(2)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Eu1 O3 2.396(6) . ?
Eu1 O1 2.426(6) . ?
Eu1 O7 2.438(7) . ?
Eu1 O2 2.497(6) . ?
Eu1 N4 2.612(9) . ?
Eu1 C1 2.818(9) . ?
Eu1 O4 2.858(6) . ?
Eu1 C5 2.985(9) . ?
Eu1 Eu1 4.0529(9) 2_666 ?
O1 C1 1.243(11) . ?
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O6 C9 1.280(10) . ?
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N4 C17 1.344(5) . ?
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C2 C3 1.363(14) . ?
C3 C4 1.396(14) 2_655 ?
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C13 C14 1.387(5) . ?
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C14 C15 1.383(5) . ?
C14 H14 0.9300 . ?
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O4 Eu1 O3 125.5(2) 2_666 . ?
O5 Eu1 O3 77.2(2) . . ?
O6 Eu1 O3 86.1(2) . . ?
O4 Eu1 O1 133.94(19) 2_666 . ?
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O4 Eu1 O7 84.5(3) 2_666 . ?
O5 Eu1 O7 140.9(3) . . ?
O6 Eu1 O7 74.1(3) . . ?
O3 Eu1 O7 140.1(3) . . ?
O1 Eu1 O7 93.5(3) . . ?
O4 Eu1 O2 84.4(2) 2_666 . ?
O5 Eu1 O2 74.5(2) . . ?
O6 Eu1 O2 141.3(2) . . ?
O3 Eu1 O2 131.4(2) . . ?
O1 Eu1 O2 52.4(2) . . ?
O7 Eu1 O2 70.0(3) . . ?
O4 Eu1 N4 148.9(2) 2_666 . ?
O5 Eu1 N4 134.2(2) . . ?
O6 Eu1 N4 74.7(2) . . ?
O3 Eu1 N4 67.6(2) . . ?
O1 Eu1 N4 70.6(2) . . ?
O7 Eu1 N4 73.8(3) . . ?
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O4 Eu1 C1 110.1(2) 2_666 . ?
O5 Eu1 C1 75.8(3) . . ?
O6 Eu1 C1 151.6(3) . . ?
O3 Eu1 C1 108.1(2) . . ?
O1 Eu1 C1 26.1(2) . . ?
O7 Eu1 C1 79.6(3) . . ?
O2 Eu1 C1 26.5(2) . . ?
N4 Eu1 C1 87.9(3) . . ?
O4 Eu1 O4 77.44(19) 2_666 . ?
O5 Eu1 O4 67.74(18) . . ?
O6 Eu1 O4 67.72(19) . . ?
O3 Eu1 O4 48.46(18) . . ?
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O7 Eu1 O4 140.2(2) . . ?
O2 Eu1 O4 141.0(2) . . ?
N4 Eu1 O4 105.4(2) . . ?
C1 Eu1 O4 139.9(2) . . ?
O4 Eu1 C5 102.7(2) 2_666 . ?
O5 Eu1 C5 73.5(2) . . ?
O6 Eu1 C5 73.9(2) . . ?
O3 Eu1 C5 23.4(2) . . ?
O1 Eu1 C5 104.7(2) . . ?
O7 Eu1 C5 144.8(3) . . ?
O2 Eu1 C5 144.3(2) . . ?
N4 Eu1 C5 84.0(3) . . ?
C1 Eu1 C5 127.3(3) . . ?
O4 Eu1 C5 25.3(2) . . ?
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O5 Eu1 Eu1 66.18(13) . 2_666 ?
O6 Eu1 Eu1 67.37(14) . 2_666 ?
O3 Eu1 Eu1 82.20(14) . 2_666 ?
O1 Eu1 Eu1 142.73(17) . 2_666 ?
O7 Eu1 Eu1 119.1(2) . 2_666 ?
O2 Eu1 Eu1 119.49(18) . 2_666 ?
N4 Eu1 Eu1 132.59(19) . 2_666 ?
C1 Eu1 Eu1 137.4(2) . 2_666 ?
O4 Eu1 Eu1 33.95(11) . 2_666 ?
C5 Eu1 Eu1 59.25(17) . 2_666 ?
C1 O1 Eu1 94.9(5) . . ?
C1 O2 Eu1 91.2(5) . . ?
C5 O3 Eu1 106.1(5) . . ?
C5 O4 Eu1 174.3(6) . 2_666 ?
C5 O4 Eu1 82.9(5) . . ?
Eu1 O4 Eu1 102.56(19) 2_666 . ?
C9 O5 Eu1 141.3(5) 2_666 . ?
C9 O6 Eu1 136.6(5) . . ?
C13 N4 C17 113.9(11) . . ?
C13 N4 Eu1 121.2(7) . . ?
C17 N4 Eu1 124.2(8) . . ?
O1 C1 O2 121.1(8) . . ?
O1 C1 C2 119.7(8) . . ?
O2 C1 C2 119.1(8) . . ?
O1 C1 Eu1 59.1(4) . . ?
O2 C1 Eu1 62.4(4) . . ?
C2 C1 Eu1 171.4(8) . . ?
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C4 C2 C1 121.6(9) . . ?
C3 C2 C1 120.2(9) . . ?
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C2 C3 H3 119.4 . . ?
C4 C3 H3 119.4 2_655 . ?
C2 C4 C3 120.5(10) . 2_655 ?
C2 C4 N1 120(2) . . ?
C3 C4 N1 119(2) 2_655 . ?
O3 C5 O4 121.3(8) . . ?
O3 C5 C6 121.2(7) . . ?
O4 C5 C6 117.4(8) . . ?
O3 C5 Eu1 50.5(4) . . ?
O4 C5 Eu1 71.8(4) . . ?
C6 C5 Eu1 165.2(6) . . ?
C8 C6 C7 118.6(8) . . ?
C8 C6 C5 121.1(8) . . ?
C7 C6 C5 120.2(8) . . ?
C6 C7 C8 119.8(8) . 2_566 ?
C6 C7 N2 122.5(13) . . ?
C8 C7 N2 117.4(13) 2_566 . ?
C6 C8 C7 121.6(9) . 2_566 ?
C6 C8 H8 119.2 . . ?
C7 C8 H8 119.2 2_566 . ?
O5 C9 O6 123.8(7) 2_666 . ?
O5 C9 C10 118.7(8) 2_666 . ?
O6 C9 C10 117.3(8) . . ?
C11 C10 C12 119.2(8) . . ?
C11 C10 C9 120.0(8) . . ?
C12 C10 C9 120.8(8) . . ?
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C10 C11 H11 119.1 . . ?
C12 C11 H11 119.1 2_676 . ?
C10 C12 C11 118.9(9) . 2_676 ?
C10 C12 N3 123.1(12) . . ?
C11 C12 N3 117.9(13) 2_676 . ?
N4 C13 C14 126.0(12) . . ?
N4 C13 H13 117.0 . . ?
C14 C13 H13 117.0 . . ?
C15 C14 C13 119.0(12) . . ?
C15 C14 H14 120.5 . . ?
C13 C14 H14 120.5 . . ?
C14 C15 C16 116.2(12) . . ?
C14 C15 C15 122.3(12) . 2_565 ?
C16 C15 C15 121.5(12) . 2_565 ?
C15 C16 C17 120.8(15) . . ?
C15 C16 H16 119.6 . . ?
C17 C16 H16 119.6 . . ?
N4 C17 C16 124.0(15) . . ?
N4 C17 H17 118.0 . . ?
C16 C17 H17 118.0 . . ?

