

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh50AM12_0m

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: hh50AM12_0m

Bond precision: C-C = 0.0016 Å

Wavelength=0.71073

Cell: a=10.5861(3) b=12.9206(4) c=14.6139(5)
alpha=71.1776(5) beta=79.6221(5) gamma=70.7566(5)
Temperature: 100 K

	Calculated	Reported
Volume	1780.17(10)	1780.17(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C37 H51 Cl2 Mo N3 O	?
Sum formula	C37 H51 Cl2 Mo N3 O	C37 H51 Cl2 Mo N3 O
Mr	720.65	720.64
Dx, g cm ⁻³	1.344	1.344
Z	2	2
Mu (mm ⁻¹)	0.551	0.551
F000	756.0	756.0
F000'	753.35	
h,k,lmax	14,17,20	14,17,20
Nref	9984	9968
Tmin,Tmax	0.756,0.914	0.681,0.746
Tmin'	0.741	

Correction method= MULTI-SCAN

Data completeness= 0.998

Theta(max)= 29.572

R(reflections)= 0.0189(9518)

wR2(reflections)= 0.0504(9968)

S = 1.046

Npar= 426

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 C3D	has ADP max/min Ratio	3.1	prolat
PLAT732 ALERT 1 C	Angle Calc	167.43(2), Rep 167.43(1)	2.22	su-Rat
	CL1 -MO1 -CL2	1.555 1.555 1.555 #	15	
PLAT911 ALERT 3 C	Missing # FCF Refl Between THmin & STh/L=	0.600	4	Report

● Alert level G

PLAT002 ALERT 2 G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003 ALERT 2 G	Number of Uiso or Uij Restrained non-H Atoms ...	4	Report
PLAT176 ALERT 4 G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT177 ALERT 4 G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- Cl1 ..	12.9	su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- Cl2 ..	12.4	su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- N2 ..	7.0	su
PLAT301 ALERT 3 G	Main Residue Disorder Percentage =	5	Note
PLAT380 ALERT 4 G	Incorrectly? Oriented X(sp ²)-Methyl Moiety	C8	Check
PLAT860 ALERT 3 G	Number of Least-Squares Restraints	5	Note
PLAT910 ALERT 3 G	Missing # of FCF Reflections Below Th(Min)	2	Report
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	10	Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

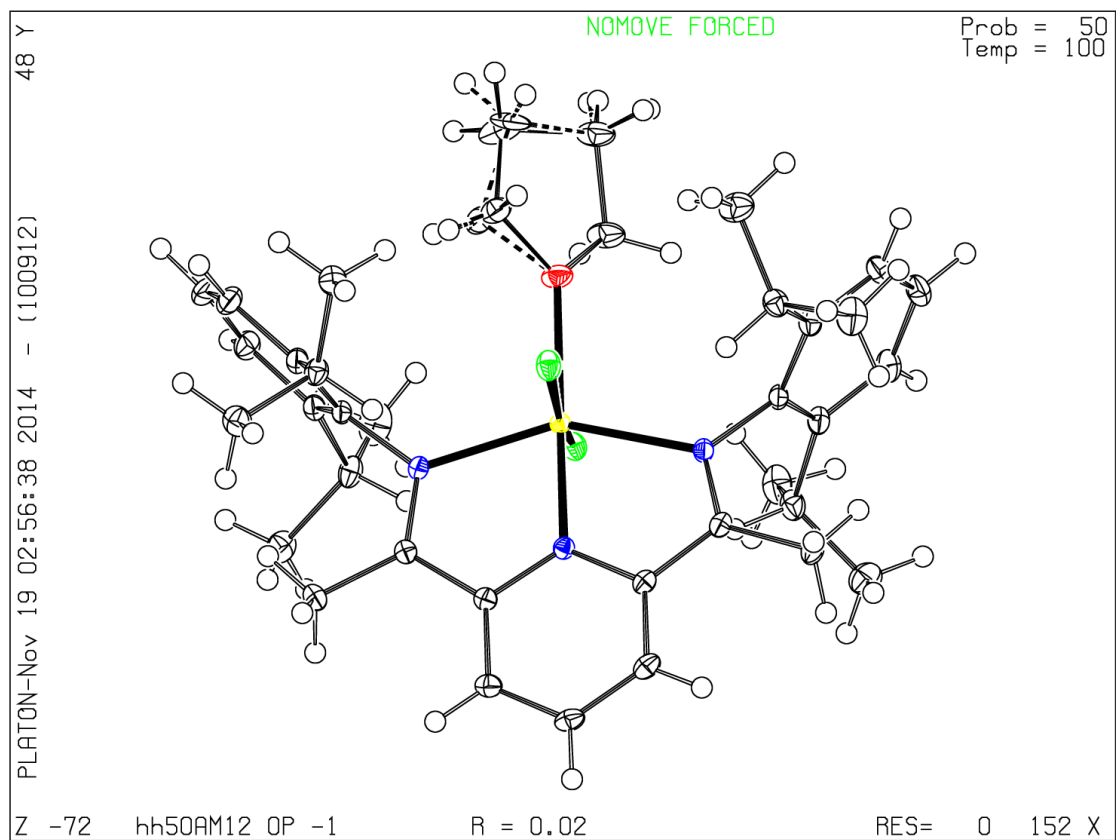
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh85AM29_0m

