# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PRG-I-85_D2_Ep_Boc

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: PRG-I-85_D2_Ep_Boc

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Bond precision: C-C = 0.0061 A Wavelength=1.54184

Cell: a=19.0015(1) b=19.5618(2) c=19.8094(2)
alpha=90 beta=102.508(1) gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 7188.46(11) | 7188.46(11) |
| Space group | P 21 | P 1 21 1 |
| Hall group | P 2yb | P 2yb |
| Moiety formula | C40 H59 N7 O2, C32 H34 N2 O3 S [+ solvent] | C72 H93 N9 O5 S |
| Sum formula | C72 H93 N9 O5 S [+ solvent] | C72 H93 N9 O5 S |
| Mr | 1196.61 | 1196.61 |
| Dx,g cm-3 | 1.106 | 1.106 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.811 | 0.811 |
| F000 | 2576.0 | 2576.0 |
| F000’ | 2584.20 | |
| h,k,lmax | 23,23,24 | 23,23,24 |
| Nref | 27504[ 14184] | 22005 |
| Tmin,Tmax | 0.881,0.956 | 0.845,1.000 |
| Tmin’ | 0.678 | |

Correction method= # Reported T Limits: Tmin=0.845 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.55/0.80 Theta(max)= 70.476

R(reflections)= 0.0496( 18788) wR2(reflections)= 0.1425( 22005)

S = 1.068 Npar= 1597

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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 C

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        4.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        5.0 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N202     --N203     .        5.5 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C26 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C211 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C225 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00613 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        19 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage        60 %
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
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## Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .     0.027 Note
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       172 A**3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
             C40 H59 N7 O2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         4 Note
             C32 H34 N2 O3 S
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        61 Note
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).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       204 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         2 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   7 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.

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**PLATON version of 13/07/2021; check.def file version of 13/07/2021**

**Datablock PRG-I-85_D2_Ep_Boc** - ellipsoid plot