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data_UCY-5-acetone

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'C19 H14 Ce N O8, O'
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 'C19 H14 Ce N O9'
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
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 'Ce'  'Ce'  -0.2486   2.6331
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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_angle_gamma                 90.00
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_cell_formula_units_Z             8
_cell_measurement_temperature     100(2)
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'Empirical absorption correction (CrysAlis RED, Oxford
Diffraction)'

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Source'
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Atlas'
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_diffrn_reflns_number             19630
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_diffrn_reflns_limit_k_max        17
_diffrn_reflns_limit_l_min        -16
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1997)'
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 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
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_computing_publication_material   'WINGX (Farrugia, 1999)'
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          5289
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_refine_ls_number_restraints      46
_refine_ls_R_factor_all           0.0471
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1 d . . .
O1 O 0.89482(12) 0.3310(3) 0.2903(3) 0.0539(10) Uani 1 1
d . . .
O2 O 0.88564(12) 0.1817(3) 0.2410(3) 0.0541(10) Uani 1 1
d . . .
O3 O 0.73112(10) 0.3513(2) -0.0050(3) 0.0372(7) Uani 1 1
d . . .
O4 O 0.79363(11) 0.4388(2) 0.1227(3) 0.0472(8) Uani 1 1 d . . .
O5 O 0.77065(12) 0.3131(3) -0.1485(3) 0.0509(9) Uani 1 1
d . . .
O6 O 0.80164(12) 0.2509(3) 0.2330(3) 0.0453(8) Uani 1 1 d . . .
O7 O 0.86040(18) 0.4176(4) 0.0364(5) 0.0948(18) Uani 1 1
d . . .
O8 O 0.8508(4) 0.1911(7) -0.0305(9) 0.063(2) Uani 0.50 1 d
PU . .
O8A O 0.8708(5) 0.2234(8) 0.0133(13) 0.084(3) Uani 0.50 1 d
PU . .
O9 O 0.55005(19) 0.4064(4) 0.8267(7) 0.129(3) Uani 1 1 d . . .
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C1 C 0.90797(16) 0.2484(4) 0.3187(4) 0.0394(10) Uani 1 1
d . . .
C2 C 0.95025(17) 0.2250(3) 0.4472(5) 0.0416(11) Uani 1 1
d . . .
C3 C 0.96344(16) 0.1334(4) 0.4843(4) 0.0438(11) Uani 1 1
d . . .
H3 H 0.9445 0.0851 0.4306 0.053 Uiso 1 1 calc R . .
C4 C 1.00460(16) 0.1124(4) 0.6008(4) 0.0455(12) Uani 1 1
d . . .
H4 H 1.0131 0.0504 0.6255 0.055 Uiso 1 1 calc R . .
C5 C 1.03309(18) 0.1852(4) 0.6807(5) 0.0551(15) Uani 1 1
d . . .
C6 C 1.0188(3) 0.2763(4) 0.6444(7) 0.088(3) Uani 1 1 d . . .
H6 H 1.0377 0.3249 0.6976 0.106 Uiso 1 1 calc R . .
C7 C 0.9773(2) 0.2967(4) 0.5311(7) 0.079(2) Uani 1 1 d . . .
H7 H 0.9671 0.3584 0.5103 0.095 Uiso 1 1 calc R . .
C8 C 0.57811(18) 0.6668(4) -0.2003(5) 0.0587(16) Uani 1 1 d
D . .
C9 C 0.74947(15) 0.4256(3) 0.0591(4) 0.0352(9) Uani 1 1 d . . .
C10 C 0.71751(14) 0.4995(3) 0.0566(4) 0.0329(9) Uani 1 1
d . . .
C11 C 0.67027(15) 0.5061(3) -0.0446(4) 0.0353(9) Uani 1 1
d . . .
H11 H 0.6575 0.4626 -0.1096 0.042 Uiso 1 1 calc R . .
C12 C 0.64207(15) 0.5787(3) -0.0480(4) 0.0386(10) Uani 1 1
d . . .
C13 C 0.66014(15) 0.6388(3) 0.0541(4) 0.0401(10) Uani 1 1
d . . .
H13 H 0.6407 0.6849 0.0543 0.048 Uiso 1 1 calc R . .
C14 C 0.70752(15) 0.6297(3) 0.1559(4) 0.0351(9) Uani 1 1
d . . .
C15 C 0.73572(14) 0.5617(3) 0.1552(4) 0.0327(9) Uani 1 1
d . . .
H15 H 0.7677 0.5571 0.2222 0.039 Uiso 1 1 calc R . .
C16 C 0.72746(17) 0.6946(4) 0.2681(4) 0.0387(10) Uani 1 1
d . . .
C17 C 0.8800(5) 0.1767(9) -0.0530(14) 0.157(4) Uani 1 1 d
DU . .
C18 C 0.8786(5) 0.0882(8) -0.1179(13) 0.171(4) Uani 1 1 d
DU . .
H18A H 0.8876 0.1015 -0.1753 0.257 Uiso 1 1 calc R . .
H18B H 0.8467 0.0629 -0.1635 0.257 Uiso 1 1 calc R . .
H18C H 0.9005 0.0436 -0.0565 0.257 Uiso 1 1 calc R . .
C19 C 0.9276(5) 0.2235(11) -0.0016(18) 0.190(5) Uani 1 1 d
DU . .
H19A H 0.9413 0.2005 -0.0454 0.286 Uiso 1 1 calc R . .
H19B H 0.9489 0.2098 0.0864 0.286 Uiso 1 1 calc R . .
H19C H 0.9231 0.2899 -0.0133 0.286 Uiso 1 1 calc R . .
N1 N 0.59441(13) 0.5864(3) -0.1594(4) 0.0437(10) Uani 1 1
d . . .
H16 H 0.592(2) 0.722(3) -0.154(5) 0.052 Uiso 1 1 d D . .

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0.00385(8)
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0.0078(16)
O2 0.0399(18) 0.0461(19) 0.0312(18) -0.0047(16) -0.0078(15)
0.0181(16)
O3 0.0314(15) 0.0309(16) 0.0336(17) 0.0018(12) 0.0085(14)
0.0040(12)
O4 0.0242(15) 0.0344(17) 0.057(2) 0.0027(15) 0.0069(15)
0.0036(13)
O5 0.0317(18) 0.083(2) 0.0241(17) 0.0141(17) 0.0068(15) -
0.0059(17)
O6 0.0344(18) 0.058(2) 0.0322(18) 0.0091(17) 0.0116(15) -
0.0043(17)
O7 0.082(3) 0.113(4) 0.079(3) 0.012(3) 0.039(3) -0.047(3)
O8 0.085(4) 0.058(4) 0.041(4) 0.011(3) 0.032(3) 0.018(3)
O8A 0.083(5) 0.075(5) 0.083(5) 0.008(3) 0.039(4) 0.016(3)
O9 0.065(3) 0.100(4) 0.206(7) -0.044(5) 0.066(4) -0.005(3)
C1 0.025(2) 0.048(3) 0.026(2) 0.004(2) 0.0034(19) 0.008(2)
C2 0.024(2) 0.047(3) 0.033(3) -0.003(2) 0.003(2) 0.0047(18)
C3 0.031(2) 0.045(3) 0.032(2) -0.004(2) 0.004(2) 0.006(2)
C4 0.031(2) 0.047(3) 0.033(2) -0.005(2) 0.002(2) 0.010(2)
C5 0.037(3) 0.052(3) 0.037(3) -0.011(2) -0.004(2) 0.012(2)
C6 0.058(4) 0.055(4) 0.059(4) -0.018(3) -0.024(3) 0.012(3)
C7 0.056(4) 0.045(3) 0.057(4) -0.009(3) -0.017(3) 0.016(3)
C8 0.039(3) 0.050(3) 0.037(3) -0.015(2) -0.009(2) 0.012(2)
C9 0.031(2) 0.032(2) 0.029(2) 0.0082(18) 0.0088(18) 0.0070(17)
C10 0.027(2) 0.032(2) 0.028(2) 0.0047(17) 0.0085(17) 0.0047(17)
C11 0.027(2) 0.038(2) 0.025(2) -0.0001(17) 0.0054(18)
0.0088(17)
C12 0.029(2) 0.045(3) 0.023(2) -0.0032(18) 0.0027(18)
0.0067(19)
C13 0.028(2) 0.051(3) 0.027(2) -0.0040(19) 0.0064(18)
0.0103(19)
C14 0.029(2) 0.046(3) 0.021(2) -0.0021(18) 0.0086(17)
0.0009(18)
C15 0.0244(19) 0.037(2) 0.023(2) 0.0061(17) 0.0051(16)
0.0024(17)
C16 0.029(2) 0.054(3) 0.027(2) -0.007(2) 0.012(2) -0.001(2)
C17 0.154(5) 0.187(6) 0.171(6) -0.031(4) 0.116(4) 0.009(4)
C18 0.186(6) 0.182(6) 0.174(6) -0.028(4) 0.118(5) 0.037(4)
C19 0.165(5) 0.222(7) 0.221(7) 0.001(5) 0.131(5) -0.015(4)
N1 0.0286(18) 0.049(2) 0.0282(19) -0.0059(17) 0.0006(16)
0.0115(17)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Ce1 O8A 2.456(13) . ?
Ce1 O4 2.518(3) . ?
Ce1 O7 2.520(4) . ?
Ce1 O2 2.529(3) . ?
Ce1 O1 2.543(3) . ?
Ce1 O8 2.554(10) . ?
Ce1 O3 2.711(3) . ?
Ce1 C1 2.898(4) . ?
Ce1 C9 2.989(4) . ?
O1 C1 1.242(6) . ?
O2 C1 1.275(6) . ?
O3 C9 1.272(5) . ?
O3 Ce1 2.452(3) 7_655 ?
O4 C9 1.246(5) . ?
O5 C16 1.236(6) 6_565 ?
O6 C16 1.261(6) 4_645 ?
O8 O8A 0.746(14) . ?
O8 C17 1.186(14) . ?
O8A C17 1.247(16) . ?
C1 C2 1.492(6) . ?
C2 C3 1.379(6) . ?
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C17 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C17 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
C17 C19 H19A 109.5 . . ?
C17 C19 H19B 109.5 . . ?
H19A C19 H19B 109.5 . . ?
C17 C19 H19C 109.5 . . ?
H19A C19 H19C 109.5 . . ?
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_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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-838.

