

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SR681

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: SR681

Bond precision:	C-C = 0.0037 A	Wavelength=0.71073
Cell:	a=18.9136(8) b=10.7740(5) c=24.7556(9)	
	alpha=90 beta=108.265(2) gamma=90	
Temperature:	150 K	
	Calculated	Reported
Volume	4790.4(4)	4790.4(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 H48 F24 K4 N4 O4	C32 H48 F24 K4 N4 O4
Sum formula	C32 H48 F24 K4 N4 O4	C32 H48 F24 K4 N4 O4
Mr	1165.15	1165.14
Dx,g cm-3	1.616	1.616
Z	4	4
Mu (mm-1)	0.505	0.505
F000	2368.0	2368.0
F000'	2373.26	
h,k,lmax	24,13,32	24,13,32
Nref	10975	10958
Tmin,Tmax	0.913,0.941	0.840,0.941
Tmin'	0.813	
Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.941		
AbsCorr = MULTI-SCAN		
Data completeness=	0.998	Theta(max)= 27.483
R(reflections)=	0.0402(8014)	wR2(reflections)= 0.1166(10958)
S =	1.056	Npar= 668

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)	13	Note
PLAT939_ALERT_3_B	Large Value of Not (SHELXL) Weight Optimized S .	234.75	Check

Alert level C

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	4.7	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	F12	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	F15	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N2	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	5	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Note

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
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	7	Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C2	Check
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	C12	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C13	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C22	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	C32	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C33	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)..	11	% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C18B .. C18B ..	2.72	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F1 .. F11 ..	2.82	Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.29	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	283	Check
	01 -C1 -K1 1.555 1.555 1.555	41.16	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	458	Check
	03 -C21 -K3 1.555 1.555 1.555	41.34	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	563	Check
	04 -C31 -K1 1.555 1.555 1.555	43.76	Deg.
PLAT793_ALERT_4_G	The Model has Chirality at C1 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C11 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C21 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C22 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C31 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3	Note

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

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

