

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SR629

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: SR629

Bond precision: C-C = 0.0036 Å Wavelength=0.71073

Cell: a=13.9764(4) b=14.1787(4) c=16.1077(4)
 alpha=84.831(1) beta=81.560(1) gamma=80.187(1)

Temperature: 150 K

	Calculated	Reported
Volume	3104.31(15)	3104.31(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H64 F24 K4 N4 O4	C48 H64 F24 K4 N4 O4
Sum formula	C48 H64 F24 K4 N4 O4	C48 H64 F24 K4 N4 O4
Mr	1373.44	1373.43
Dx,g cm-3	1.469	1.469
Z	2	2
Mu (mm-1)	0.402	0.402
F000	1408.0	1408.0
F000'	1410.71	
h,k,lmax	18,18,20	18,18,20
Nref	14282	14178
Tmin,Tmax	0.821,0.894	0.805,0.894
Tmin'	0.821	

Correction method= # Reported T Limits: Tmin=0.805 Tmax=0.894
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 27.521

R(reflections)= 0.0418(10584) wR2(reflections)= 0.1101(14178)

S = 1.010 Npar= 759

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min)

16 Note

🟢 Alert level C

PLAT220_ALERT_2_C	Non-Solvent Resd 1	C	Ueq(max)/Ueq(min) Range	4.4	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1	H	Uiso(max)/Uiso(min) Range	4.8	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	F5	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	F24	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	F25	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	F28	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C37	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C59	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C79	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C58	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C78	Check
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H37A .. H35F ..		1.86	Ang.
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600		8	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers			1	Check

🟠 Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	5	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C77 -- C78 ..	9.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C78 -- C79 ..	8.3	s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C3	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C7	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C23	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C27	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C43	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C47	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C63	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C67	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1) ..	4	% Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.23	Ratio
PLAT793_ALERT_4_G	The Model has Chirality at C22 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C23 (Centro SPGR)	S	Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	81 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain1 **ALERT level B** = A potentially serious problem, consider carefully14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight18 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

22 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

5 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.

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