Oxford Diffraction (2008). <i>CrysAlis CCD and CrysAlis
RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;


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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
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are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
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P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.38788(19) 0.3215(3) 0.5332(5) 0.0498(13) Uani 1 1 d .
B .
O3 O 0.26695(16) 0.3489(3) 0.5309(4) 0.0356(10) Uani 1 1
d . . .
O4 O 0.29820(16) 0.0688(3) 0.4818(5) 0.0451(12) Uani 1 1 d .
B .
O5 O 0.27688(17) 0.1888(4) 0.7081(4) 0.0448(11) Uani 1 1 d .
B .
O6 O 0.29733(18) 0.2499(4) 0.3606(4) 0.0404(10) Uani 1 1
d . . .
O8 O 0.3614(2) 0.3168(5) 0.7478(5) 0.0631(15) Uani 1 1 d . B .
N1 N 0.59800(19) 0.4152(4) 0.3569(5) 0.0380(12) Uani 1 1
d . . .
C1 C 0.4082(2) 0.2584(5) 0.4951(6) 0.0406(15) Uani 1 1 d . B .
C2 C 0.4516(3) 0.2799(5) 0.4526(7) 0.0415(17) Uani 1 1 d . . .
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C3 C 0.4799(3) 0.2109(5) 0.4299(8) 0.0515(19) Uani 1 1 d . B .
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C4 C 0.5222(3) 0.2305(5) 0.4006(8) 0.051(2) Uani 1 1 d . . .
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C9 C 0.2527(2) 0.0777(4) 0.4505(6) 0.0382(15) Uani 1 1 d . . .
C10 C 0.2218(2) 0.0017(4) 0.3928(6) 0.0363(14) Uani 1 1 d . . .
C11 C 0.1742(2) -0.0053(5) 0.3976(6) 0.0386(14) Uani 1 1 d .
B .
H11 H 0.1613 0.0377 0.4367 0.046 Uiso 1 1 calc R . .
C12 C 0.1454(2) -0.0781(4) 0.3426(6) 0.0357(14) Uani 1 1
d . . .
C13 C 0.1640(2) -0.1376(4) 0.2772(6) 0.0351(13) Uani 1 1 d .
B .
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d . . .
C15 C 0.2405(2) -0.0607(4) 0.3314(6) 0.0364(14) Uani 1 1 d .
B .
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C16 C 0.2320(2) 0.1940(5) 0.7019(6) 0.0369(14) Uani 1 1 d . . .
C17 C 0.3844(12) 0.116(2) 0.813(3) 0.048(7) Uani 0.25 1 d
PU . .
H17A H 0.4015 0.0690 0.8626 0.072 Uiso 0.25 1 calc PR A 1
H17B H 0.3566 0.1336 0.8371 0.072 Uiso 0.25 1 calc PR A 1
H17C H 0.4056 0.1664 0.8170 0.072 Uiso 0.25 1 calc PR A 1
O7 O 0.3691(16) 0.084(3) 0.698(4) 0.085(13) Uani 0.25 1 d PU B
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O7A O 0.3763(3) 0.1168(7) 0.7175(8) 0.055(2) Uani 0.75 1 d PU
B 2
C18 C 0.3469(6) 0.3502(11) 0.8404(12) 0.115(5) Uani 1 1 d U . .
H18A H 0.3731 0.3835 0.8907 0.173 Uiso 1 1 calc R B .
H18B H 0.3382 0.3014 0.8827 0.173 Uiso 1 1 calc R . .
H18C H 0.3193 0.3889 0.8121 0.173 Uiso 1 1 calc R . .
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O2 0.044(3) 0.045(3) 0.077(3) -0.015(3) 0.045(3) -0.017(2)
O3 0.030(2) 0.031(2) 0.055(3) -0.0025(19) 0.0269(19) -
0.0003(17)
O4 0.028(2) 0.034(2) 0.083(3) -0.001(2) 0.032(2) 0.0020(18)
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O5 0.028(2) 0.068(3) 0.051(3) 0.008(2) 0.031(2) -0.003(2)
O6 0.038(3) 0.045(2) 0.051(3) 0.000(2) 0.033(2) 0.002(2)
O8 0.069(4) 0.067(4) 0.053(3) -0.009(3) 0.017(3) -0.008(3)
N1 0.031(3) 0.045(3) 0.049(3) -0.008(2) 0.029(2) -0.006(2)
C1 0.023(3) 0.053(4) 0.051(4) 0.003(3) 0.018(3) -0.005(3)
C2 0.029(4) 0.056(5) 0.049(4) 0.001(3) 0.026(3) -0.006(3)
C3 0.044(4) 0.048(5) 0.073(5) 0.002(4) 0.034(4) -0.004(3)
C4 0.040(4) 0.050(5) 0.076(6) 0.000(4) 0.036(4) 0.001(3)
C5 0.029(3) 0.053(4) 0.051(4) 0.000(3) 0.027(3) -0.006(3)
C6 0.038(4) 0.047(4) 0.054(4) -0.006(3) 0.030(3) -0.009(3)
C7 0.032(3) 0.049(4) 0.053(4) -0.008(3) 0.029(3) -0.007(3)
C8 0.036(4) 0.052(4) 0.049(4) -0.004(3) 0.026(3) -0.001(3)
C9 0.035(3) 0.034(3) 0.056(4) -0.001(3) 0.030(3) -0.008(3)
C10 0.029(3) 0.032(3) 0.058(4) -0.001(3) 0.030(3) -0.004(2)
C11 0.039(4) 0.033(3) 0.054(4) 0.002(3) 0.031(3) -0.002(3)
C12 0.032(3) 0.036(3) 0.049(4) -0.001(3) 0.028(3) -0.003(3)
C13 0.031(3) 0.038(3) 0.044(3) -0.001(3) 0.023(3) 0.000(3)
C14 0.030(3) 0.041(3) 0.044(3) -0.001(3) 0.023(3) -0.001(3)
C15 0.029(3) 0.036(3) 0.055(4) 0.000(3) 0.030(3) 0.000(3)
C16 0.035(3) 0.038(4) 0.046(4) 0.002(3) 0.025(3) 0.000(3)
C17 0.051(9) 0.051(9) 0.042(9) -0.002(7) 0.012(7) 0.007(7)
O7 0.085(14) 0.085(14) 0.085(14) 0.000(5) 0.024(6) 0.000(5)
O7A 0.050(4) 0.055(4) 0.057(4) 0.001(3) 0.011(3) 0.012(3)
C18 0.130(8) 0.127(8) 0.094(6) -0.008(6) 0.041(6) -0.005(6)