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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: hh85AM29_0m

Bond precision: C-C = 0.0031 A

Wavelength=0.71073

Cell: a=20.5549(6) b=12.5715(4) c=29.0368(9)
alpha=90 beta=107.0914(5) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	7171.9(4)	7171.9(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C38 H49 Mo2 N3 S2	?
Sum formula	C38 H49 Mo2 N3 S2	C38 H49 Mo2 N3 S2
Mr	803.80	803.80
Dx,g cm-3	1.489	1.489
Z	8	8
Mu (mm-1)	0.847	0.847
F000	3312.0	3312.0
F000'	3287.14	
h,k,lmax	28,17,40	28,17,40
Nref	10075	10071
Tmin,Tmax	0.759,0.798	0.701,0.746
Tmin'	0.692	

Correction method= # Reported T Limits: Tmin=0.701 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000

Theta(max)= 29.574

R(reflections)= 0.0334(9383)

wR2(reflections)= 0.0657(10071)

S = 1.229

Npar= 468

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

PLAT220 ALERT 2 C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.5 Ratio
PLAT906 ALERT 3 C	Large K value in the Analysis of Variance	4.017 Check
PLAT972 ALERT 2 C	Check Calcd Residual Density 0.74A From Mo2	-1.87 eA-3

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 Uij Restrained non-H Atoms ...	10 Report
PLAT083 ALERT 2 G	SHELXL Second Parameter in WGHT Unusually Large	25.01 Why ?
PLAT176 ALERT 4 G	The CIF-Embedded .res File Contains SADI Records	1 Report
PLAT177 ALERT 4 G	The CIF-Embedded .res File Contains DELU Records	1 Report
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mol -- S1 ..	6.0 s.u.
PLAT301 ALERT 3 G	Main Residue Disorder Percentage =	11 Note
PLAT860 ALERT 3 G	Number of Least-Squares Restraints	21 Note
PLAT910 ALERT 3 G	Missing # of FCF Reflection(s) Below Theta(Min)	1 Note
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	3 Note
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density	15 Note

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0 ALERT type 5 Informative message, check
-
-

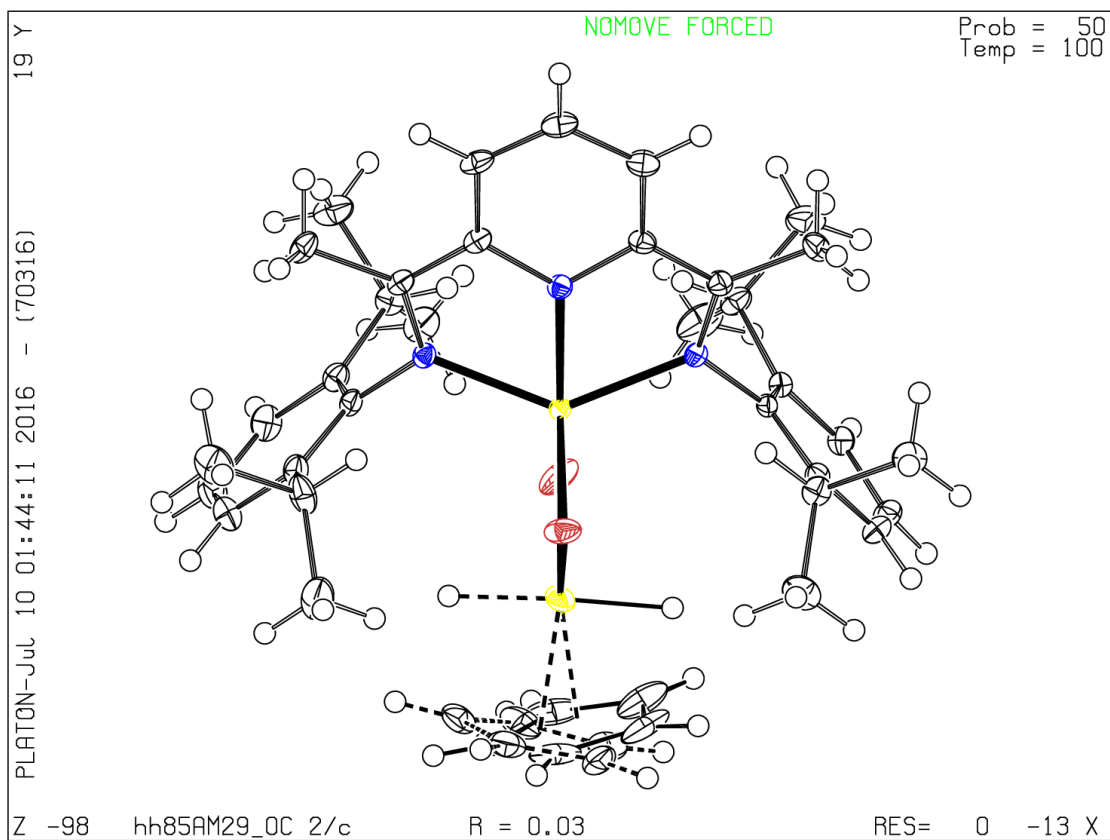
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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh52AM14r_0m-5

