

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lng_a

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: lng_a

Bond precision:	C-C = 0.0065 A	Wavelength=0.71073	
Cell:	a=10.609 (5)	b=12.079 (4)	c=22.527 (6)
	alpha=99.318 (9)	beta=98.930 (12)	gamma=94.48 (2)
Temperature:	100 K		
	Calculated	Reported	
Volume	2798.3 (18)	2798.3 (18)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C41 H44 F28 Gd Li O17	C41 H44 F28 Gd Li O16.68, 0.32 (O)	
Sum formula	C41 H44 F28 Gd Li O17	C41 H44 F28 Gd Li O17	
Mr	1504.95	1504.95	
Dx, g cm ⁻³	1.786	1.786	
Z	2	2	
Mu (mm ⁻¹)	1.343	1.343	
F000	1490.0	1490.0	
F000'	1491.09		
h, k, lmax	16, 18, 34	16, 18, 34	
Nref	21685	18970	
Tmin, Tmax	0.923, 0.935	0.624, 0.747	
Tmin'	0.851		

Correction method= # Reported T Limits: Tmin=0.624 Tmax=0.747
AbsCorr = MULTI SCAN

Data completeness= 0.875 Theta (max)= 33.336

R(reflections)= 0.0572 (15394)

wR2(reflections)=
0.1325 (18970)

S = 1.082

Npar= 947

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

PLAT220_ALERT_2_B	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	10.0	Ratio
PLAT242_ALERT_2_B	Low	'MainMol'		Ueq as Compared to Neighbors of	017	Check

Alert level C

PLAT213_ALERT_2_C	Atom C37			has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1	F	Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1	O	Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	10.0	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O8A	--C20	.	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O16A	--C38	.	0.16	Ang.
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)			016A	Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4				Please	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			3.196	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			78	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers			..	1	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.92Ang		From O5	-2.50	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H38A	.		-0.37	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H38B	.		-0.33	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H40A	.		-0.31	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H40C	.		-0.38	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				26	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...			13	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large				8.46	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				2	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records				1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records				3	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records				3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records				6	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par				0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar				0.0020	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par				0.0050	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par				0.0020	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar				0.0040	Report
PLAT242_ALERT_2_G	Low	'MainMol'		Ueq as Compared to Neighbors of	C6	Check
PLAT242_ALERT_2_G	Low	'MainMol'		Ueq as Compared to Neighbors of	C16	Check
PLAT242_ALERT_2_G	Low	'MainMol'		Ueq as Compared to Neighbors of	C26	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)			17%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)			04A	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)			08A	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)			011A	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O16	.			108.1	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F26	..C40	.	2.51	Ang.
			x,1+y,z =		1_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F27	..C40	.	2.82	Ang.
			x,1+y,z =		1_565	Check

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6	..F6	.	2.62	Ang.
		-x,-y,-z =		2_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6	..F18	.	2.76	Ang.
		-1+x,-1+y,z =		1_445	Check
PLAT793_ALERT_4_G	Model has Chirality at C7	(Centro SPGR)		S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C36	(Centro SPGR)		R	Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd1	(III)	.	3.40	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			115	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please	Do !
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			2635	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			1.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			1	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 27 ALERT type 2 Indicator that the structure model may be wrong or deficient
 13 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

