



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4

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: 4

Bond precision: C-C = 0.0050 Å

Wavelength=0.71073

Cell: a=15.1694 (3) b=17.2445 (3) c=17.9990 (3)
 alpha=85.702 (2) beta=89.358 (2) gamma=69.858 (2)
Temperature: 123 K

	Calculated	Reported
Volume	4407.42 (15)	4407.42 (15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C78 H122 Fe2 K2 Mo6 O6 S8	C78 H122 Fe2 K2 Mo6 O6 S8
Sum formula	C78 H122 Fe2 K2 Mo6 O6 S8	C78 H122 Fe2 K2 Mo6 O6 S8
Mr	2177.78	2177.77
Dx, g cm ⁻³	1.641	1.641
Z	2	2
Mu (mm ⁻¹)	1.475	1.475
F000	2216.0	2216.0
F000'	2199.96	
h, k, lmax	18, 21, 22	18, 21, 22
Nref	18037	17944
Tmin, Tmax	0.863, 0.863	0.831, 1.145
Tmin'	0.863	

Correction method= # Reported T Limits: Tmin=0.831 Tmax=1.145
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 26.372

R(reflections)= 0.0306(13722)

wR2(reflections)=
0.0640(17944)

S = 1.004

Npar= 1032

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 FCF Reflection(s) Below Theta(Min) [Deg]= 3.35 Note

1	0	0,	2	0	0,	-1	1	0,	0	1	0,	1	1	0,	2	1	0,
-1	2	0,	0	2	0,	1	2	0,	2	2	0,	-1	-2	1,	0	-2	1,
-2	-1	1,	-1	-1	1,	0	-1	1,	1	-1	1,	-2	0	1,	-1	0	1,
0	0	1,	1	0	1,	2	0	1,	-1	1	1,	0	1	1,	1	1	1,

(15 More NOT listed: see .ckf listing file)

Author Response: This alert is due to blinds of the beamstop or the 2D detection system

Alert level C

PLAT213_ALERT_2_C Atom C8	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C Atom C9	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C Atom C10	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C Atom C20	has ADP max/min Ratio	3.1	prolat
PLAT213_ALERT_2_C Atom C69A	has ADP max/min Ratio	3.6	prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range		4.5	Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O1 --C1	.	6.5	s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 --C2	.	5.5	s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O5 --C74	.	0.17	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C72 --C73	.	0.19	Ang.
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours		K2	Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for		C78A	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600		11	Report
8 20 0, 14 2 13, 13 4 14, 13 5 14, 13 4 15, 13 5 15,			
13 6 15, 12 6 16, 12 7 16, 12 8 16, 11 8 17,			
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF		4	Note
0 2 0, -1 -1 1, -1 1 1, 0 0 2,			

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		3	Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms		10	Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)		0.002	Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records		15	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		1	Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records		1	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used		0.0200	Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for O4 --C67A	.	6.2	s.u.

PLAT232_ALERT_2_G	Hirshfeld	Test Diff	(M-X)	Mo3	--S3	.	5.0 s.u.	
PLAT232_ALERT_2_G	Hirshfeld	Test Diff	(M-X)	Fe1	--C1	.	7.6 s.u.	
PLAT232_ALERT_2_G	Hirshfeld	Test Diff	(M-X)	Fe2	--C2	.	7.4 s.u.	
PLAT299_ALERT_4_G	Atom Site	Occupancy	Constrained at				0.5 Check	
	C58	C58A	C59	C59A	C60	C60A	C61	
	C62	C62A	H58A	H58B	H58C	H58D	H58E	
	H59A	H59B	H59C	H59D	H59E	H59F	H60A	
	H60C	H60D	H60E	H60F	H61A	H61B	H61C	
	H61E	H61F	H62A	H62B	H62C	H62D	H62E	
PLAT300_ALERT_4_G	Atom Site	Occupancy	of O5				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of O6				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of O5A				Constrained at	0.4 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of O6A				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C67				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C68				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C69				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C70				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C71				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C72				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C73				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C74				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C76A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C77A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C78A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C67A				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C68A				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C69A				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C70A				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C71A				Constrained at	0.4 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C72A				Constrained at	0.4 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C73A				Constrained at	0.4 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C74A				Constrained at	0.4 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C76				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C77				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of C78				Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H67A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H67B				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H68A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H68B				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H69A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H69B				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H70A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H70B				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H71A				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H71B				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H72A				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H72B				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H73A				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H73B				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H74A				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H74B				Constrained at	0.6 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H75A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H75B				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H76C				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H76D				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H77A				Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site	Occupancy	of H77B				Constrained at	0.55 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H78A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78B	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H67C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H67D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H68C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H68D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H69C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H69D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H70C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H70D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H71C	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H71D	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H72C	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H72D	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H73C	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H73D	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H74C	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H74D	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H75C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H75D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H76A	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H76B	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H77C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H77D	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78C	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78D	Constrained at	0.45	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		18%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C2	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C58A	Check
PLAT774_ALERT_1_G	Check X-Y Bond in CIF: K1 --K2 ..		4.48	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		331	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		43	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.1	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		1.646	Note
	Predicted wR2: Based on SigI**2 3.89 or SHELX Weight		6.37	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 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
 84 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

Datablock 4 - ellipsoid plot