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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: hh52AM14r_0m-5

Bond precision: C-C = 0.0087 A

Wavelength=0.71073

Cell: a=11.1885(11) b=14.8249(14) c=26.397(3)
alpha=96.3680(15) beta=101.6756(15) gamma=110.1426(14)
Temperature: 100 K

	Calculated	Reported
Volume	3947.2(7)	3947.2(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C43 H53 Mo2 N3 S2	?
Sum formula	C43 H53 Mo2 N3 S2	C43 H53 Mo2 N3 S2
Mr	867.88	867.88
Dx,g cm-3	1.460	1.460
Z	4	4
Mu (mm-1)	0.775	0.775
F000	1792.0	1792.0
F000'	1779.62	
h,k,lmax	13,18,32	13,18,32
Nref	16121	15663
Tmin,Tmax	0.857,0.981	0.813,0.928
Tmin'	0.678	

Correction method= # Reported T Limits: Tmin=0.813 Tmax=0.928
AbsCorr = MULTI-SCAN

Data completeness= 0.972

Theta(max)= 26.372

R(reflections)= 0.0402(14509)

wR2(reflections)= 0.1069(15663)

S = 1.093

Npar= 922

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

PLAT029 ALERT 3 C	_diffn_measured_fraction_theta_full value Low .	0.974	Note
PLAT213 ALERT 2 C	Atom C18A has ADP max/min Ratio	3.7	oblate
PLAT342 ALERT 3 C	Low Bond Precision on C-C Bonds	0.00874	Ang.
PLAT601 ALERT 2 C	Structure Contains Solvent Accessible VOIDS of .	80	Ang3
PLAT911 ALERT 3 C	Missing # FCF Refl Between THmin & STh/L= 0.600	853	Report



Alert level G

PLAT083 ALERT 2 G	SHELXL Second Parameter in WGHT Unusually Large	20.63	Why ?
PLAT870 ALERT 4 G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT910 ALERT 3 G	Missing # of FCF Reflection(s) Below Theta(Min)	1	Note
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	309	Note
PLAT931 ALERT 5 G	Found Twin Law () [1 0 0] Estimated BASF	0.26	Check

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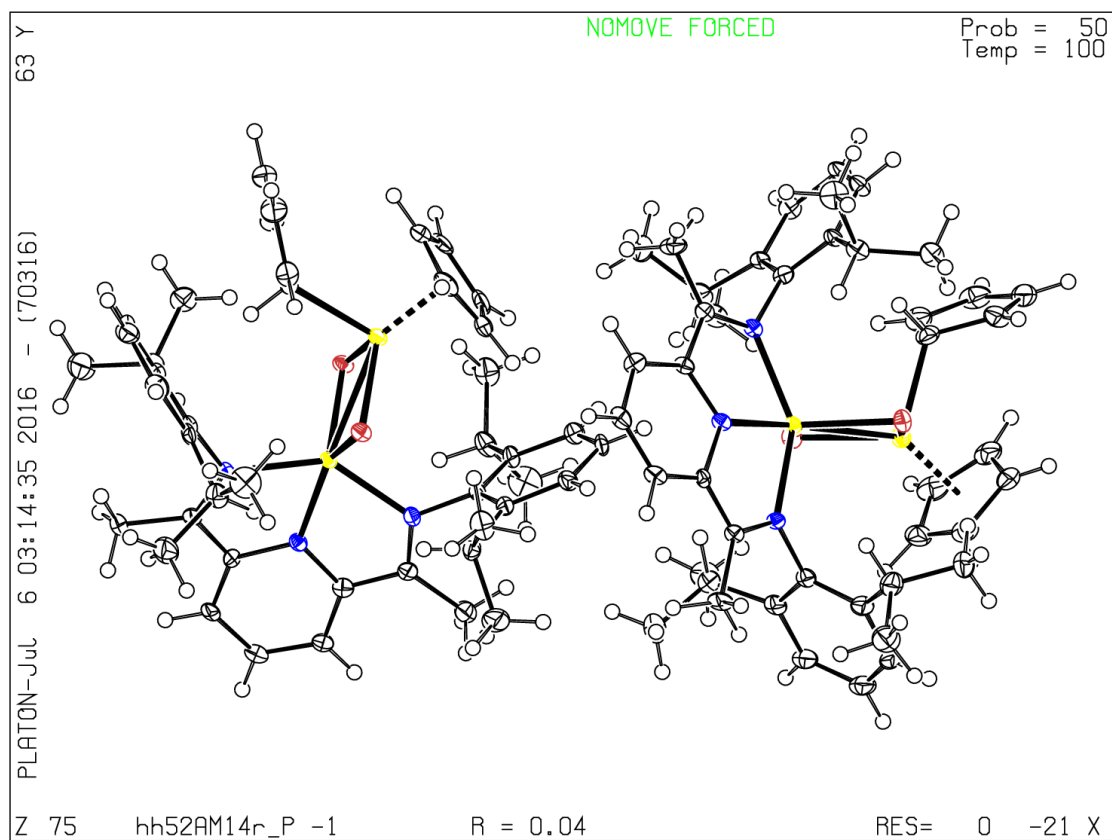
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PLATON version of 06/05/2016; check.def file version of 05/05/2016

