# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SE_S36

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: SE_S36

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Bond precision: C-C = 0.0037 A Wavelength=1.54178

Cell: a=23.4801(3) b=23.6834(2) c=24.6001(3)
alpha=75.386(1) beta=70.306(1) gamma=67.900(1)
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 11809.2(3) | 11809.2(3) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | 2(C40 H52 N6 O), C40 H50 N6, 3(C40 H43 N3 O3), 2(C6 H14) [+ sol | 3(C40 H43 N3 O3), 2(C40 H52 N6 O), C40 H50 N6, 2(C6 H14), 2[C6H |
| Sum formula | C252 H311 N27 O11 [+ solvent] | C264 H339 N27 O11 |
| Mr | 3894.28 | 4066.60 |
| Dx,g cm-3 | 1.095 | 1.144 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.523 | 0.541 |
| F000 | 4200.0 | 4400.0 |
| F000' | 4211.15 | |
| h,k,lmax | 29,29,31 | 29,28,30 |
| Nref | 49956 | 46453 |
| Tmin,Tmax | 0.878,0.922 | 0.866,1.000 |
| Tmin' | 0.873 | |

Correction method= # Reported T Limits: Tmin=0.866 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.930 Theta(max)= 77.035

R(reflections)= 0.0617( 38127)

wR2(reflections)= 0.1787( 46453)

S = 1.015 Npar= 2727

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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.

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**Alert level B**

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 0.87 eA-3

**Author Response: Arises from unmodelled minor disorder of macrocycle linker.**

PLAT417_ALERT_2_B Short Inter D-H..H-D H00N ..H00S . 1.96 Ang.
x,y,z = 1_555 Check

**Author Response: Arises from intra- and inter-molecular H-bonded hydroxy groups of a single rotaxane of the structure which are geometrically close.**

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**Alert level C**

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -0.638
Test value = -0.600
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -0.64 eA-3
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C07M Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C045 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C07X 0.174 Check
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C07M - C07R . 1.38 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.844 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 286 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.53Ang From O013 . -0.63 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.42Ang From O00N . -0.51 eA-3

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**Alert level G**

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C264 H339 N27 O11
Atom count from the _atom_site data: C252 H311 N27 O11
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

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 symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z    2
From the CIF: _chemical_formula_sum  C264 H339 N27 O11
TEST: Compare cell contents of formula and atom_site data

atom    Z*formula  cif sites diff
C        528.00    504.00   24.00
H        678.00    622.00   56.00
N         54.00     54.00    0.00
O         22.00     22.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         16 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          5 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.20 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         13 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         6% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )         9% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H034     ..H5A      .       2.08 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H05R     ..H2A      .       2.06 Ang.
                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O003     ..C026     .       2.96 Ang.
                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C032     ..C03D     .       3.13 Ang.
                                                    x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        516 Note
PLAT793_ALERT_4_G Model has Chirality at C024        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C02H        (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C03L        (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C04R        (Centro SPGR)          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         49 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       3042 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.5 Low
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
  2 **ALERT level B** = A potentially serious problem, consider carefully
 16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 29 **ALERT level G** = General information/check it is not something unexpected

  7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
 11 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.

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**PLATON version of 12/09/2022; check.def file version of 09/08/2022**

**Datablock SE_S36** - ellipsoid plot