

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lcsm16

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: lcsm16

Bond precision: C-C = 0.0271 Å Wavelength=1.54184

Cell: a=6.8570(9) b=25.484(3) c=13.743(2)
 alpha=90 beta=92.460(14) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2399.3(5)	2399.3(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H9 Fe O6 [+ solvent]	C21 H9 Fe O6
Sum formula	C21 H9 Fe O6 [+ solvent]	C21 H9 Fe O6
Mr	413.13	413.13
Dx, g cm ⁻³	1.144	1.144
Z	4	4
Mu (mm ⁻¹)	5.288	5.288
F000	836.0	836.0
F000'	834.17	
h,k,lmax	6,23,12	6,23,12
Nref	1865	1853
Tmin,Tmax	0.948,0.948	0.249,1.000
Tmin'	0.948	

Correction method= # Reported T Limits: Tmin=0.249 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 44.312

R(reflections)= 0.1525(1022) wR2(reflections)= 0.4306(1853)

S = 1.426 Npar= 197

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 A

THETM01_ALERT_3_A The value of $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.4531$

Author Response: Crystals diffracted to 1.1 Å of resolution, so the data had to be trimmed accordingly

Alert level B

PLAT084_ALERT_3_B High wR_2 Value (i.e. > 0.25) 0.43 Report

Author Response: Due to the poor resolution of the data acquired, the model was based on ill shaped electron density map. As consequence the wR_2 and R_1 values are larger than normal values

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 8 Report
C2 C3 C4 C5 C6 C7 etc.

Author Response: In order to maximize the data/parameter ratio, the disordered atoms were refined isotropically

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.02706 Å.

Author Response: It is caused by the low resolution data.

Alert level C

PLAT018_ALERT_1_C $\text{_diffraction_measured_fraction_theta_max}$.NE. *_full ! Check
PLAT082_ALERT_2_C High R_1 Value 0.15 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.41 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT369_ALERT_2_C Long C(sp²)-C(sp²) Bond C20 - C20_b . 1.53 Å.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.604 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.453 13 Report
PLAT922_ALERT_1_C wR_2 in the CIF and FCF Differ by 0.0028 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H6 -0.38 eÅ⁻³
PLAT977_ALERT_2_C Check Negative Difference Density on H16 -0.33 eÅ⁻³
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 34 Report

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.20	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records		2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C23	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		21%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1	..C14	2.98	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2	..C14	3.14	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4	..C17	3.12	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4	..C18	3.20	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C5	..C10	2.94	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C5	..C9	3.14	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C7	..C12	3.10	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C7	..C13	3.12	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C8	..C13	3.17	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C9	..C13	3.17	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C18	..C14	3.16	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19	..C24	3.17	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C21	..C25	3.16	Ang.
		2-x,1-y,1-z =	3_766	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C23	..C27	3.16	Ang.
		2-x,1-y,1-z =	3_766	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		!	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III)		3.58	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		289	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		!	Info
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		30%	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		4	Note
PLAT954_ALERT_1_G	Reported (CIF) and Actual (FCF) Kmax Differ by		1	Units

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

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

29 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
15 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.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