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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Ce1 O3 2.443(4) . ?
Ce1 O6 2.447(5) . ?
Ce1 O4 2.514(5) . ?
Ce1 O7A 2.534(9) . ?
Ce1 O2 2.535(4) . ?
Ce1 O1 2.557(5) . ?
Ce1 O8 2.559(6) . ?
Ce1 O7 2.68(4) . ?
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Ce1 O3 2.713(4) 7_556 ?
Ce1 C1 2.897(7) . ?
Ce1 C9 2.998(7) . ?
O1 C1 1.261(10) . ?
O2 C1 1.258(10) . ?
O3 C9 1.279(8) 7_556 ?
O3 Ce1 2.713(4) 7_556 ?
O4 C9 1.260(8) . ?
O5 C16 1.271(8) . ?
O6 C16 1.271(9) 7_556 ?
O8 C18 1.385(15) . ?
N1 C8 1.271(9) . ?
N1 C12 1.419(8) 3 ?
C1 C2 1.506(9) . ?
C2 C7 1.379(10) . ?
C2 C3 1.384(11) . ?
C3 C4 1.385(11) . ?
C3 H3 0.9300 . ?
C4 C5 1.385(11) . ?
C4 H4 0.9300 . ?
C5 C6 1.407(10) . ?
C5 C8 1.475(9) . ?
C6 C7 1.391(9) . ?
C6 H6 0.9300 . ?
C7 H7 0.9300 . ?
C8 H16 0.95(2) . ?
C9 O3 1.279(8) 7_556 ?
C9 C10 1.485(9) . ?
C10 C15 1.385(9) . ?
C10 C11 1.387(8) . ?
C11 C12 1.411(9) . ?
C11 H11 0.9300 . ?
C12 C13 1.388(9) . ?
C12 N1 1.419(8) 3_445 ?
C13 C14 1.392(9) . ?
C13 H13 0.9300 . ?
C14 C15 1.378(9) . ?
C14 C16 1.504(9) 6 ?
C15 H15 0.9300 . ?
C16 O6 1.271(9) 7_556 ?
C16 C14 1.504(9) 6_556 ?
C17 O7A 1.10(3) . ?
C17 O7 1.41(5) . ?
C17 H17A 0.9600 . ?
C17 H17B 0.9600 . ?
C17 H17C 0.9600 . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
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O3 Ce1 O4 122.48(15) . . ?
O6 Ce1 O4 76.31(18) . . ?
O5 Ce1 O7A 74.8(3) . . ?
O3 Ce1 O7A 148.0(3) . . ?
O6 Ce1 O7A 140.7(3) . . ?
O4 Ce1 O7A 77.5(3) . . ?
O5 Ce1 O2 142.97(18) . . ?
O3 Ce1 O2 88.77(16) . . ?
O6 Ce1 O2 74.80(18) . . ?
O4 Ce1 O2 126.35(15) . . ?
O7A Ce1 O2 98.4(3) . . ?
O5 Ce1 O1 146.31(19) . . ?
O3 Ce1 O1 132.61(16) . . ?
O6 Ce1 O1 73.73(19) . . ?
O4 Ce1 O1 77.47(17) . . ?
O7A Ce1 O1 72.4(3) . . ?
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O3 Ce1 O7 153.8(10) . . ?
O6 Ce1 O7 133.0(9) . . ?
O4 Ce1 O7 65.8(8) . . ?
O7A Ce1 O7 11.8(8) . . ?
O2 Ce1 O7 105.9(9) . . ?
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O8 Ce1 O7 84.9(9) . . ?
O5 Ce1 O3 66.97(15) . 7_556 ?
O3 Ce1 O3 74.48(15) . 7_556 ?
O6 Ce1 O3 69.10(15) . 7_556 ?
O4 Ce1 O3 49.72(13) . 7_556 ?
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C9 O3 Ce1 90.0(4) 7_556 7_556 ?
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C9 O4 Ce1 99.8(4) . . ?
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C7 C2 C3 120.5(6) . . ?
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C4 C3 H3 120.1 . . ?
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C2 C7 H7 119.8 . . ?
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N1 C8 C5 123.3(7) . . ?
N1 C8 H16 128(10) . . ?
C5 C8 H16 108(10) . . ?
O4 C9 O3 120.5(6) . 7_556 ?
O4 C9 C10 119.4(6) . . ?
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C11 C12 N1 116.8(6) . 3_445 ?
C12 C13 C14 120.4(6) . . ?
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C14 C15 C10 120.4(6) . . ?
C14 C15 H15 119.8 . . ?
C10 C15 H15 119.8 . . ?
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O6 C16 C14 117.4(6) 7_556 6_556 ?
O5 C16 C14 118.1(6) . 6_556 ?
O7A C17 O7 21.4(19) . . ?
O7A C17 H17A 125.4 . . ?
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O7A C17 H17B 111.2 . . ?
O7 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
O7A C17 H17C 89.5 . . ?
O7 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
C17 O7 Ce1 106(3) . . ?
C17 O7A Ce1 130.3(18) . . ?
O8 C18 H18A 109.5 . . ?
O8 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
O8 C18 H18C 109.5 . . ?
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H18B C18 H18C 109.5 . . ?

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

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_cell_angle_beta                  103.394(12)
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1997)'
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_computing_publication_material    ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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d . . .
O2 O -0.22972(18) -0.1542(4) 0.5385(4) 0.0225(11) Uani 1 1
d . . .
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O4 O 0.1175(2) 0.1816(5) 0.4709(5) 0.0347(14) Uani 1 1 d . . .
O5 O -0.19946(19) 0.2473(4) 0.8725(4) 0.0230(11) Uani 1 1
d . . .
O6 O -0.27047(18) 0.1744(4) 0.8205(4) 0.0258(12) Uani 1 1
d . . .
O7 O -0.3517(3) -0.2973(6) 0.2741(6) 0.056(2) Uani 1 1 d . . .
O8 O -0.3631(3) -0.0968(7) 0.3179(7) 0.066(3) Uani 1 1 d DU . .
N1 N -0.0947(2) 0.0888(5) 0.6462(6) 0.0289(15) Uani 1 1 d . . .
C1 C -0.2489(3) -0.0789(5) 0.5601(6) 0.0209(14) Uani 1 1
d . . .
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d . . .
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C5 C -0.1605(3) 0.1379(6) 0.7328(6) 0.0238(15) Uani 1 1 d . . .
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C10 C -0.0033(3) 0.1139(7) 0.5904(7) 0.0310(18) Uani 1 1
d . . .
H10 H -0.0124 0.0523 0.5972 0.037 Uiso 1 1 calc R . .
C14 C -0.0172(4) 0.2796(7) 0.6067(11) 0.052(3) Uani 1 1 d . . .
H14 H -0.0361 0.3281 0.6223 0.062 Uiso 1 1 calc R . .
C13 C 0.0250(4) 0.2985(7) 0.5741(11) 0.051(3) Uani 1 1 d . . .
H13 H 0.0353 0.3598 0.5711 0.061 Uiso 1 1 calc R . .
C12 C 0.0520(3) 0.2255(7) 0.5459(7) 0.0310(19) Uani 1 1 d . . .
C11 C 0.0379(3) 0.1338(6) 0.5552(7) 0.0296(17) Uani 1 1 d . . .
H11 H 0.0563 0.0853 0.5375 0.036 Uiso 1 1 calc R . .
C15 C 0.0960(3) 0.2467(7) 0.5045(7) 0.0313(18) Uani 1 1 d . . .
C16 C -0.2275(3) 0.1883(5) 0.8183(6) 0.0210(15) Uani 1 1
d . . .
C17 C -0.3810(5) -0.3424(11) 0.2125(12) 0.070(4) Uani 1 1 d
U . .
C18 C -0.3715(7) -0.4090(14) 0.1350(16) 0.110(6) Uani 1 1 d
U . .
H18A H -0.3383 -0.4053 0.1323 0.165 Uiso 1 1 calc R . .
H18B H -0.3914 -0.3951 0.0653 0.165 Uiso 1 1 calc R . .
H18C H -0.3785 -0.4709 0.1560 0.165 Uiso 1 1 calc R . .
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C19 C -0.4335(10) -0.348(2) 0.214(2) 0.175(11) Uani 1 1 d U . .
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H19B H -0.4408 -0.4097 0.2353 0.262 Uiso 1 1 calc R . .
H19C H -0.4528 -0.3348 0.1435 0.262 Uiso 1 1 calc R . .
C21 C -0.3779(11) -0.034(2) 0.1374(17) 0.184(9) Uani 1 1 d
DU . .
H21A H -0.3976 -0.0844 0.1032 0.276 Uiso 1 1 calc R . .
H21B H -0.3485 -0.0326 0.1133 0.276 Uiso 1 1 calc R . .
H21C H -0.3947 0.0241 0.1192 0.276 Uiso 1 1 calc R . .
C20 C -0.3684(13) -0.045(2) 0.2380(19) 0.190(7) Uani 1 1 d
DU . .
C22 C -0.3534(14) 0.032(3) 0.276(3) 0.253(10) Uani 1 1 d DU . .
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O3 0.036(3) 0.028(3) 0.076(5) 0.016(3) 0.037(3) 0.004(3)
O4 0.028(3) 0.043(4) 0.040(3) -0.013(3) 0.024(3) -0.011(3)
O5 0.023(3) 0.026(3) 0.023(3) -0.003(2) 0.011(2) 0.000(2)
O6 0.019(2) 0.033(3) 0.029(3) -0.005(2) 0.012(2) -0.002(2)
O7 0.071(5) 0.068(5) 0.025(3) -0.005(3) 0.004(3) -0.037(4)
O8 0.045(4) 0.107(7) 0.048(4) 0.019(5) 0.013(4) 0.037(5)
N1 0.019(3) 0.041(4) 0.031(3) -0.008(3) 0.016(3) -0.005(3)
C1 0.020(3) 0.023(4) 0.023(3) -0.001(3) 0.012(3) 0.000(3)
C2 0.021(3) 0.018(3) 0.023(3) 0.003(3) 0.007(3) 0.002(3)
C3 0.016(3) 0.025(4) 0.020(3) -0.001(3) 0.010(3) -0.002(3)
C4 0.022(3) 0.022(4) 0.020(3) 0.002(3) 0.012(3) 0.002(3)
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C6 0.019(3) 0.032(4) 0.023(3) -0.001(3) 0.012(3) 0.000(3)
C7 0.020(3) 0.026(4) 0.029(4) -0.003(3) 0.017(3) -0.002(3)
C8 0.025(4) 0.042(5) 0.042(5) -0.005(4) 0.020(4) -0.007(4)
C9 0.027(4) 0.042(5) 0.038(5) -0.009(4) 0.016(4) -0.007(4)
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C13 0.036(5) 0.032(5) 0.094(9) -0.003(6) 0.036(6) -0.005(4)
C12 0.023(4) 0.044(5) 0.031(4) 0.001(4) 0.015(3) -0.006(4)
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C16 0.023(3) 0.022(4) 0.020(3) 0.003(3) 0.010(3) 0.007(3)
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0.0004(10)
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0.0000(10)
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C20 0.191(7) 0.191(7) 0.190(7) 0.0016(10) 0.0441(19) 0.0001(10)
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0.0003(10)

