checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SCD22_118_Fddd_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: SCD22_118_Fddd_sq

```
Bond precision:   C-C = 0.0149 A          Wavelength=0.71073

Cell:             a=13.9439(6)     b=30.2750(15)     c=31.0542(15)
                  alpha=90         beta=90           gamma=90
Temperature:      296 K
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	Calculated	Reported
Volume	13109.6(11)	13109.6(11)
Space group	F d d d	F d d d
Hall group	-F 2uv 2vw	-F 2uv 2vw
Moiety formula	C44 H40 N14 Nd2 O10 [+ solvent]	C44 H40 N14 Nd2 O10 [+ANIONS + solvent]
Sum formula	C44 H40 N14 Nd2 O10 [+ solvent]	C44 H40 N14 Nd2 O10 [+ANIONS + solvent]
Mr	1213.38	1213.38
Dx,g cm-3	1.230	1.230
Z	8	8
Mu (mm-1)	1.619	1.619
F000	4816.0	4816.0
F000'	4814.56	
h,k,lmax	17,37,38	17,37,38
Nref	3236	3205
Tmin,Tmax	0.947,0.960	0.452,0.499
Tmin'	0.930	

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Correction method= # Reported T Limits: Tmin=0.452 Tmax=0.499
AbsCorr = EMPIRICAL

Data completeness= 0.990           Theta(max)= 26.000
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R(reflections)= 0.0994(1868) wR2(reflections)= 0.3252(3205)

S = 1.148 Npar= 161

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

```
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Nd1      --O1       .       10.3 s.u.
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Nd1      --N1       .       11.2 s.u.
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Nd1      --N3       .       11.0 s.u.
```

Alert level C

```
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.33 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O3       --N4       .        5.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2       --N4       .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Nd1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01491 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C10      - C11      .       1.53 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C44 H40 N14 Nd2 O10
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -10.256 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.194 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         30 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          4 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.07Ang From C11             1.55 eA-3
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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    8
           From the CIF: _chemical_formula_sum  C44 H40 N14 Nd2 O10 [+anions + sol
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        352.00    352.00    0.00
           H        320.00    320.00    0.00
           N        112.00    112.00    0.00
           Nd        16.00     16.00    0.00
           O         80.00     80.00    0.00
           [+ani      8.00      0.00    8.00
           +          8.00      0.00    8.00
           solve      8.00      0.00    8.00
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Nd1      --O2       .        7.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Nd1      --N2       .        9.0 s.u.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
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PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         31 Note
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
   3 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
   4 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* 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 12/09/2022; check.def file version of 09/08/2022

Datablock SCD22_118_Fddd_sq - ellipsoid plot