

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shengyi1cult_auto

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: shengyi1cult_auto

Bond precision: C-C = 0.0025 Å Wavelength=1.54184

Cell: a=14.7786(5) b=15.3778(4) c=16.3190(5)
 alpha=62.436(3) beta=66.796(3) gamma=72.923(3)
Temperature: 100 K

	Calculated	Reported
Volume	2993.44(18)	2993.46(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C41 H21 N5 O [+ solvent]	C41 H21 N5 O
Sum formula	C41 H21 N5 O [+ solvent]	C41 H21 N5 O
Mr	599.63	599.63
Dx, g cm ⁻³	1.331	1.331
Z	4	4
Mu (mm ⁻¹)	0.651	0.651
F000	1240.0	1240.0
F000'	1243.54	
h, k, lmax	18, 19, 20	18, 18, 20
Nref	12676	12106
Tmin, Tmax	0.901, 0.907	0.837, 1.000
Tmin'	0.901	

Correction method= # Reported T Limits: Tmin=0.837 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.955 Theta(max)= 76.957

R(reflections)= 0.0471(10892)	wR2(reflections)=
S = 1.071	0.1139(12106)
Npar= 973	

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

PLAT410_ALERT_2_B Short Intra H...H Contact H3A ..H28A . 1.87 Ang.
x,y,z = 1_555 Check

Author Response: The assignment of the titled atoms are checked carefully and confirmed that they are correct.



Alert level C

PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C14C -C19C . 1.37 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H12 ..H25 . 1.93 Ang.
x,y,z = 1_555 Check

Author Response: The assignment of the titled atoms are checked carefully and confirmed that they are correct.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.805 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 82 Report



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 23 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 6 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 23 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C39A --C41A . 5.4 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.88 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1C Constrained at 0.12 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of C14	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19	Constrained at	0.88	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19B	Constrained at	0.45	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		15%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)		15%	Note
PLAT411_ALERT_2_G	Short Inter H...H Contact H4A ..H16C .		2.13	Ang.
	1+x,y,-1+z =	1_654		Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H4A ..H17C .		2.01	Ang.
	1+x,y,-1+z =	1_654		Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1C ..C41A .		2.88	Ang.
	x,y,z =	1_555		Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4A ..C16C .		3.03	Ang.
	1+x,y,-1+z =	1_654		Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4A ..C17C .		3.09	Ang.

		1+x,y,-1+z =	1_654	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C41A ..C19C .	3.05	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C41A ..C14C .	3.16	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C42A ..C19C .	3.10	Ang.
		x,y,z =	1_555	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		110	A**3
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		354	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		444	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		16	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 88 **ALERT level G** = General information/check it is not something unexpected

1 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
 20 ALERT type 3 Indicator that the structure quality may be low
 56 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

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.

