

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.
Please wait while processing

CIF dictionary
Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0106 Å Wavelength=0.71073
 Cell: a=10.7178(4) b=15.0809(6) c=15.7745(9)
 alpha=71.510(6) beta=75.508(2) gamma=88.493(8)
 Temperature: 293 K

	Calculated	Reported
Volume	2337.2(2)	2337.270(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Mo5 O23 P2, 4(C6 H14 N), 0.5(H4 O2), 2(H4 N)	C24 H66 Mo5 N6 O24 P2
Sum formula	C24 H66 Mo5 N6 O24 P2	C24 H66 Mo5 N6 O24 P2
Mr	1364.47	1364.46
Dx, g cm-3	1.939	1.939
Z	2	2
Mu (mm-1)	1.458	1.458
F000	1368.0	1368.0
F000'	1351.76	
h,k,lmax	13,19,20	13,19,20
Nref	10177	10169
Tmin,Tmax	0.493,0.600	0.702,0.899
Tmin'	0.327	

Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.899 AbsCorr =
PSI-SCAN
 Data completeness= 0.999 Theta(max)= 26.973
 R(reflections)= 0.0458(9203) wR2(reflections)= 0.1219(8866)
 S = 1.246 Npar= 559

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

[PLAT430_ALERT_2_A](#) Short Inter D...A Contact O23 .. O23 .. 2.41 Ang.

Alert level C

[PLAT234_ALERT_4_C](#) Large Hirshfeld Difference C21 -- C22 .. 0.23 Ang.

[PLAT234_ALERT_4_C](#) Large Hirshfeld Difference C23 -- C24 .. 0.20 Ang.

[PLAT243_ALERT_4_C](#) High 'Solvent' Ueq as Compared to Neighbors of C3 Check

And 3 other PLAT243 Alerts

[Less ...](#)

[PLAT243_ALERT_4_C](#) High 'Solvent' Ueq as Compared to Neighbors of C9 Check

[PLAT243_ALERT_4_C](#) High 'Solvent' Ueq as Compared to Neighbors of C21 Check

[PLAT243_ALERT_4_C](#) High 'Solvent' Ueq as Compared to Neighbors of C23 Check

[PLAT244_ALERT_4_C](#) Low 'Solvent' Ueq as Compared to Neighbors of C20 Check

[PLAT244_ALERT_4_C](#) Low 'Solvent' Ueq as Compared to Neighbors of C24 Check

[PLAT250_ALERT_2_C](#) Large U3/U1 Ratio for Average U(i,j) Tensor 3.9 Note

[PLAT342_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.01063 Ang.

[PLAT360_ALERT_2_C](#) Short C(sp3)-C(sp3) Bond C3 - C4 .. 1.42 Ang.

[PLAT360_ALERT_2_C](#) Short C(sp3)-C(sp3) Bond C21 - C22 .. 1.40 Ang.

[PLAT410_ALERT_2_C](#) Short Intra H...H Contact H46 .. H56 . 1.99 Ang.

[PLAT410_ALERT_2_C](#) Short Intra H...H Contact H49 .. H67 . 1.93 Ang.

[PLAT414_ALERT_2_C](#) Short Intra D-H..H-X H43 .. H55 .. 1.98 Ang.

[PLAT415_ALERT_2_C](#) Short Inter D-H..H-X H46 .. H64 .. 2.13 Ang.

