

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shengyi8cult_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: shengyi8cult_auto

Bond precision:	C-C = 0.0016 Å	Wavelength=1.54184	
Cell:	a=11.37795 (11)	b=7.57095 (7)	c=39.0727 (3)
	alpha=90	beta=94.7078 (9)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	3354.44 (5)	3354.44 (5)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C22 H12 N4	C22 H12 N4	
Sum formula	C22 H12 N4	C22 H12 N4	
Mr	332.36	332.36	
Dx, g cm ⁻³	1.316	1.316	
Z	8	8	
Mu (mm ⁻¹)	0.639	0.639	
F000	1376.0	1376.0	
F000'	1379.86		
h, k, lmax	14, 9, 48	14, 9, 48	
Nref	6889	6720	
Tmin, Tmax	0.774, 0.826	0.857, 1.000	
Tmin'	0.774		

Correction method= # Reported T Limits: Tmin=0.857 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.975 Theta(max)= 74.678

R(reflections)= 0.0338 (6019)	wR2(reflections)=
S = 1.021	0.0872 (6720)
Npar= 524	

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 C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Sth/L= 0.600 21 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	13	Report
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00007	Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00030	Ang.
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	17	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	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
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
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 C4A --C7A .	8.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C5A --C8A .	6.6	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C4 --C7 .	6.5	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C5 --C8 .	6.1	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of C21A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26A Constrained at	0.56	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25B Constrained at	0.44	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26B Constrained at	0.44	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	23%	Note

PLAT411_ALERT_2_G	Short Inter H...H Contact	H12	..H25B	.	2.05	Ang.
			x,y,z =		1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C2A	..C23A	.	3.14	Ang.
			1-x,2-y,1-z =		3_676	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				171	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			145	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF				1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				3.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				24	Info

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

0 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
 18 ALERT type 3 Indicator that the structure quality may be low
 28 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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock shengyi8cult_auto - ellipsoid plot