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 are estimated using the full covariance matrix.  The cell
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 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Gd1 O2 2.682(5) . ?
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O3 C15 1.266(12) . ?
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H21B C21 H21C 109.5 . . ?
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C20 C22 H22B 109.5 . . ?
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1997)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick,
1997)'
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```
 DIAMOND (Brandenburg, 2006)
 MERCURY (Bruno et al. 2002)
;

_computing_publication_material   'WINGX (Farrugia, 1999)'
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;
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Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
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Cryst</i>.
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-838.

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Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1020P)^2^+2.7273P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          6227
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_refine_ls_R_factor_all           0.0557
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d . . .
O1 O 0.6550(5) 0.2907(5) 0.2267(5) 0.0634(14) Uani 1 1 d . . .
O2 O 0.8128(5) 0.2614(4) 0.1582(3) 0.0463(10) Uani 1 1 d . . .
O3 O 1.1500(4) 0.5011(4) 0.4988(3) 0.0409(9) Uani 1 1 d . . .
O4 O 1.1225(4) 0.4300(5) 0.3189(3) 0.0484(10) Uani 1 1 d . . .
O5 O 0.9210(6) 0.2749(4) 0.4065(4) 0.0526(12) Uani 1 1 d . . .
O6 O 0.9978(6) 0.6789(4) 0.4016(4) 0.0534(12) Uani 1 1 d . . .
O7 O 0.6952(6) 0.5552(6) 0.2524(5) 0.0705(15) Uani 1 1 d . . .
O8 O 0.9162(7) 0.5343(5) 0.1598(4) 0.0622(13) Uani 1 1 d . . .
N1 N 0.765(3) 0.025(3) 0.007(2) 0.281(12) Uani 1 1 d U . .
N2 N 1.3326(12) 0.3706(10) 0.2730(9) 0.104(3) Uani 1 1 d U . .
N3 N 0.9745(10) 0.0832(9) 0.2967(8) 0.0897(19) Uani 1 1 d U . .
N4 N 0.599(2) 0.697(2) 0.1787(17) 0.184(4) Uani 1 1 d DU . .
N5 N 1.0221(15) 0.6675(13) 0.0850(12) 0.131(2) Uani 1 1 d U . .
C1 C 0.6928(6) 0.2286(5) 0.1611(5) 0.0395(12) Uani 1 1 d . . .
C2 C 0.5933(6) 0.1089(5) 0.0785(5) 0.0428(13) Uani 1 1 d . . .
C3 C 0.6385(8) 0.0319(7) 0.0099(6) 0.0523(15) Uani 1 1 d U . .
C4 C 0.4552(8) 0.0777(7) 0.0686(6) 0.0595(18) Uani 1 1 d . . .
H4 H 0.4245 0.1294 0.1140 0.071 Uiso 1 1 calc R . .
C5 C 1.1998(5) 0.4708(5) 0.4243(5) 0.0378(11) Uani 1 1 d . . .
C6 C 1.3542(5) 0.4840(5) 0.4621(5) 0.0359(11) Uani 1 1 d . . .
C7 C 1.4431(6) 0.5473(6) 0.5751(5) 0.0456(14) Uani 1 1 d . . .
H7 H 1.4046 0.5784 0.6259 0.055 Uiso 1 1 calc R . .
C8 C 1.4124(8) 0.4352(8) 0.3866(8) 0.0631(15) Uani 1 1 d U . .
C9 C 0.9668(8) 0.2482(5) 0.5012(5) 0.0483(15) Uani 1 1 d . . .
C10 C 0.9815(8) 0.1182(5) 0.4984(5) 0.0519(16) Uani 1 1 d . . .
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C11 C 0.9802(10) 0.0409(9) 0.4006(8) 0.0734(18) Uani 1 1 d
U . .
C12 C 1.0034(9) 0.0767(6) 0.5980(6) 0.062(2) Uani 1 1 d . . .
H12 H 1.0071 0.1289 0.6641 0.075 Uiso 1 1 calc R . .
C13 C 0.670(2) 0.6427(17) 0.256(2) 0.166(7) Uani 1 1 d U . .
C14 C 0.460(2) 0.610(2) 0.1156(19) 0.187(5) Uani 1 1 d DU . .
H14A H 0.4047 0.6434 0.0569 0.281 Uiso 1 1 calc R . .
H14B H 0.4149 0.5985 0.1678 0.281 Uiso 1 1 calc R . .
H14C H 0.4702 0.5323 0.0808 0.281 Uiso 1 1 calc R . .
C15 C 0.594(2) 0.827(2) 0.209(2) 0.183(5) Uani 1 1 d U . .
H15A H 0.6276 0.8563 0.2913 0.274 Uiso 1 1 calc R . .
H15B H 0.4994 0.8326 0.1746 0.274 Uiso 1 1 calc R . .
H15C H 0.6530 0.8769 0.1815 0.274 Uiso 1 1 calc R . .
C16 C 1.0175(18) 0.6101(16) 0.1664(14) 0.125(3) Uani 1 1 d
U . .
C17 C 0.9147(18) 0.6457(16) -0.0210(14) 0.133(3) Uani 1 1 d
U . .
H17A H 0.9213 0.7191 -0.0484 0.199 Uiso 1 1 calc R . .
H17B H 0.8259 0.6234 -0.0141 0.199 Uiso 1 1 calc R . .
H17C H 0.9222 0.5793 -0.0744 0.199 Uiso 1 1 calc R . .
C18 C 1.1424(18) 0.7672(16) 0.1006(14) 0.135(3) Uani 1 1 d
U . .
H18A H 1.1288 0.7886 0.0289 0.202 Uiso 1 1 calc R . .
H18B H 1.2268 0.7398 0.1255 0.202 Uiso 1 1 calc R . .
H18C H 1.1502 0.8384 0.1575 0.202 Uiso 1 1 calc R . .

