

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Imm28

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: Imm28

Bond precision:	C-C = 0.0060 A	Wavelength=1.54184
Cell:	a=25.6890 (5) alpha=90	b=8.1881 (2) beta=98.540 (2) c=20.2875 (5) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4220.04 (17)	4220.04 (17)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C18 H36 K N2 O6, C12 H8 Br2 N4, 2 (C4 H8 O)	C12 H8 Br2 N4, C18 H36 K N2 O6, 2 (C4 H8 O)
Sum formula	C38 H60 Br2 K N6 O8	C38 H60 Br2 K N6 O8
Mr	927.82	927.84
Dx, g cm ⁻³	1.460	1.460
Z	4	4
Mu (mm ⁻¹)	3.784	3.784
F000	1932.0	1932.0
F000'	1932.95	
h, k, lmax	32, 10, 25	32, 10, 25
Nref	4434	4384
Tmin, Tmax	0.695, 0.815	0.166, 1.000
Tmin'	0.377	

Correction method= # Reported T Limits: Tmin=0.166 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 76.394

R(reflections)= 0.0712 (4093)

wR2(reflections)=
0.1906 (4384)

S = 1.146

Npar= 344

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		Please Check
	Calc: C18 H36 K N2 O6, C12 H8 Br2 N4, 2(C4 H8 O)		
	Rep.: C12 H8 Br2 N4, C18 H36 K N2 O6, 2(C4 H8 O)		
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	04	0.145 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	05	0.145 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		5.790 Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H1HA	.	-0.38 eA-3



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 U(i,j) Restrained non-H-Atoms		28 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		21.23 Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		1 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		6 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records		2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		13 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		4 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records		4 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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	21.42	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	4.58	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)	8.44	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)	4.56	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4	98.2	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O5	104.8	Degree
PLAT411_ALERT_2_G	Short Inter H...H Contact H1DA ..H19A	2.04	Ang.
	1-x,-y,1-z =	5_656	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	16	Note
	H1AA H1AB H1BA H1BB H1CA H1CB H1DA H1DB		
	H1EA H1EB H1FA H1FB H1GA H1GB H1HA H1HB		
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	622	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	49	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	5.547	Note
	Predicted wR2: Based on SigI**2 3.44 or SHELX Weight 16.63		
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

5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
32 **ALERT level G** = General information/check it is not something unexpected

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