Datablock hh52AM14r_0m-5 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh148AM54r_0m

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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: hh148AM54r_0m

Bond precision: C-C = 0.0035 A

Wavelength=0.71073

Cell: a=42.8652(17) b=49.0867(19) c=12.2689(5)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	25815.1(18)	25815.1(18)
Space group	F d d 2	F d d 2
Hall group	F 2 -2d	F 2 -2d
Moiety formula	4(C38 H49 Mo2 N3 S2), 4(C18 H36 N2 Na O6), C14 H16, 2(C7 H8), 2	?
Sum formula	C260 H390 Mo8 N22 Na4 O26 S8	C65 H97.50 Mo2 N5.50 Na O6.50 S2
Mr	5355.90	1338.97
Dx, g cm ⁻³	1.378	1.378
Z	4	16
Mu (mm ⁻¹)	0.515	0.515
F000	11280.0	11280.0
F000'	11232.83	
h,k,lmax	61,70,17	61,70,17
Nref	19708[10276]	19698
Tmin,Tmax	0.908,0.961	0.881,0.928
Tmin'	0.833	

Correction method= # Reported T Limits: Tmin=0.881 Tmax=0.928
AbsCorr = NONE

Data completeness= 1.92/1.00

Theta(max)= 30.508

R(reflections)= 0.0243(18438)

wR2(reflections)= 0.0569(19698)

S = 1.065

Npar= 875

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

PLAT250 ALERT 2 B	Large U3/U1 Ratio for Average U(i,j) Tensor	4.8 Note
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● Alert level C

PLAT250 ALERT 2 C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.4 Note
PLAT413 ALERT 2 C	Short Inter XH3 .. XHn H33C .. H3I ..	2.06 Ang.
PLAT910 ALERT 3 C	Missing # of FCF Reflection(s) Below Theta(Min)	6 Note

● Alert level G

PLAT002 ALERT 2 G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT003 ALERT 2 G	Number of Uiso or Uij Restrained non-H Atoms ...	27 Report
PLAT045 ALERT 1 G	Calculated and Reported Z Differ by a Factor ...	0.25 Check
PLAT083 ALERT 2 G	SHELXL Second Parameter in WGHT Unusually Large	12.07 Why ?
PLAT174 ALERT 4 G	The CIF-Embedded .res File Contains FLAT Records	2 Report
PLAT176 ALERT 4 G	The CIF-Embedded .res File Contains SADI Records	2 Report
PLAT177 ALERT 4 G	The CIF-Embedded .res File Contains DELU Records	1 Report
PLAT178 ALERT 4 G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo2 -- S2 ..	6.0 s.u.
PLAT300 ALERT 4 G	Atom Site Occupancy of <C1T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C1U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C2T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C2U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C3T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C3U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C4T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C4U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C5T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C5U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C6T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C6U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C7T is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <C7U is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H2D is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H2E is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H3H is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H3I is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H4H is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H4I is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H5E is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H5F is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H6D is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H6E is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H7F is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H7G is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H7H is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H7I is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H7J is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <H7K is Constrained at	0.25 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C1S is Constrained at	0.5 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C2S is Constrained at	0.5 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C3S is Constrained at	0.5 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C4S is Constrained at	0.5 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C5S is Constrained at	0.5 Check

PLAT300 ALERT 4 G	Atom Site Occupancy of *C6S	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C7S	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H2C	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H3G	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H4G	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H5D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H6C	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H7C	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H7D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H7E	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *O1D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *N1D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C1D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C2D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C3D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *C4D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H1C	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H1D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H1E	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H3D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H3E	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H3F	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H4D	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H4E	is Constrained at	0.5	Check
PLAT300 ALERT 4 G	Atom Site Occupancy of *H4F	is Constrained at	0.5	Check
PLAT301 ALERT 3 G	Main Residue Disorder	Percentage =	5	Note
PLAT302 ALERT 4 G	Anion/Solvent Disorder	Percentage =	100	Note
PLAT304 ALERT 4 G	Non-Integer Number of Atoms (7.50) in Resd. #		3	Check
PLAT304 ALERT 4 G	Non-Integer Number of Atoms (7.50) in Resd. #		4	Check
PLAT304 ALERT 4 G	Non-Integer Number of Atoms (7.50) in Resd. #		5	Check
PLAT789 ALERT 4 G	Atoms with Negative _atom_site_disorder_group #		30	Check
PLAT860 ALERT 3 G	Number of Least-Squares Restraints		481	Note
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density		9	Note