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0.00226(10)
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O2 0.046(2) 0.038(2) 0.036(2) -0.0037(16) 0.0101(17) -
0.0084(17)
O3 0.0252(17) 0.049(2) 0.044(2) 0.0038(17) 0.0124(16)
0.0103(16)
O4 0.0283(19) 0.072(3) 0.0347(19) 0.0050(19) 0.0071(16)
0.0079(19)
O5 0.081(3) 0.0244(19) 0.038(2) 0.0093(16) 0.008(2) 0.010(2)
O6 0.081(3) 0.0233(19) 0.038(2) 0.0061(16) 0.009(2) 0.0031(19)
O7 0.055(3) 0.082(4) 0.086(4) 0.045(3) 0.019(3) 0.039(3)
O8 0.091(4) 0.047(3) 0.049(3) 0.019(2) 0.027(3) 0.012(3)
N1 0.281(12) 0.281(12) 0.281(12) 0.072(3) 0.109(5) 0.073(3)
N2 0.104(3) 0.105(3) 0.102(3) 0.0242(12) 0.0394(14) 0.0267(12)
N3 0.092(2) 0.090(2) 0.0874(19) 0.0268(11) 0.0348(12)
0.0219(10)
N4 0.184(4) 0.184(4) 0.184(5) 0.0477(15) 0.0707(19) 0.0498(15)
N5 0.133(3) 0.131(3) 0.130(3) 0.0351(12) 0.0518(13) 0.0334(11)
C1 0.038(3) 0.035(3) 0.029(2) 0.005(2) 0.001(2) -0.001(2)
C2 0.044(3) 0.032(3) 0.031(2) 0.000(2) 0.001(2) -0.005(2)
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C3 0.0516(17) 0.0521(17) 0.0522(17) 0.0119(10) 0.0204(11)
0.0115(10)
C4 0.049(4) 0.053(4) 0.049(4) -0.012(3) 0.010(3) -0.007(3)
C5 0.027(2) 0.043(3) 0.036(3) 0.003(2) 0.009(2) 0.006(2)
C6 0.024(2) 0.044(3) 0.036(3) 0.006(2) 0.010(2) 0.006(2)
C7 0.033(3) 0.055(4) 0.041(3) -0.007(3) 0.014(2) 0.011(2)
C8 0.045(3) 0.063(4) 0.101(4) 0.024(3) 0.046(3) 0.023(3)
C9 0.066(4) 0.022(2) 0.040(3) 0.009(2) 0.005(3) 0.001(2)
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C11 0.073(2) 0.070(2) 0.0747(19) 0.0160(11) 0.0261(12)
0.0206(10)
C12 0.098(6) 0.025(3) 0.040(3) 0.007(2) 0.006(3) 0.003(3)
C13 0.151(16) 0.117(13) 0.246(19) 0.036(13) 0.086(14) 0.068(12)
C14 0.187(5) 0.187(5) 0.188(5) 0.0475(15) 0.073(2) 0.0480(15)
C15 0.183(5) 0.182(5) 0.183(5) 0.0469(15) 0.071(2) 0.0473(16)
C16 0.125(3) 0.125(3) 0.125(3) 0.0310(14) 0.0491(15) 0.0323(12)
C17 0.133(3) 0.133(3) 0.132(3) 0.0342(13) 0.0508(12) 0.0348(12)
C18 0.135(3) 0.135(3) 0.135(3) 0.0355(13) 0.0534(15) 0.0325(10)

_geom_special_details
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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Ce1 O7 2.507(5) . ?
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Ce1 O4 2.519(4) . ?
Ce1 O2 2.543(4) . ?
Ce1 O1 2.548(4) . ?
Ce1 O3 2.753(4) . ?
Ce1 C1 2.900(5) . ?
Ce1 C5 3.006(5) . ?
Ce1 Ce1 4.1357(16) 2_766 ?
O1 C1 1.218(8) . ?
O2 C1 1.263(8) . ?
O3 C5 1.264(7) . ?
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O3 Ce1 2.441(4) 2_766 ?
O4 C5 1.259(7) . ?
O5 C9 1.254(7) . ?
O6 C9 1.259(7) 2_766 ?
O7 C13 1.070(17) . ?
O8 C16 1.209(17) . ?
N1 C3 1.36(3) . ?
N2 C8 1.386(14) . ?
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N4 C14 1.462(10) . ?
N4 C15 1.48(3) . ?
N5 C16 1.333(19) . ?
N5 C17 1.378(18) . ?
N5 C18 1.47(2) . ?
C1 C2 1.512(7) . ?
C2 C4 1.384(10) . ?
C2 C3 1.389(9) . ?
C3 C4 1.403(9) 2_655 ?
C4 C3 1.403(9) 2_655 ?
C4 H4 0.9300 . ?
C5 C6 1.493(7) . ?
C6 C7 1.395(8) . ?
C6 C8 1.399(9) . ?
C7 C8 1.387(9) 2_866 ?
C7 H7 0.9300 . ?
C8 C7 1.387(9) 2_866 ?
C9 O6 1.259(7) 2_766 ?
C9 C10 1.508(8) . ?
C10 C11 1.394(11) . ?
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C12 C11 1.379(11) 2_756 ?
C12 H12 0.9300 . ?
C14 H14A 0.9600 . ?
C14 H14B 0.9600 . ?
C14 H14C 0.9600 . ?
C15 H15A 0.9600 . ?
C15 H15B 0.9600 . ?
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C17 H17A 0.9600 . ?
C17 H17B 0.9600 . ?
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O3 Ce1 O7 82.77(17) 2_766 . ?
O5 Ce1 O7 136.23(19) . . ?
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O7 Ce1 O4 144.58(18) . . ?
O8 Ce1 O4 72.99(18) . . ?
O3 Ce1 O2 134.03(14) 2_766 . ?
O5 Ce1 O2 72.13(14) . . ?
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O7 Ce1 C5 149.37(19) . . ?
O8 Ce1 C5 90.58(18) . . ?
O4 Ce1 C5 24.36(14) . . ?
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C1 Ce1 C5 120.76(17) . . ?
O3 Ce1 Ce1 39.91(9) 2_766 2_766 ?
O5 Ce1 Ce1 65.64(10) . 2_766 ?
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O6 Ce1 Ce1 68.20(10) . 2_766 ?
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O8 Ce1 Ce1 135.43(13) . 2_766 ?
O4 Ce1 Ce1 83.59(9) . 2_766 ?
O2 Ce1 Ce1 136.64(11) . 2_766 ?
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C9 O6 Ce1 133.2(4) 2_766 . ?
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C13 N4 C15 122.4(19) . . ?
C14 N4 C15 113(2) . . ?
C16 N5 C17 125.2(15) . . ?
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O1 C1 C2 119.6(6) . . ?
O2 C1 C2 118.1(5) . . ?
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O2 C1 Ce1 61.1(3) . . ?
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C4 C2 C1 119.7(6) . . ?
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N1 C3 C2 135.3(14) . . ?
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C2 C4 C3 119.9(7) . 2_655 ?
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C3 C4 H4 120.0 2_655 . ?
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C8 C7 H7 119.3 2_866 . ?
C6 C7 H7 119.3 . . ?
N2 C8 C7 117.3(7) . 2_866 ?
N2 C8 C6 123.2(7) . . ?
C7 C8 C6 119.5(8) 2_866 . ?
O5 C9 O6 125.5(5) . 2_766 ?
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O6 C9 C10 117.3(5) 2_766 . ?
C11 C10 C12 119.4(7) . . ?
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C12 C11 N3 117.4(8) 2_756 . ?
C10 C11 N3 122.5(8) . . ?
C11 C12 C10 120.7(7) 2_756 . ?
C11 C12 H12 119.7 2_756 . ?
C10 C12 H12 119.7 . . ?
O7 C13 N4 135(2) . . ?
N4 C14 H14A 109.5 . . ?
N4 C14 H14B 109.5 . . ?
H14A C14 H14B 109.5 . . ?
N4 C14 H14C 109.5 . . ?
H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
N4 C15 H15A 109.5 . . ?
N4 C15 H15B 109.5 . . ?
H15A C15 H15B 109.5 . . ?
N4 C15 H15C 109.5 . . ?
H15A C15 H15C 109.5 . . ?
H15B C15 H15C 109.5 . . ?
O8 C16 N5 124.9(15) . . ?
N5 C17 H17A 109.5 . . ?
N5 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
N5 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
N5 C18 H18A 109.5 . . ?
N5 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
N5 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?

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 'x, y, z'
 '-x, -y, -z'

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_cell_angle_beta                  110.673(5)
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_cell_formula_units_Z             2
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Source'
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 DIAMOND (Brandenburg, 2006)
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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<b>30</b>, 565.

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-838.

