

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 6\_cr2\_pristine\_a

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: 6\_cr2\_pristine\_a

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Bond precision:    N- C = 0.0096 Å                      Wavelength=0.68890

Cell:                      a=8.9443(8)                      b=9.3385(8)                      c=9.7258(11)  
                                    alpha=86.983(9)                      beta=82.127(9)                      gamma=70.611(8)

Temperature:            30 K

	Calculated	Reported
Volume	759.04(13)	759.04(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 Mo N7, 0.17(O2), 1.659(O), 4(K)	C7 K4 Mo N7 O1.659, 0.341(O)
Sum formula	C7 K4 Mo N7 O2	C7 K4 Mo N7 O2
Mr	466.48	466.48
Dx, g cm <sup>-3</sup>	2.041	2.041
Z	2	2
Mu (mm <sup>-1</sup> )	1.791	1.791
F000	450.0	450.0
F000'	447.80	
h,k,lmax	11,12,12	11,12,12
Nref	3767	3635
Tmin,Tmax	0.938,0.982	0.998,1.000
Tmin'	0.931	

Correction method= # Reported T Limits: Tmin=0.998 Tmax=1.000  
AbsCorr = EMPIRICAL

Data completeness= 0.965                      Theta(max)= 27.338

R(reflections)= 0.0671( 2415)

wR2(reflections)=  
0.1805( 3635)

S = 1.060

Npar= 200

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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.

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#### Alert level A

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.83Ang From MolA 5.17 eA-3

**Author Response: The residual density near molybdenum is due to partial photoinduced changes in the crystal structure caused by a strong synchrotron X-ray source.**

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#### Alert level B

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 5.13 eA-3

**Author Response: The residual density near molybdenum is due to partial photoinduced changes in the crystal structure caused by a strong synchrotron X-ray source.**

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PLAT306\_ALERT\_2\_B Isolated Oxygen Atom (H-atoms Missing ?) ..... 01A Check

**Author Response: The water molecules in the structure are disordered, so we decided not to model the positions of the hydrogen atoms, since the refinement led to an unphysical result.**

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#### Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

PLAT029\_ALERT\_3\_C \_diffrn\_measured\_fraction\_theta\_full value Low . 0.976 Why?

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C7 Mo N7, 0.17(O2), 1.659(O), 4(K)

Rep.: C7 K4 Mo N7 O1.659, 0.341(O)

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.43 Report

PLAT213\_ALERT\_2\_C Atom C3A has ADP max/min Ratio ..... 3.3 prolat

PLAT213\_ALERT\_2\_C Atom C4A has ADP max/min Ratio ..... 3.4 prolat

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.8 Ratio

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.267 Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 64 Report

-4	-8	2,	-6	-7	2,	-4	-8	3,	-3	-8	3,	5	-4	4,	4	-5	5,
1	7	5,	4	-4	6,	7	3	6,	-1	-8	7,	-2	-7	7,	-1	-7	7,
-1	-6	7,	-1	-5	7,	4	-3	7,	-3	-7	8,	-2	-7	8,	-1	-7	8,
0	-7	8,	1	-7	8,	-3	-6	8,	-2	-6	8,	-1	-6	8,	0	-6	8,
1	-6	8,	-2	-5	8,	-1	-5	8,	0	-5	8,	1	-5	8,	2	-5	8,
0	-4	8,	3	-3	8,	-3	-2	8,	-2	1	8,	3	5	8,	-3	-6	9,
-2	-6	9,	-1	-6	9,	0	-6	9,	1	-6	9,	-2	-5	9,	-1	-5	9,

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      0 -5  9,   1 -5  9,   2 -5  9,   -1 -4  9,   0 -4  9,   1 -4  9,
     -1 -2  9,   -1 -1  9,   -1  0  9,   0  1  9,   0  2  9,   1  2  9,
     -2 -5 10,   -1 -5 10,   0 -5 10,   1 -5 10,   -1 -4 10,   0 -4 10,
      1 -4 10,   2 -4 10,   0 -3 11,   1 -3 11,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.50Ang From K1A              1.80 eA-3

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**Author Response: The residual density near molybdenum is due to partial photoinduced changes in the crystal structure caused by a strong synchrotron X-ray source.**

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.65Ang From MolA          -1.55 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      MolA          1.41 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      K1A          1.31 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From O1A      .          1.09 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.90Ang From O2A      .          0.62 eA-3

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#### Alert level G

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ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
                    not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          1 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..        Please Check
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd   2)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd   4)        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd   2)        0.68 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd   4)        0.66 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O2A Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #          3 Note
O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #          4 Note
O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #          5 Note
K
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #          6 Note
K
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....              6 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..        Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
O  1  0,   0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          66 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
O  1  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....            4.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....            1.550 Note
Predicted wr2: Based on SigI**2 11.64 or SHELX Weight 17.03
PLAT984_ALERT_1_G The K-f' = 0.1940 Deviates from the B&C-Value          0.1927 Check
PLAT984_ALERT_1_G The Mo-f' = -1.8750 Deviates from the B&C-Value        -1.8622 Check
PLAT985_ALERT_1_G The K-f" = 0.2390 Deviates from the B&C-Value          0.2361 Check
PLAT985_ALERT_1_G The Mo-f" = 0.6620 Deviates from the B&C-Value          0.6534 Check

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain  
2 **ALERT level B** = A potentially serious problem, consider carefully

16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
25 **ALERT level G** = General information/check it is not something unexpected

9 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  
6 ALERT type 3 Indicator that the structure quality may be low  
11 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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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.

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