

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) LGG_TDI_8_6TH_0m_sq_sq_sq

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: LGG_TDI_8_6TH_0m_sq_sq_sq

Bond precision: C-C = 0.0115 Å Wavelength=1.54178

Cell: a=14.1622 (18) b=40.113 (6) c=44.706 (6)
 alpha=112.494 (6) beta=92.089 (5) gamma=99.573 (5)
Temperature: 180 K

	Calculated	Reported
Volume	22998 (6)	22998 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C118 H88 N4 O8 [+ solvent]	?
Sum formula	C118 H88 N4 O8 [+ solvent]	C118 H88 N4 O8
Mr	1689.93	1689.92
Dx, g cm ⁻³	0.976	0.976
Z	8	8
Mu (mm ⁻¹)	0.480	0.480
F000	7104.0	7104.0
F000'	7124.24	
h, k, lmax	15, 44, 49	15, 44, 49
Nref	66812	66478
Tmin, Tmax	0.944, 0.953	0.536, 0.752
Tmin'	0.908	

Correction method= # Reported T Limits: Tmin=0.536 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 59.299

R(reflections)= 0.1186 (26939)	wR2(reflections)=
S = 1.198	0.3187 (66478)
Npar= 4658	

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

THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\text{wavelength}$ is less than 0.575

Calculated $\sin(\theta_{\max})/\text{wavelength} = 0.5577$

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01146 Ang.



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.122

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.122	Report
PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	41%	Check
PLAT082_ALERT_2_C	High R1 Value	0.12	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.32	Report
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 3 C Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 4 C Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range	4.2	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 3 H Uiso(max)/Uiso(min) Range	4.4	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 4 H Uiso(max)/Uiso(min) Range	5.2	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5_2	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C16_3	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5_4	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C16_4	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5_5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C49_5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5_6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C49_6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5_8	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C16_8	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C7_1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C47_1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C48_1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C53_1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56_1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56_2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1_3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C7_3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C10_3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C47_3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56_3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C6_4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C7_4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C10_4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56_4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C7_5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C10_5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C48_5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56_5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C2_6	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C7_6	Check

PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10_6	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C47_6	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C56_6	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C7_7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10_7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C48_7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C56_7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10_8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C46_8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C47_8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C48_8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C53_8	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C56_8	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	O1_1	0.139	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	O1_3	0.148	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	O1_5	0.167	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	O1_7	0.159	Check
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H26_7 ..H43_8 .	1.95	Ang.
			x,y,z =	1_555	Check
PLAT411_ALERT_2_C	Short	Inter H...H Contact	H5_1 ..H4_6 .	2.02	Ang.
			x,y,z =	1_555	Check
PLAT413_ALERT_2_C	Short	Inter XH3 .. XHn	H55B_6 ..H51_7 .	2.14	Ang.
			1+x,y,z =	1_655	Check
PLAT905_ALERT_3_C	Negative	K value in the Analysis of Variance	...	-19.453	Report
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.558	336	Report
PLAT918_ALERT_3_C	Reflection(s)	with I(obs) much Smaller I(calc)	.	1	Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	520	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	520	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	20.00	Why ?
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C18_1 -C31_1 .	1.44	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C18_3 -C31_3 .	1.44	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C18_4 -C31_4 .	1.44	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C18_5 -C31_5 .	1.44	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C28_6 -C41_6 .	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C18_8 -C31_8 .	1.44	Ang.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	872	Note
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4	Please	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	9376	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).	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	26	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

68 ALERT type 2 Indicator that the structure model may be wrong or deficient
14 ALERT type 3 Indicator that the structure quality may be low
6 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.

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