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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
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 Refinement of F^2^ against ALL reflections.  The weighted R-
factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R
are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.7935(6) 0.2837(5) 0.1192(5) 0.0534(13) Uani 1 1 d . . .
O3 O 1.1220(5) 0.4440(6) 0.3000(5) 0.0586(14) Uani 1 1 d . . .
O4 O 1.1514(5) 0.5107(4) 0.4968(5) 0.0447(11) Uani 1 1 d . . .
O5 O 0.9290(6) 0.2810(4) 0.3971(5) 0.0583(15) Uani 1 1 d . . .
O6 O 0.9870(8) 0.6830(4) 0.3923(5) 0.0704(19) Uani 1 1 d . . .
O7 O 0.6903(8) 0.5650(8) 0.2286(8) 0.093(2) Uani 1 1 d . . .
O8 O 0.9148(8) 0.5564(6) 0.1254(6) 0.0725(18) Uani 1 1 d . . .
N1 N 1.326(4) 0.377(3) 0.271(3) 0.314(14) Uani 1 1 d U . .
N2 N 0.436(4) 0.126(3) 0.184(3) 0.334(17) Uiso 1 1 d . . .
N3 N 0.967(3) 0.088(3) 0.277(2) 0.286(12) Uani 1 1 d DU . .
C1 C 0.6833(7) 0.2418(7) 0.1388(7) 0.0478(17) Uani 1 1 d . . .
C2 C 0.5882(8) 0.1163(7) 0.0678(7) 0.0496(17) Uani 1 1 d . . .
C3 C 0.4695(11) 0.0673(10) 0.0872(10) 0.087(4) Uani 1 1 d . . .
C4 C 0.6203(10) 0.0499(9) -0.0214(10) 0.077(3) Uani 1 1 d . . .
H4 H 0.7003 0.0824 -0.0375 0.093 Uiso 1 1 calc R . .
C5 C 1.2017(7) 0.4797(7) 0.4149(7) 0.0466(16) Uani 1 1 d . . .
C6 C 1.3557(7) 0.4897(7) 0.4574(7) 0.0468(16) Uani 1 1 d . . .
C7 C 1.4095(8) 0.4314(10) 0.3816(8) 0.071(3) Uani 1 1 d . . .
C8 C 1.4454(8) 0.5558(9) 0.5737(9) 0.071(3) Uani 1 1 d . . .
H8 H 1.4088 0.5939 0.6255 0.085 Uiso 1 1 calc R . .
C9 C 0.9743(10) 0.2490(6) 0.5006(8) 0.057(2) Uani 1 1 d . . .
C10 C 0.9881(11) 0.1198(6) 0.4999(8) 0.065(2) Uani 1 1 d . . .
C11 C 0.9708(14) 0.0431(7) 0.3878(8) 0.083(4) Uani 1 1 d D . .
C12 C 1.0196(14) 0.0766(7) 0.6099(9) 0.086(4) Uani 1 1 d . . .
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H12 H 1.0350 0.1285 0.6846 0.103 Uiso 1 1 calc R . .
C13 C 0.628(3) 0.636(2) 0.198(3) 0.192(11) Uani 1 1 d D . .
C14 C 0.610(6) 0.694(4) 0.080(3) 0.42(2) Uani 1 1 d DU . .
H14A H 0.6196 0.7802 0.1023 0.624 Uiso 1 1 calc R . .
H14B H 0.5181 0.6547 0.0154 0.624 Uiso 1 1 calc R . .
H14C H 0.6818 0.6830 0.0491 0.624 Uiso 1 1 calc R . .
C15 C 0.602(6) 0.728(4) 0.289(4) 0.40(2) Uani 1 1 d DU . .
H15A H 0.6133 0.8064 0.2653 0.603 Uiso 1 1 calc R . .
H15B H 0.6691 0.7357 0.3740 0.603 Uiso 1 1 calc R . .
H15C H 0.5076 0.6985 0.2858 0.603 Uiso 1 1 calc R . .
C16 C 0.997(2) 0.634(2) 0.106(2) 0.157(7) Uani 1 1 d DU . .
C17 C 0.943(3) 0.688(3) -0.014(3) 0.264(13) Uani 1 1 d DU . .
H17A H 0.9428 0.7718 0.0100 0.396 Uiso 1 1 calc R . .
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H17C H 1.0042 0.6861 -0.0595 0.396 Uiso 1 1 calc R . .
C18 C 1.160(2) 0.663(3) 0.136(3) 0.232(12) Uani 1 1 d DU . .
H18A H 1.1846 0.5874 0.1217 0.348 Uiso 1 1 calc R . .
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0.01091(13)
O1 0.040(3) 0.052(3) 0.079(4) -0.032(3) 0.016(3) -0.001(2)
O2 0.050(3) 0.043(3) 0.050(3) -0.013(2) 0.014(2) -0.002(2)
O3 0.038(3) 0.085(4) 0.044(3) -0.005(3) 0.007(2) 0.022(3)
O4 0.030(2) 0.047(3) 0.052(3) -0.007(2) 0.014(2) 0.0133(19)
O5 0.078(4) 0.022(2) 0.054(3) 0.001(2) 0.003(3) 0.016(2)
O6 0.112(5) 0.023(2) 0.053(3) -0.002(2) 0.008(3) 0.017(3)
O7 0.069(4) 0.115(6) 0.120(6) 0.060(5) 0.034(4) 0.064(4)
O8 0.097(5) 0.052(3) 0.071(4) 0.019(3) 0.036(4) 0.015(3)
N1 0.314(14) 0.315(14) 0.314(14) 0.063(3) 0.122(5) 0.085(4)
N3 0.286(12) 0.285(12) 0.286(12) 0.058(3) 0.111(5) 0.077(3)
C1 0.038(3) 0.043(4) 0.043(4) -0.011(3) 0.002(3) 0.005(3)
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C3 0.064(6) 0.074(6) 0.093(7) -0.053(6) 0.036(5) -0.015(5)
C4 0.058(5) 0.066(6) 0.085(6) -0.037(5) 0.035(5) -0.015(4)
C5 0.034(3) 0.053(4) 0.051(4) 0.000(3) 0.014(3) 0.016(3)
C6 0.033(3) 0.053(4) 0.047(4) -0.007(3) 0.011(3) 0.012(3)
C7 0.035(4) 0.104(7) 0.053(5) -0.026(5) 0.008(3) 0.014(4)
C8 0.035(4) 0.092(7) 0.070(5) -0.030(5) 0.016(4) 0.018(4)
C9 0.080(6) 0.019(3) 0.054(4) 0.003(3) 0.007(4) 0.012(3)
C10 0.097(7) 0.021(3) 0.050(4) 0.001(3) 0.002(4) 0.014(4)
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C13 0.163(19) 0.18(2) 0.30(3) 0.13(2) 0.10(2) 0.125(17)
C14 0.42(2) 0.42(2) 0.42(2) 0.084(4) 0.161(8) 0.112(6)
C15 0.40(2) 0.40(2) 0.40(2) 0.081(4) 0.156(8) 0.108(6)
C16 0.157(7) 0.157(7) 0.157(7) 0.0316(17) 0.061(3) 0.042(2)
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C17 0.264(13) 0.264(13) 0.264(13) 0.054(3) 0.102(5) 0.071(4)
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 All esds (except the esd in the dihedral angle between two
l.s. planes)
 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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Ce1 O2 2.541(5) . ?
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Ce1 O4 2.726(5) . ?
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Ce1 C5 3.009(7) . ?
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O1 C1 1.251(9) . ?
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O5 C9 1.244(9) . ?
O6 C9 1.259(9) 2_766 ?
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O8 C16 1.20(2) . ?
N1 C7 1.26(3) . ?
N2 C3 1.42(4) . ?
N3 C11 1.416(10) . ?
C1 C2 1.503(9) . ?
C2 C3 1.354(13) . ?
C2 C4 1.385(11) . ?
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C5 C6 1.485(9) . ?
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C9 O6 1.259(9) 2_766 ?
C9 C10 1.506(9) . ?
C10 C12 1.365(12) . ?
C10 C11 1.405(12) . ?
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C12 C11 1.388(11) 2_756 ?
C12 H12 0.9300 . ?
C13 C15 1.531(10) . ?
C13 C14 1.541(10) . ?
C14 H14A 1.1473 . ?
C14 H14B 1.1503 . ?
C14 H14C 1.1477 . ?
C15 H15A 0.9630 . ?
C15 H15B 0.9632 . ?
C15 H15C 0.9632 . ?
C16 C17 1.547(10) . ?
C16 C18 1.562(10) . ?
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C17 H17B 0.9600 . ?
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O4 Ce1 O3 123.45(16) 2_766 . ?
O6 Ce1 O3 91.2(2) . . ?
O5 Ce1 O3 75.5(2) . . ?
O4 Ce1 O8 146.78(19) 2_766 . ?
O6 Ce1 O8 74.3(2) . . ?
O5 Ce1 O8 138.4(2) . . ?
O3 Ce1 O8 73.2(2) . . ?
O4 Ce1 O1 85.19(18) 2_766 . ?
O6 Ce1 O1 139.8(2) . . ?
O5 Ce1 O1 72.7(2) . . ?
O3 Ce1 O1 128.31(19) . . ?
O8 Ce1 O1 107.1(2) . . ?
O4 Ce1 O2 132.08(17) 2_766 . ?
O6 Ce1 O2 148.9(2) . . ?
O5 Ce1 O2 74.30(18) . . ?
O3 Ce1 O2 81.68(18) . . ?
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O1 Ce1 O2 51.11(17) . . ?
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C2 C3 N2 121.8(16) . . ?
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C6 C8 C7 122.2(7) . 2_866 ?
C6 C8 H8 118.9 . . ?
C7 C8 H8 118.9 2_866 . ?
O5 C9 O6 125.3(6) . 2_766 ?
O5 C9 C10 118.1(7) . . ?
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O7 C13 C14 127(3) . . ?
C15 C13 C14 105(3) . . ?
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C13 C14 H14B 128.2 . . ?
H14A C14 H14B 86.1 . . ?
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H14A C14 H14C 86.2 . . ?
H14B C14 H14C 86.0 . . ?
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C13 C15 H15B 110.0 . . ?
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C13 C15 H15C 110.0 . . ?
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;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A.,
Burla, M. C.,
Polidori, G. & Camalli, M. (1994). <i>J. Appl. Cryst.</i>
<b>27</b>, 435--436.

