

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SR437

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: SR437

Bond precision: C-C = 0.0059 Å Wavelength=0.71073

Cell: a=13.5114(7) b=13.5114(7) c=17.556(3)
 alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	3205.0(6)	3205.0(6)
Space group	P -4 21 c	P -4 21 c
Hall group	P -4 2n	P -4 2n
Moiety formula	C48 H64 F24 K4 N4 O4	C12 H16 F6 K1 N1 O1
Sum formula	C48 H64 F24 K4 N4 O4	C12 H16 F6 K N O
Mr	1373.43	343.36
Dx,g cm-3	1.423	1.423
Z	2	8
Mu (mm-1)	0.389	0.389
F000	1408.0	1408.0
F000'	1410.71	
h,k,lmax	17,17,22	17,17,22
Nref	3691[2061]	3501
Tmin,Tmax	0.882,0.962	0.794,0.962
Tmin'	0.859	

Correction method= # Reported T Limits: Tmin=0.794 Tmax=0.962
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.95 Theta(max)= 27.500

R(reflections)= 0.0466(2146) wR2(reflections)= 0.0942(3501)

S = 0.963 Npar= 191

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	Non-Solvent Resd 1	C	Ueq(max)/Ueq(min)	Range	4.1	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	F1	--	C1	..	7.0 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C8	--	C9	..	0.18 Ang.
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds			0.00589 Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance				2.122 Check
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage					89 %
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.					0 Note



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ					Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...					0.25 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of					C3 Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					181 Do !
	O1 -K1 -C6 -C7	-158.00	10.00	8.667	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					182 Do !
	O1 -K1 -C6 -C7	-66.00	10.00	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					183 Do !
	O1 -K1 -C6 -C7	-74.00	10.00	2.755	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					184 Do !
	F2 -K1 -C6 -C7	31.00	10.00	2.755	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					185 Do !
	N5 -K1 -C6 -C7	-4.00	10.00	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					186 Do !
	F1 -K1 -C6 -C7	-7.00	10.00	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					187 Do !
	C13 -K1 -C6 -C7	86.00	10.00	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					188 Do !
	C12 -K1 -C6 -C7	62.00	10.00	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					189 Do !
	C2 -K1 -C6 -C7	-47.00	10.00	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					190 Do !
	K1 -K1 -C6 -C7	-111.00	10.00	7.647	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					191 Do !
	K1 -K1 -C6 -C7	-141.00	10.00	8.667	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #					193 Do !
	K1 -C6 -C7 -C8	18.00	0.00	1.555	1.555	1.555
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)					1.36 Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					87 Check
	O1 -C2 -K1	1.555	1.555	1.555		42.81 Deg.
PLAT792_ALERT_1_G	The Model has Chirality at C2			(Polar	SPGR)	R Verify
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)					4 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=			0.600		4 Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
16 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.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

