checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SCD23_110_R-3_sq

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: SCD23_110_R-3_sq

Bond precision: C-C = 0.0122 A Wavelength=0.71073

Cell: a=31.8437(6) b=31.8437(6) c=19.8704(9)
alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	17449.6(10)	17449.5(10)
Space group	R -3	R -3 :H
Hall group	-R 3	-R 3
Moiety formula	C162 H138 N36 Nd6 O42 [+ solvent]	C162 H138 N36 Nd6 O42 [+ solvent]
Sum formula	C162 H138 N36 Nd6 O42 [+ solvent]	C162 H138 N36 Nd6 O42 [+ solvent]
Mr	4126.53	4126.53
Dx,g cm-3	1.178	1.178
Z	3	3
Mu (mm-1)	1.379	1.379
F000	6174.0	6174.0
F000'	6172.92	
h,k,lmax	39,39,24	39,39,24
Nref	7616	5911
Tmin,Tmax	0.743,0.876	0.372,0.499
Tmin'	0.728	

Correction method= # Reported T Limits: Tmin=0.372 Tmax=0.499
AbsCorr = EMPIRICAL

Data completeness= 0.776 Theta(max)= 25.992

R(reflections)= 0.0390(4852)

wR2(reflections)= 0.1107(5911)

S = 1.091 Npar= 378

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

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 1645 Report

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Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C3 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C3 --C4 . 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Nd1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C26 Check
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O7 -H8W . 83.32 Degree
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01222 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C22 - C26 . 1.53 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -3.173 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From O7 . -0.67 eA-3

Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 3
From the CIF: _chemical_formula_sum C162 H138 N36 Nd6 O42 [+ solvent]
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	486.00	486.00	0.00
H	414.00	414.00	0.00
N	108.00	108.00	0.00
Nd	18.00	18.00	0.00
O	126.00	126.00	0.00
[+	3.00	0.00	3.00
solve	3.00	0.00	3.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.987 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 132.28 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Nd1 --O2 . 6.0 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact C27 ..C27 . 3.15 Ang.
5/3-x,1/3-y,4/3-z = 13_656 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Nd1 (III) . 3.65 Info

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PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         60 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         13 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  14 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  16 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   2 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* or *IUCrData*, 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 06/07/2023; check.def file version of 30/06/2023

Datablock SCD23_110_R-3_sq - ellipsoid plot