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0 ALERT type 5 Informative message, check

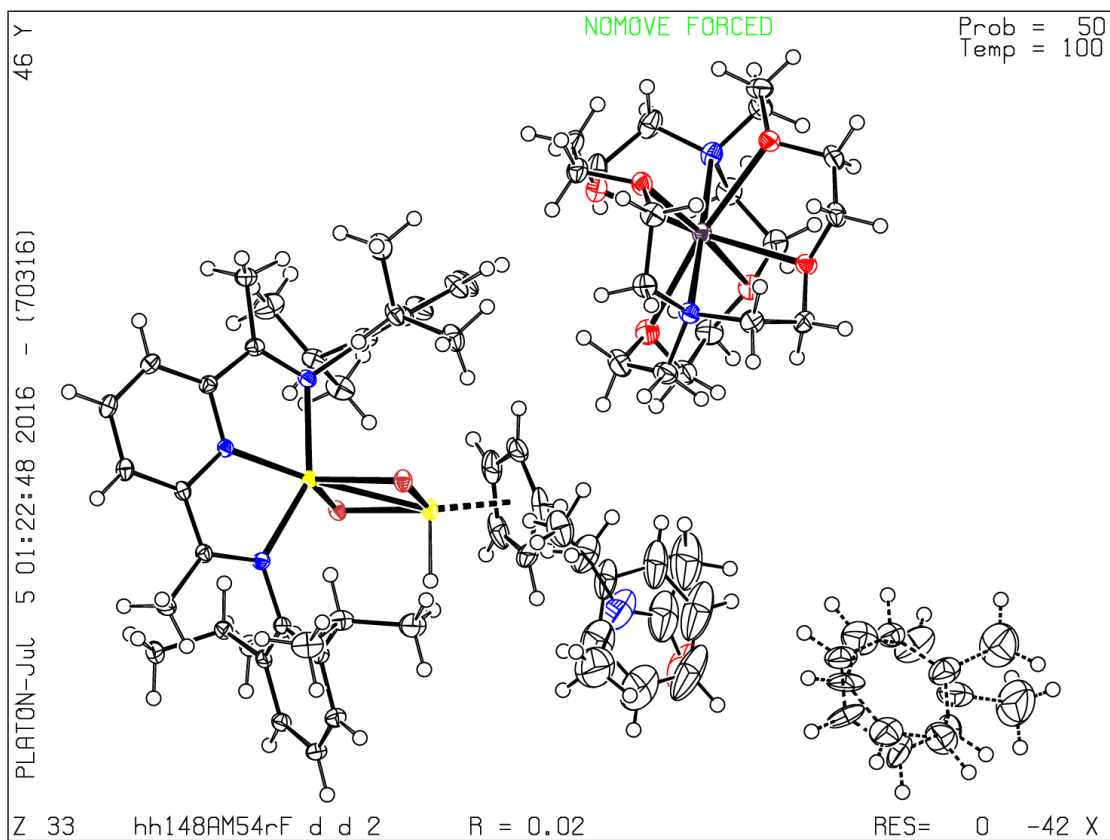
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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh172AM60_0m

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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: hh172AM60_0m

Bond precision: C-C = 0.0028 Å

Wavelength=0.71073

Cell: a=12.7387(3) b=16.7266(4) c=19.0589(4)
alpha=104.0257(11) beta=107.7631(11) gamma=91.0793(12)
Temperature: 100 K

	Calculated	Reported
Volume	3733.11(15)	3733.11(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H12 B F24, C38 H49 Mo2 N3 S2, C4 H10 O	?
Sum formula	C74 H71 B F24 Mo2 N3 O S2	C74 H71 B F24 Mo2 N3 O S2
Mr	1741.15	1741.14
Dx, g cm ⁻³	1.549	1.549
Z	2	2
Mu (mm ⁻¹)	0.498	0.498
F000	1762.0	1762.0
F000'	1756.77	
h,k,lmax	18,23,27	18,23,27
Nref	22780	22766
Tmin,Tmax	0.810,0.848	0.805,0.862
Tmin'	0.788	

Correction method= # Reported T Limits: Tmin=0.805 Tmax=0.862

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 30.508

R(reflections)= 0.0371(20259)

wR2(reflections)= 0.0978(22766)

S = 1.043

Npar= 1028

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

PLAT213 ALERT 2 B	Atom F11A	has ADP max/min Ratio	4.4 prolat
PLAT213 ALERT 2 B	Atom F24A	has ADP max/min Ratio	4.2 prolat

Alert level C

PLAT213 ALERT 2 C	Atom F4A	has ADP max/min Ratio	3.4 prolat
PLAT213 ALERT 2 C	Atom F12A	has ADP max/min Ratio	3.2 prolat
PLAT220 ALERT 2 C	Non-Solvent Resd 1 F	Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT412 ALERT 2 C	Short Intra XH3 .. XHn	H8A .. H2N ..	1.84 Ang.
PLAT910 ALERT 3 C	Missing # of FCF Reflection(s) Below Theta(Min)		10 Note
PLAT911 ALERT 3 C	Missing # FCF Refl Between THmin & STh/L=	0.600	5 Report
PLAT971 ALERT 2 C	Check Calcd Residual Density	0.78A From F14A	1.52 eA-3
PLAT978 ALERT 2 C	Number C-C Bonds with Positive Residual Density		0 Note

