checkCIF/PLATON report

Structure factors have been supplied for datablock(s) JMIX076_C3P_2

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: JMIX076_C3P_2

Bond precision: C-C = 0.0024 A Wavelength=1.54184

Cell: a=11.4186(1) b=15.1215(1) c=20.0942(1)
alpha=95.432(1) beta=100.146(1) gamma=105.079(1)
Temperature: 100 K

	Calculated	Reported
Volume	3261.51(5)	3261.51(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H49 N7 O6, C32 H34 N2 O3 S, C H4 O	C32 H34 N2 O3 S, C36 H49 N7 O6, C H4 O
Sum formula	C69 H87 N9 O10 S	C69 H87 N9 O10 S
Mr	1234.54	1234.53
Dx,g cm-3	1.257	1.257
Z	2	2
Mu (mm-1)	0.971	0.971
F000	1320.0	1320.0
F000'	1324.48	
h,k,lmax	13,18,24	13,18,24
Nref	12456	12119
Tmin,Tmax	0.793,0.890	0.869,1.000
Tmin'	0.701	

Correction method= # Reported T Limits: Tmin=0.869 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.973 Theta(max)= 70.468

R(reflections)= 0.0468(11641) wR2(reflections)= 0.1144(12119)

S = 1.035 Npar= 818

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C126 --C127 . 7.5 s.u.

Author Response: Disorder of the sulfoxide appears to have affected the thermal ellipsoids of some of the surrounding alkyl chain atoms. Nevertheless, the atom assignments presented are in agreement with all other experimental data, and thus this is not indicative of an incorrect atom type.

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.49 Report
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C36 H49 N7 O6
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.096 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 145 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 26 Note

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes are Equal ..(Note) 0.0001 Ang.
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 3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for S124 --O125 . 6.4 s.u.

Author Response: Disorder of the sulfoxide appears to have affected the thermal ellipsoids of some of the surrounding alkyl chain atoms. Nevertheless, the atom assignments presented are in agreement with all other experimental data, and thus this is not indicative of an incorrect atom type.

PLAT230_ALERT_2_G Hirshfeld Test Diff for S124 --C123 . 10.3 s.u.

Author Response: Disorder of the sulfoxide appears to have affected the thermal ellipsoids of some of the surrounding alkyl chain atoms. Nevertheless, the atom assignments presented are in agreement with all other experimental data, and thus this is not indicative of an incorrect atom type.

PLAT230_ALERT_2_G Hirshfeld Test Diff for S124 --C126 . 15.5 s.u.

Author Response: Disorder of the sulfoxide appears to have affected the thermal ellipsoids of some of the surrounding alkyl chain atoms. Nevertheless, the atom assignments presented are in agreement with all other experimental data, and thus this is not indicative of an incorrect atom type.

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PLAT230_ALERT_2_G Hirshfeld Test Diff for    S1       --O125     .        5.1 s.u.
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Author Response: Disorder of the sulfoxide appears to have affected the thermal ellipsoids of some of the surrounding alkyl chain atoms. Nevertheless, the atom assignments presented are in agreement with all other experimental data, and thus this is not indicative of an incorrect atom type.

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PLAT230_ALERT_2_G Hirshfeld Test Diff for    S1       --C123     .       19.5 s.u.
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Author Response: Disorder of the sulfoxide appears to have affected the thermal ellipsoids of some of the surrounding alkyl chain atoms. Nevertheless, the atom assignments presented are in agreement with all other experimental data, and thus this is not indicative of an incorrect atom type.

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PLAT300_ALERT_4_G Atom Site Occupancy of S124       Constrained at       0.83 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S1         Constrained at       0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12C       Constrained at       0.83 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12D       Constrained at       0.83 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12G       Constrained at       0.83 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12H       Constrained at       0.83 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12E       Constrained at       0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12F       Constrained at       0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12I       Constrained at       0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12J       Constrained at       0.17 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )         3% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H12A     ..H12F     .       2.11 Ang.
                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C6       ..C130             3.19 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          2 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C32 H34 N2 O3 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             C H4 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        192 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  31 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 17 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 13/07/2021; check.def file version of 13/07/2021

Datablock JMIX076_C3P_2 - ellipsoid plot