Farrugia, L. J. (1997). <i>ORTEP-3 for Windows</i>. <i>J.Appl.
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RED</i>. Oxford
Diffraction Ltd, Abingdon, Oxford, England.

Sheldrick, G. M. (1997). <i>SHELXL97</i>. University of
G\"ottingen, Germany.

Spek, A. L. (2008). <i>PLATON</i>. University of Utrecht, The
Netherlands.
;

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 Refinement of F^2^ against ALL reflections.  The weighted R-
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 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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O2 O 0.8401(11) 0.1941(11) 0.2767(12) 0.122(4) Uani 1 1 d . . .
O3 O 0.3814(10) 0.0487(10) 0.1971(10) 0.107(2) Uani 1 1 d . . .
O4 O 0.6520(9) 0.0108(8) 0.0039(10) 0.099(2) Uani 1 1 d . . .
O5 O 0.5022(14) -0.1805(9) 0.1085(11) 0.116(3) Uani 1 1 d . . .
O6 O 0.5738(11) 0.2152(8) 0.1064(10) 0.106(2) Uani 1 1 d . . .
O7 O 0.5901(16) -0.0558(11) 0.3699(12) 0.124(3) Uani 1 1
d . . .
O8 O 0.7950(15) -0.0688(17) 0.261(2) 0.157(6) Uani 1 1 d . . .
N1 N 1.075(6) 0.366(5) 0.334(7) 0.34(4) Uani 1 1 d . . .
N2 N 0.183(4) 0.146(7) 0.232(5) 0.34(4) Uani 1 1 d . . .
N3 N 0.472(7) -0.407(4) -0.217(3) 0.27(2) Uani 1 1 d D . .
C1 C 0.9102(14) 0.3824(14) 0.4313(15) 0.107(4) Uani 1 1 d . . .
C2 C 0.8754(18) 0.4526(19) 0.518(2) 0.133(6) Uani 1 1 d . . .
H2 H 0.7902 0.4214 0.5286 0.159 Uiso 1 1 calc R . .
C3 C 1.0322(19) 0.4309(19) 0.413(2) 0.131(6) Uani 1 1 d . . .
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C6 C 0.1445(13) 0.0077(13) 0.0422(15) 0.102(3) Uani 1 1 d . . .
C7 C 0.0497(15) -0.0615(19) -0.0742(17) 0.122(5) Uani 1 1
d . . .
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C8 C 0.0946(16) 0.071(2) 0.1183(18) 0.128(6) Uani 1 1 d . . .
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C9 C 0.4666(17) -0.2498(11) -0.0018(16) 0.106(4) Uani 1 1
d . . .
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d . . .
C11 C 0.511(3) -0.4253(14) 0.1097(18) 0.135(6) Uani 1 1 d . . .
H11 H 0.5205 -0.3756 0.1844 0.162 Uiso 1 1 calc R . .
C12 C 0.474(3) -0.4532(14) -0.1119(18) 0.136(7) Uani 1 1 d
D . .
C13 C 0.510(5) -0.138(4) 0.401(4) 0.218(19) Uani 1 1 d D . .
C14 C 0.344(5) -0.173(6) 0.352(6) 0.33(5) Uani 1 1 d D . .
H14A H 0.3087 -0.1290 0.2851 0.497 Uiso 1 1 calc R . .
H14B H 0.3173 -0.1489 0.4215 0.497 Uiso 1 1 calc R . .
H14C H 0.3047 -0.2614 0.3201 0.497 Uiso 1 1 calc R . .
C15 C 0.540(12) -0.237(12) 0.484(13) 0.79(19) Uani 1 1 d D . .
H15A H 0.6416 -0.2267 0.5208 1.190 Uiso 1 1 calc R . .
H15B H 0.4914 -0.3194 0.4324 1.190 Uiso 1 1 calc R . .
H15C H 0.5063 -0.2259 0.5519 1.190 Uiso 1 1 calc R . .
C16 C 0.849(6) -0.143(5) 0.277(6) 0.228(19) Uani 1 1 d D . .
C17 C 0.902(11) -0.229(8) 0.203(9) 0.53(11) Uani 1 1 d D . .
H17A H 0.8820 -0.2118 0.1182 0.798 Uiso 1 1 calc R . .
H17B H 0.8536 -0.3150 0.1966 0.798 Uiso 1 1 calc R . .
H17C H 1.0037 -0.2144 0.2464 0.798 Uiso 1 1 calc R . .
C18 C 0.880(10) -0.172(9) 0.412(7) 0.38(6) Uani 1 1 d D . .
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O2 0.088(5) 0.111(6) 0.141(8) -0.032(6) 0.037(5) 0.018(5)
O3 0.080(4) 0.112(6) 0.115(6) -0.003(5) 0.029(4) 0.025(4)
O4 0.078(4) 0.084(4) 0.126(6) -0.004(4) 0.037(4) 0.024(3)
O5 0.134(8) 0.077(4) 0.124(7) 0.009(4) 0.033(6) 0.039(5)
O6 0.113(6) 0.070(4) 0.113(6) -0.003(4) 0.025(5) 0.024(4)
O7 0.144(9) 0.097(6) 0.123(7) 0.026(5) 0.043(7) 0.033(6)
O8 0.108(7) 0.161(12) 0.212(16) 0.071(11) 0.048(9) 0.067(8)
N1 0.27(5) 0.24(5) 0.49(9) -0.07(5) 0.23(6) -0.03(4)
N2 0.15(2) 0.47(9) 0.31(5) -0.16(6) 0.04(3) 0.07(4)
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C4 0.084(6) 0.085(6) 0.109(8) -0.016(6) 0.014(5) 0.019(5)
C5 0.069(5) 0.081(6) 0.130(9) -0.005(6) 0.037(6) 0.018(4)
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C16 0.23(4) 0.20(3) 0.31(6) 0.10(4) 0.12(4) 0.13(3)
C17 0.39(12) 0.38(12) 1.0(3) 0.39(17) 0.35(17) 0.30(11)
C18 0.29(9) 0.37(11) 0.52(15) 0.25(12) 0.13(10) 0.14(8)

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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell esds is used for estimating esds involving
l.s. planes.
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O6 C9 1.25(2) 2_655 ?
O7 C13 1.26(5) . ?
O8 C16 1.10(4) . ?
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N2 C8 1.34(4) . ?
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C6 C7 1.36(2) . ?
C6 C8 1.37(2) . ?
C7 C8 1.38(2) 2 ?
C7 H7 0.9300 . ?
C8 C7 1.38(2) 2 ?
C9 O6 1.25(2) 2_655 ?
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O1 Gd1 C4 26.9(4) . . ?
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H15A C15 H15B 109.5 . . ?
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H15B C15 H15C 109.5 . . ?
O8 C16 C18 112(5) . . ?
O8 C16 C17 138(5) . . ?
C18 C16 C17 109(5) . . ?
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