

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UM4139

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: UM4139

Bond precision: C-C = 0.0070 Å

Wavelength=0.71073

Cell: a=15.414(4) b=16.050(5) c=18.165(5)
 alpha=64.669(7) beta=69.128(6) gamma=76.782(7)
Temperature: 210 K

	Calculated	Reported
Volume	3779.8(19)	3779.9(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C66 H68 N8 O16, 0.412(C3), 0.514(C) [+ solvent]	C66 H68 N8 O16, [+ solvent]
Sum formula	C67.75 H68 N8 O16 [+ solvent]	C67.75 H68 N8 O16
Mr	1250.30	1250.30
Dx, g cm ⁻³	1.099	1.099
Z	2	2
Mu (mm ⁻¹)	0.079	0.079
F000	1317.0	1317.0
F000'	1317.66	
h, k, lmax	18, 19, 21	18, 19, 21
Nref	13315	13305
Tmin, Tmax	0.968, 0.988	0.826, 0.993
Tmin'	0.959	

Correction method= # Reported T Limits: Tmin=0.826 Tmax=0.993
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 24.999

R(reflections)= 0.0856(6795)

wR2(reflections)=
0.1633(13305)

S = 1.366

Npar= 921

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	4.7	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	5.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O89	--C90	.	0.17	Ang.
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	O89	Check	
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.00705	Ang.	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			12.856	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			2.169	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			3.515	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			2.128	Check	
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			8	Note	
	1 0 0, -1 1 0, 0 1 0, 1 1 0, 0 0 1,			1 0 1,		
	0 1 1, 1 1 1,					
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595		2	Report	
	2 1 1, 3 1 1,					



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C67.75 H68 N8 O16
Atom count from _chemical_formula_moiety:C66 H68 N8 O16

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	22	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	30	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
	Calc: C66 H68 N8 O16, 0.412(C3), 0.514(C)		
	Rep.: C66 H68 N8 O16,		
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for First Par	0.0100	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0500	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	11%	Note
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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	1.24	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	0.26	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)	0.26	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H7 ..H17 .	2.08	Ang.
	x,y,z =	1_555	Check

PLAT410_ALERT_2_G	Short Intra H...H Contact	H17	..H7A	.	1.98 Ang.
			x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H90A	..H10B	.	2.14 Ang.
			-x,-y,1-z =	2_556	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C68	..C2Y	.	3.17 Ang.
			x,y,z =	1_555	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure				! Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				3 Note
	H1A1	H1A2	H1A3		
PLAT721_ALERT_1_G	Bond Calc	0.96000, Rep	0.97000 Dev...		0.01 Ang.
	C10A	-H10C	1_555 1_555	 #	20 Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5A		--C25		1.77 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	...			38.70 Deg.
	C1X	-C2X	-C3X	1_555 1_555 1_555	 # 350 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				485 Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE	Suppressed			! Info
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF				1 Note
	0	1	0,		
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res	..			50.0 Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value				3.94 Note
	Predicted wR2: Based on SigI**2	4.15 or SHELX Weight	12.39		
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
 11 **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

3 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
 14 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.

