checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ip407

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ip407

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Bond precision:  C-C = 0.0117 A          Wavelength=0.71073

Cell:           a=10.049(2)       b=11.337(2)      c=14.471(3)
                alpha=82.53(3)    beta=83.02(3)    gamma=73.74(3)
Temperature:    153 K

                Calculated                Reported
Volume          1563.0(6)                 1562.9(5)
Space group     P -1                      P-1
Hall group      -P 1                      ?
Moiety formula  C56 H92 Cl2 N8 Nd2 O2     ?
Sum formula     C56 H92 Cl2 N8 Nd2 O2     C56 H92 Cl2 N8 Nd2 O2
Mr              1268.76                   1268.76
Dx,g cm-3       1.348                     1.348
Z               1                         1
Mu (mm-1)       1.771                     1.771
F000            654.0                     654.0
F000'           654.06
h,k,lmax        13,15,19                  13,15,19
Nref            8448                      8340
Tmin,Tmax                                 0.318,0.334
Tmin'

Correction method= SPHERE

Data completeness= 0.987          Theta(max)= 29.170

R(reflections)= 0.0547( 8022)     wR2(reflections)= 0.1663( 8340)

S = 1.219                 Npar= Npar = 324
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT971_ALERT_2_B Check Calcd Residual Density 0.82A From Nd 3.45 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density 0.97A From Nd 3.39 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density 0.78A From Nd -2.84 eA-3
PLAT972_ALERT_2_B Check Calcd Residual Density 0.85A From Nd -2.63 eA-3

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C25 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C24 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0117 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C25 - C26 ... 1.43 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 4.715 Check
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) ..... 5 Why ?
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 63 Why ?
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 22 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) . 3 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 10.15
PLAT971_ALERT_2_C Check Calcd Residual Density 1.27A From O 2.14 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.11A From Nd 1.98 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.22A From Nd 1.82 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.35A From Nd 1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.83A From C30 -1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.76A From Nd -1.78 eA-3

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 14.14 Why ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.03000 Degree
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C1 - C2 ... 1.44 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C21 - C22 ... 1.46 Ang.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 117 Do !
N2 -C1 -C2 -C3 -63.00 19.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 118 Do !
N1 -C1 -C2 -C3 111.00 19.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 119 Do !
ND -C1 -C2 -C3 21.00 19.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 120 Do !
C1 -C2 -C3 -C4 43.00 84.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 121 Do !
C2 -C3 -C4 -C6 16.00 0.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 122 Do !
C2 -C3 -C4 -C5 -93.00 74.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 165 Do !
N3 -C21 -C22 -C23 18.00 0.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 166 Do !
N4 -C21 -C22 -C23 1.00 21.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 167 Do !
ND -C21 -C22 -C23 -84.00 21.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 168 Do !
C21 -C22 -C23 -C24 35.00 36.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 169 Do !
C22 -C23 -C24 -C25 1.00 20.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 170 Do !
C22 -C23 -C24 -C26 -68.00 20.00 1.555 1.555 1.555 1.555
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 36 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

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  4 ALERT level B = A potentially serious problem, consider carefully
 17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 18 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
 13 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/02/2014; check.def file version of 05/02/2014

Datablock ip407 - ellipsoid plot