Alert level G

PLAT002 ALERT 2 G	Number of Distance or Angle Restraints on AtSite		8 Note
PLAT003 ALERT 2 G	Number of Uiso or Uij Restrained non-H Atoms ...		10 Report
PLAT176 ALERT 4 G	The CIF-Embedded .res File Contains SADI Records		2 Report
PLAT177 ALERT 4 G	The CIF-Embedded .res File Contains DELU Records		1 Report
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mol	-- N1 ..	8.2 s.u.
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C7A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C8A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C15A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C16A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C23A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C24A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C31A Check
PLAT242 ALERT 2 G	Low 'MainMol' Ueq as Compared to Neighbors of		C32A Check
PLAT301 ALERT 3 G	Main Residue Disorder	Percentage =	5 Note
PLAT434 ALERT 2 G	Short Inter HL..HL Contact F9A	.. F9A ..	2.81 Ang.
PLAT860 ALERT 3 G	Number of Least-Squares Restraints		31 Note

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

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 20 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

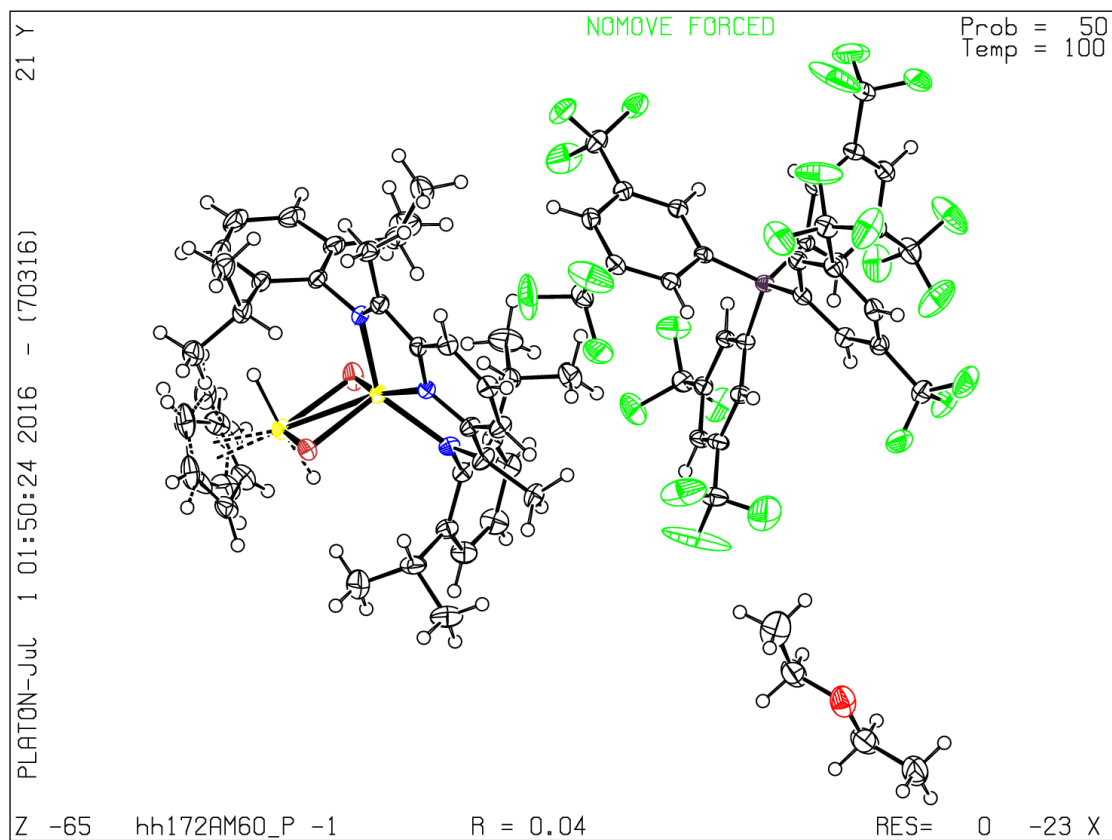
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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh166AM58_0m

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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: hh166AM58_0m

Bond precision: C-C = 0.0023 A

Wavelength=0.71073

Cell: a=11.6274(6) b=11.9639(6) c=18.4816(10)
alpha=75.9380(8) beta=81.0945(8) gamma=65.2264(7)
Temperature: 100 K

	Calculated	Reported
Volume	2260.3(2)	2260.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C39 H49 F3 Mo2 N3 O3 S3, C ? F3 O3 S	
Sum formula	C40 H49 F6 Mo2 N3 O6 S4	C40 H49 F6 Mo2 N3 O6 S4
Mr	1101.94	1101.94
Dx, g cm-3	1.619	1.619
Z	2	2
Mu (mm-1)	0.812	0.812
F000	1120.0	1120.0
F000'	1114.61	
h,k,lmax	15,15,24	15,15,24
Nref	11215	11204
Tmin,Tmax	0.677,0.866	0.767,0.825
Tmin'	0.664	

