



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 5

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: 5

Bond precision:	C-C = 0.0088 Å		Wavelength=0.71073
Cell:	a=20.9534 (11)	b=17.3538 (7)	c=20.5697 (10)
	alpha=90	beta=114.468 (6)	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	6807.9 (6)	6807.9 (6)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C31 H45 Fe Mo3 O S4	C31 H45 Fe Mo3 O S4	
Sum formula	C31 H45 Fe Mo3 O S4	C31 H45 Fe Mo3 O S4	
Mr	905.58	905.58	
Dx, g cm ⁻³	1.767	1.767	
Z	8	8	
Mu (mm ⁻¹)	1.767	1.767	
F000	3640.0	3640.0	
F000'	3606.01		
h, k, lmax	26, 21, 25	26, 21, 25	
Nref	13919	13906	
Tmin, Tmax	0.979, 0.982	0.836, 1.000	
Tmin'	0.965		

Correction method= # Reported T Limits: Tmin=0.836 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 26.372

R(reflections)= 0.0550(8919)

wR2(reflections)=
0.0863(13906)

S = 1.003

Npar= 751

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

PLAT213_ALERT_2_C Atom C6A	has ADP max/min Ratio	3.1 oblate
PLAT213_ALERT_2_C Atom C23A	has ADP max/min Ratio	3.8 oblate
PLAT213_ALERT_2_C Atom C24A	has ADP max/min Ratio	3.1 oblate
PLAT213_ALERT_2_C Atom O1B	has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C Atom C6B	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C Atom C7B	has ADP max/min Ratio	3.5 prolat
PLAT213_ALERT_2_C Atom C9B	has ADP max/min Ratio	4.0 prolat
PLAT213_ALERT_2_C Atom C12B	has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C Atom C26B	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom C31B	has ADP max/min Ratio	3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range		3.4 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range		4.3 Ratio
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours		C1B Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds		0.00882 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance		13.756 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance		2.706 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H30C .		-0.31 eA-3



Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms		5 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records		2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records		1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records		1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used		0.0100 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2A --S2A .		5.2 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels		18 Note
H9BA H9BB H9BC H8AA H8AB H8AC H9AA H9AB		
H9AC H7AA H7AB H7AC H7BA H7BB H7BC H8BA		
H8BB H8BC		
PLAT860_ALERT_3_G Number of Least-Squares Restraints		30 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 1 0 0, 1 1 0, -1 1 1, 0 1 1,		1.99 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		8 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		3.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value		1.485 Note
Predicted wR2: Based on SigI**2 5.81 or SHELX Weight		8.60 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully
17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

1 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
7 ALERT type 3 Indicator that the structure quality may be low
5 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

