

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SR556

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: SR556

Bond precision:	C-C = 0.0041 A	Wavelength=0.71073
Cell:	a=14.2195(4) b=11.8504(4) c=39.8155(13)	
	alpha=90 beta=97.526(1) gamma=90	
Temperature:	150 K	
	Calculated	Reported
Volume	6651.4(4)	6651.4(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C104 H112 F48 K8 N8 O8 [+ solvent]	C104 H112 F48 K8 N8 O8
Sum formula	C104 H112 F48 K8 N8 O8 [+ solvent]	C104 H112 F48 K8 N8 O8
Mr	2826.82	2826.82
Dx, g cm ⁻³	1.411	1.411
Z	2	2
Mu (mm ⁻¹)	0.378	0.378
F000	2880.0	2880.0
F000'	2885.46	
h,k,lmax	18,15,51	18,15,51
Nref	15246	15220
Tmin,Tmax	0.901,0.945	0.889,0.945
Tmin'	0.825	
Correction method= # Reported T Limits: Tmin=0.889 Tmax=0.945		
AbsCorr = MULTI-SCAN		
Data completeness=	0.998	Theta(max)= 27.480
R(reflections)=	0.0453(9649)	wR2(reflections)= 0.1185(15220)
S =	0.989	Npar= 797

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)	19	Note
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	2	Check
PLAT990_ALERT_1_B	Deprecated RES file style based SQUEEZE job	!	Note

Alert level C

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C1 -- C6 ..	6.3	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C12 -- C14 ..	5.5	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	F16	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	F107	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C7	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00409	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	10.000	Check

Alert level G

PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C18	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C44	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C48	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C74	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C78	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C104	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C108	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.21	Ratio
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: K1 -- K4 ..	4.01	Ang.
PLAT793_ALERT_4_G	The Model has Chirality at N69 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C12 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C14 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C42 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C44 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C72 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C102 (Centro SPGR)	R	Verify
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	10	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 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
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.

