

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) fe1-tbbtclo4h2o

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: fe1-tbbtclo4h2o

Bond precision:	C-C = 0.0034 A	Wavelength=1.54184	
Cell:	a=8.9918(1)	b=18.0165(2)	c=13.4614(2)
	alpha=90	beta=91.565(1)	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	2179.94(5)	2179.94(5)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C30 H34 Fe N18 O2, 2(Cl O4), 4(H2 O)	C30 H34 Fe N18 O2, 2(Cl O4), 4(H2 O)	
Sum formula	C30 H42 Cl2 Fe N18 O14	C30 H42 Cl2 Fe N18 O14	
Mr	1005.57	1005.56	
Dx, g cm-3	1.532	1.532	
Z	2	2	
Mu (mm-1)	4.640	4.640	
F000	1040.0	1040.0	
F000'	1042.55		
h,k,lmax	10,21,16	10,21,16	
Nref	3895	3890	
Tmin,Tmax		0.620,0.642	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.620 Tmax=0.642
AbsCorr = SPHERE

Data completeness= 0.999 Theta(max)= 67.079

R(reflections)= 0.0454(3565)	wR2(reflections)= 0.1271(3890)
S = 1.061	Npar= 327

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

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11	0.157	Check	
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O2	- H2A	.	1.03 Ang.	
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O3	- H3D	.	1.04 Ang.	
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H1A	..H2B	.	2.11 Ang.
		x,y,z	=	1_555	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H2B	..H3D	.	2.10 Ang.
		x,y,z	=	1_555	Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be	LIST 4		Please	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.597		5	Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		4	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.		2	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		3	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C11		Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H10A	..N2	.	2.65 Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1	(II)	.	2.00 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		3	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		84%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.3	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

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
12 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
5 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.