PLAT417_ALERT_2_C Short Inter D-H..H-D H58 .. H60 .. 2.14 Ang.
 PLAT417_ALERT_2_C Short Inter D-H..H-D H59 .. H60 .. 2.13 Ang.
 PLAT430_ALERT_2_C Short Inter D...A Contact O4 .. O22 .. 2.86 Ang.
 PLAT737_ALERT_1_C D...A Calc 2.936(4), Rep 2.935(10) 2.5 s.u.-R
 N1 -O11 1.555 1.555 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 2.858(4), Rep 2.858(10) 2.5 s.u.-R
 N1 -O1 1.555 2.575 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 2.806(4), Rep 2.806(10) 2.5 s.u.-R
 N1 -O9 1.555 1.555 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 2.926(4), Rep 2.925(10) 2.5 s.u.-R
 N2 -O7 1.555 2.576 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 3.021(3), Rep 3.021(10) 3.3 s.u.-R
 N2 -O19 1.555 1.555 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 3.092(4), Rep 3.092(10) 2.5 s.u.-R
 N2 -O23 1.555 1.555 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 2.985(4), Rep 2.985(10) 2.5 s.u.-R
 N2 -O18 1.555 2.476 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 3.139(4), Rep 3.139(10) 2.5 s.u.-R
 C7 -O8 1.555 2.576 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 3.261(4), Rep 3.261(10) 2.5 s.u.-R
 N3 -O18 1.555 1.555 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 2.981(4), Rep 2.981(10) 2.5 s.u.-R
 N3 -O14 1.555 1.555 # 137 Check
 PLAT737_ALERT_1_C D...A Calc 2.807(4), Rep 2.806(10) 2.5 s.u.-R
 N3 -O8 1.555 1.455 # 137 Check
 PLAT758_ALERT_4_C D-H..A Calc 160.00, Rep 159.62(18) Senseless s.u.
 N1 -H1 -O11 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 162.00, Rep 161.54(19) Senseless s.u.
 N1 -H3 -O9 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 150.00, Rep 149.68(18) Senseless s.u.
 N2 -H16 -O19 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 128.00, Rep 127.81(18) Senseless s.u.
 N2 -H16 -O23 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 153.00, Rep 153.0(2) Senseless s.u.
 N3 -H29 -O18 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 176.00, Rep 176.0(2) Senseless s.u.
 N3 -H30 -O14 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 172.00, Rep 172.1(4) Senseless s.u.
 N4 -H44 -O23 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 168.00, Rep 168.0(6) Senseless s.u.
 C19 -H46 -O3 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 132.00, Rep 131.8(2) Senseless s.u.
 N5 -H59 -N3 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 141.00, Rep 141.0(5) Senseless s.u.
 N6 -H62 -O5 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 143.00, Rep 142.6(5) Senseless s.u.
 N6 -H63 -O7 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 136.00, Rep 136.5(6) Senseless s.u.
 N6 -H64 -C20 1.555 1.555 1.555 # 317 Check
 PLAT758_ALERT_4_C D-H..A Calc 132.00, Rep 132.3(4) Senseless s.u.
 C20 -H68 -N6 1.555 1.555 1.555 # 317 Check

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 24 Report
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.76 mm
 PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 190 Units
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
 PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C19 -- C24 .. 8.3 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- O6 .. 6.2 s.u.
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- O5 .. 5.7 s.u.
 PLAT300_ALERT_4_G Atom Site Occupancy of Ow1 is Constrained at 0.5 Check

And 5 other PLAT300 Alerts

Less ...

PLAT300_ALERT_4_G Atom Site Occupancy of Ow2 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H47 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H48 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H65 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H66 is Constrained at 0.5 Check

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6).. 100 % Note
 PLAT344_ALERT_2_G Unusual sp3 Angle Range in Solvent/Ion for . C20 Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact N6 .. C19 .. 2.82 Ang.

PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C6 H14 N	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C6 H14 N	3	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C6 H14 N	4	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H4 N	7	Note
PLAT793_ALERT_4_G	The Model has Chirality at P1 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at P2 (Centro SPGR)	S	Verify
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT882_ALERT_1_G	Missing datum for _diffn_reflns_av_unetI/netI .		Please Check

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

- 16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
37 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

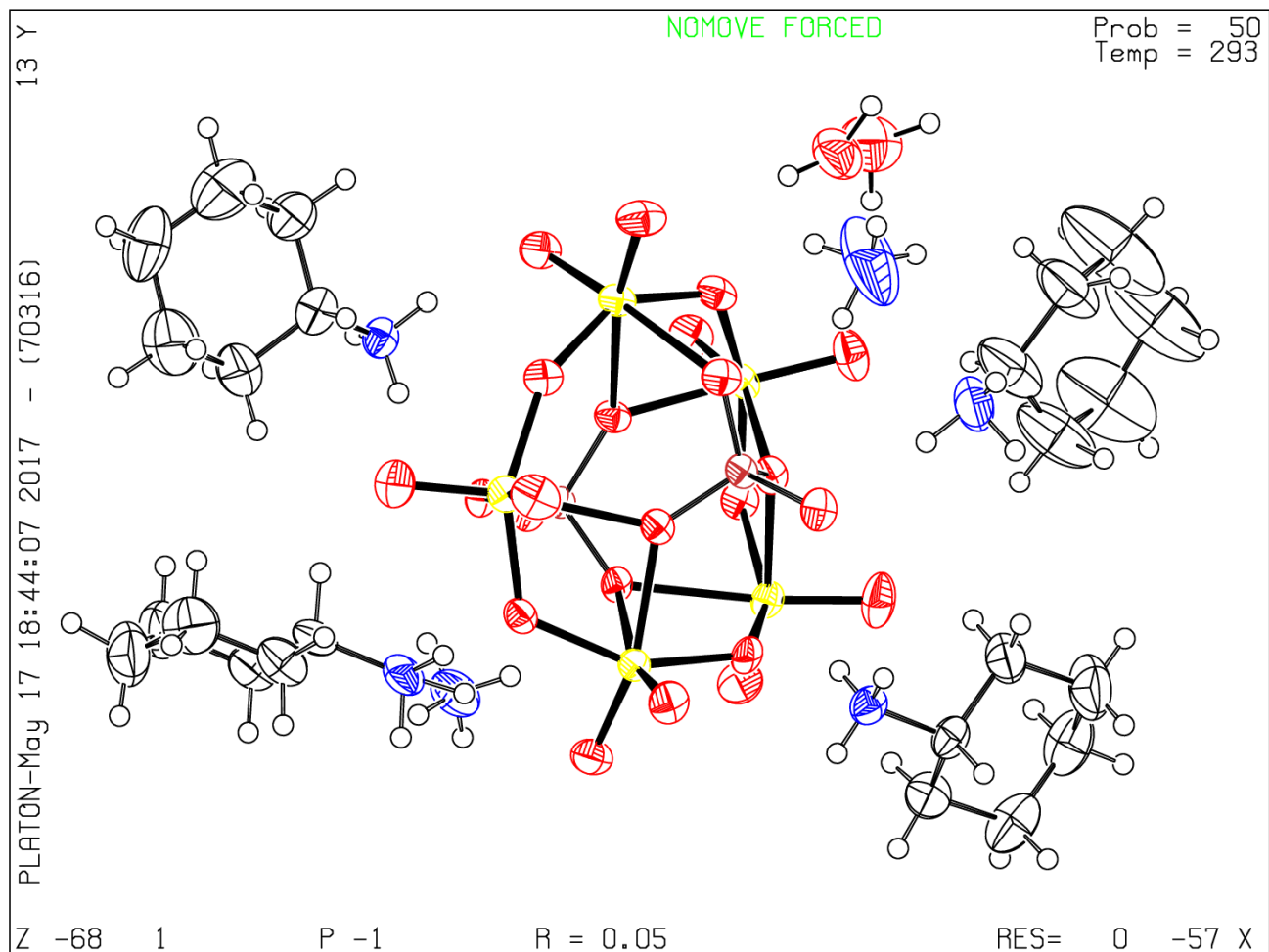
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 27/03/2017; check.def file version of 24/03/2017

Datablock 1 - ellipsoid plot



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