Correction method= # Reported T Limits: Tmin=0.767 Tmax=0.825

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 28.282

R(reflections)= 0.0208(10726)

wR2(reflections)= 0.0512(11204)

S = 1.072

Npar= 621

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

PLAT220 ALERT 2 C	Non-Solvent Resd 1 Mo Ueq(max)/Ueq(min) Range	4.0 Ratio
PLAT222 ALERT 3 C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	7.7 Ratio
PLAT601 ALERT 2 C	Structure Contains Solvent Accessible VOIDS of .	35 Ang3
PLAT911 ALERT 3 C	Missing # FCF Refl Between THmin & STh/L= 0.600	3 Report



Alert level G

PLAT002 ALERT 2 G	Number of Distance or Angle Restraints on AtSite	14 Note
PLAT003 ALERT 2 G	Number of Uiso or Uij Restrained non-H Atoms ...	10 Report
PLAT176 ALERT 4 G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT177 ALERT 4 G	The CIF-Embedded .res File Contains DELU Records	1 Report
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- S1 ..	6.6 s.u.
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo2D -- S1 ..	14.3 s.u.
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo2D -- S2 ..	17.0 s.u.
PLAT244 ALERT 4 G	Low 'Solvent' Ueq as Compared to Neighbors of	C1T Check
PLAT301 ALERT 3 G	Main Residue Disorder Percentage =	11 Note
PLAT432 ALERT 2 G	Short Inter X...Y Contact O1T .. C4 ..	2.92 Ang.
PLAT432 ALERT 2 G	Short Inter X...Y Contact O1T .. C3 ..	2.98 Ang.
PLAT434 ALERT 2 G	Short Inter HL..HL Contact F4T .. F4T ..	2.80 Ang.
PLAT860 ALERT 3 G	Number of Least-Squares Restraints	41 Note
PLAT910 ALERT 3 G	Missing # of FCF Reflection(s) Below Theta(Min)	2 Note
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	7 Note
PLAT978 ALERT 2 G	Number C-C Bonds with Positive Residual Density	16 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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 0 ALERT type 5 Informative message, check

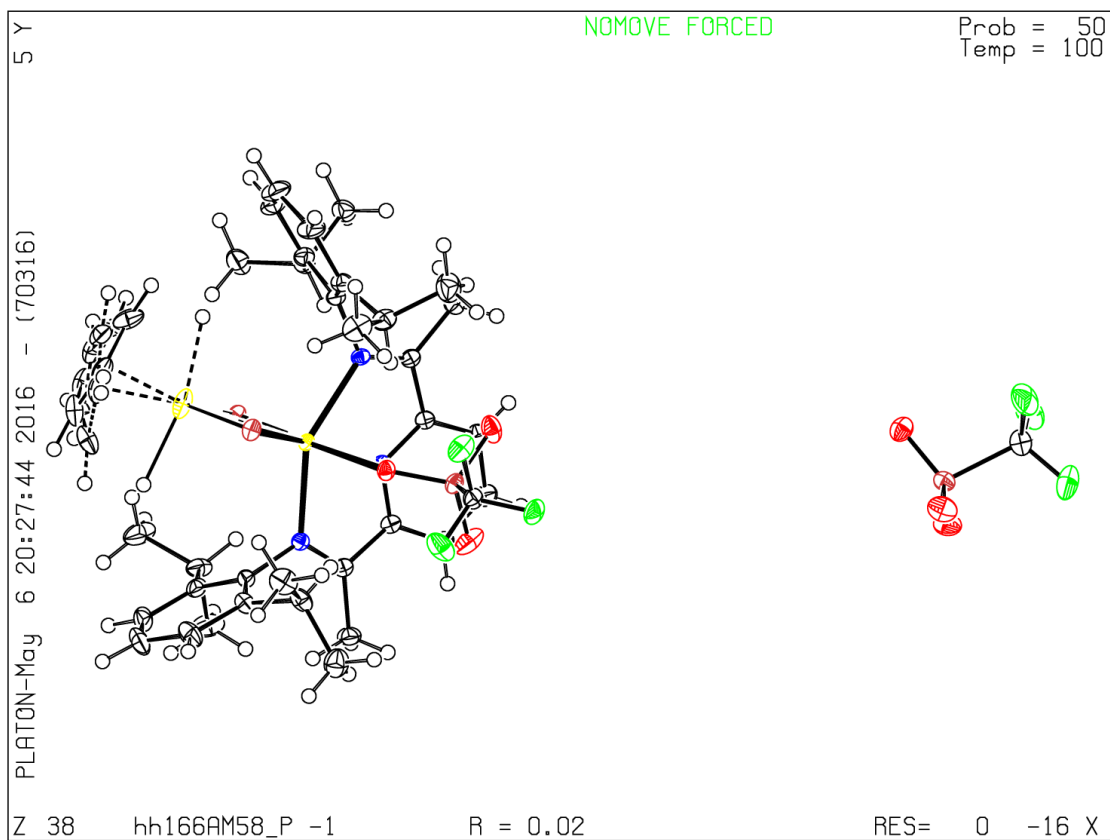
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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hh75AM22_0m

