

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20250508sl-r-rh_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: 20250508sl-r-rh_auto

Bond precision:	C-C = 0.0063 A	Wavelength=1.54184	
Cell:	a=12.1490 (1) alpha=90	b=12.3348 (1) beta=90	c=22.9651 (2) gamma=90
Temperature:	109 K		
	Calculated	Reported	
Volume	3441.45 (5)	3441.45 (5)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C36 H35 Cl N3 O Rh, C H Cl3	C36 H35 Cl N3 O Rh, C H Cl3	
Sum formula	C37 H36 Cl4 N3 O Rh	C37 H36 Cl4 N3 O Rh	
Mr	783.40	783.40	
Dx, g cm-3	1.512	1.512	
Z	4	4	
Mu (mm-1)	7.140	7.140	
F000	1600.0	1600.0	
F000'	1609.48		
h,k,lmax	15,15,28	15,15,28	
Nref	7154 [4004]	6757	
Tmin,Tmax	0.300,0.343	0.264,1.000	
Tmin'	0.192		

Correction method= # Reported T Limits: Tmin=0.264 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.94 Theta(max)= 75.633

R(reflections)= 0.0309 (6692)	wR2(reflections)= 0.0766 (6757)
S = 1.021	Npar= 417

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

PLAT214_ALERT_2_C	Atom Cl2	(Anion/Solvent) ADP max/min Ratio	4.8	prolat
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C37	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl2	0.120	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H26A ..H29A .	1.99	Ang.
		x,y,z =	1_555	Check
PLAT411_ALERT_2_C	Short Inter H...H Contact	H20 ..H29B .	2.13	Ang.
		1-x,-1/2+y,3/2-z =	3_646	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	5	Report
	7 10 0, 7 10 1, 0 2 2, 0 8 17, 0 6 20,			



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	6.91	Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00010	Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00020	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1 ..C37 .	3.00	Ang.
		x,y,z =	1_555	Check
PLAT791_ALERT_4_G	Model has Chirality at C1	(Sohncke SpGr)		R Verify
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
	0 0 2,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	105	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
	0 2 2,			
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.695	Note
	Predicted wR2: Based on SigI**2	1.63 or SHELX Weight	7.50	
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
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
5 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.