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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: hh75AM22_0m

Bond precision: C-C = 0.0018 Å

Wavelength=0.71073

Cell: a=12.1696(2) b=14.8304(3) c=16.7360(3)
alpha=64.6153(5) beta=70.7927(5) gamma=73.5133(5)
Temperature: 100 K

	Calculated	Reported
Volume	2540.65(8)	2540.65(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H54 Mo2 N5 S2, 2(B F4), 2(C2 H3 N)	?
Sum formula	C46 H60 B2 F8 Mo2 N7 S2	C46 H60 B2 F8 Mo2 N7 S2
Mr	1140.72	1140.63
Dx, g cm ⁻³	1.491	1.491
Z	2	2
Mu (mm ⁻¹)	0.645	0.645
F000	1166.1	1166.0
F000'	1160.17	
h,k,lmax	17,20,23	17,20,23
Nref	14871	14859
Tmin,Tmax	0.749,0.877	0.703,0.747
Tmin'	0.734	

Correction method= # Reported T Limits: Tmin=0.703 Tmax=0.747

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 30.033

R(reflections)= 0.0193(13854)

wR2(reflections)= 0.0493(14859)

S = 1.029

Npar= 693

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

PLAT244 ALERT 4 C	Low 'Solvent' Ueq as Compared to Neighbors of	B2 Check
PLAT731 ALERT 1 C	Bond Calc 2.8148(4), Rep 2.81475(13)	3 su-Rat
	MO1 -MO2 1.555 1.555 # 23	
PLAT732 ALERT 1 C	Angle Calc 102.60(2), Rep 102.60(1)	2.22 su-Rat
	S1 -MO1 -S2 1.555 1.555 1.555 # 39	
PLAT732 ALERT 1 C	Angle Calc 105.99(2), Rep 105.99(1)	2.22 su-Rat
	S1 -MO2 -S2 1.555 1.555 1.555 # 208	
PLAT911 ALERT 3 C	Missing # FCF Refl Between THmin & STh/L= 0.600	4 Report

● Alert level G

PLAT002 ALERT 2 G	Number of Distance or Angle Restraints on AtSite	15 Note
PLAT003 ALERT 2 G	Number of Uiso or Uij Restrained non-H Atoms ...	15 Report
PLAT171 ALERT 4 G	The CIF-Embedded .res File Contains EADP Records	3 Report
PLAT172 ALERT 4 G	The CIF-Embedded .res File Contains DFIX Records	3 Report
PLAT176 ALERT 4 G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT177 ALERT 4 G	The CIF-Embedded .res File Contains DELU Records	1 Report
PLAT230 ALERT 2 G	Hirshfeld Test Diff for C2S -- C3S ..	5.4 su
PLAT230 ALERT 2 G	Hirshfeld Test Diff for C4S -- C5S ..	5.9 su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- S1 ..	10.5 su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- S2 ..	12.3 su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo1 -- N3S ..	12.3 su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo2 -- S2 ..	9.5 su
PLAT232 ALERT 2 G	Hirshfeld Test Diff (M-X) Mo2 -- N1S ..	14.5 su
PLAT300 ALERT 4 G	Atom Site Occupancy of >F1 is Constrained at	0.532 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of >F2 is Constrained at	0.532 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of >F3 is Constrained at	0.532 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of >F4 is Constrained at	0.532 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of >B1 is Constrained at	0.532 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F1D is Constrained at	0.364 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F2D is Constrained at	0.364 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F3D is Constrained at	0.364 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F4D is Constrained at	0.364 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <B1D is Constrained at	0.364 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F1E is Constrained at	0.105 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F2E is Constrained at	0.105 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F3E is Constrained at	0.105 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <F4E is Constrained at	0.105 Check
PLAT300 ALERT 4 G	Atom Site Occupancy of <B1E is Constrained at	0.105 Check
PLAT302 ALERT 4 G	Anion/Solvent Disorder Percentage =	31 Note
PLAT304 ALERT 4 G	Non-Integer Number of Atoms (2.66) in Resd. #	2 Check
PLAT304 ALERT 4 G	Non-Integer Number of Atoms (1.82) in Resd. #	4 Check
PLAT304 ALERT 4 G	Non-Integer Number of Atoms (0.52) in Resd. #	5 Check
PLAT380 ALERT 4 G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C21 Check
PLAT860 ALERT 3 G	Number of Least-Squares Restraints	88 Note
PLAT910 ALERT 3 G	Missing # of FCF Reflection(s) Below Th(Min) ...	1 Report
PLAT912 ALERT 4 G	Missing # of FCF Reflections Above STh/L= 0.600	8 Note

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

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

9 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
26 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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