checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2_cr1_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: 2_cr1_pristine_a

```
Bond precision:   N- C = 0.0119 A          Wavelength=0.68890

Cell:           a=8.9957(10)        b=9.3395(11)       c=9.7432(12)
                alpha=86.908(11)    beta=82.149(11)    gamma=70.48(1)
Temperature:    30 K
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	Calculated	Reported
Volume	764.27(16)	764.27(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 Mo N7, 0.168(O2), 1.665(O), 4(K)	C7 K4 Mo N7 O2
Sum formula	C7 K4 Mo N7 O2	C7 K4 Mo N7 O2
Mr	466.48	466.48
Dx,g cm-3	2.027	2.027
Z	2	2
Mu (mm-1)	1.779	1.779
F000	450.0	450.0
F000'	447.80	
h,k,lmax	12,13,13	12,13,13
Nref	4492	4033
Tmin,Tmax	0.938,0.982	0.998,1.000
Tmin'	0.915	

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

Data completeness= 0.898           Theta(max)= 29.071

R(reflections)= 0.0788( 2484)                    wR2(reflections)=
                                                 0.2044( 4033)
S = 1.071                  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.

Alert level A

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.83Ang From Mo1A 6.12 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.

Alert level B

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 6.20 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.

PLAT213_ALERT_2_B Atom N7A has ADP max/min Ratio ..... 5.0 prolat

Author Response: This is due to the onset of cyanide dissociation induced by a powerful synchrotron X-ray source.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1A 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.

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 . 0.979 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C7 Mo N7, 0.168(O2), 1.665(O), 4(K)
Rep.: C7 K4 Mo N7 O2
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.54 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 7.300 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 58 Report
-7 2 1, 1 8 3, -6 2 4, 2 8 4, 3 8 4, -5 0 6,
-5 1 6, -4 1 7, -4 2 7, 1 7 7, -3 1 8, -3 3 8,
-1 4 8, 0 4 8, -1 5 8, 0 5 8, 1 5 8, -1 6 8,
0 6 8, 1 6 8, -1 7 8, 0 7 8, 2 -1 9, 3 0 9,

```
                3  1  9,    3  2  9,  -2  3  9,  -1  3  9,   3  3  9,  -2  4  9,
               -1  4  9,    0  4  9,   1  4  9,  -2  5  9,  -1  5  9,   0  5  9,
                1  5  9,    2  5  9,  -1  6  9,   0  6  9,   1  6  9,   2  6  9,
                1  7  9,    2  7  9,  -2  3 10,  -1  3 10,   0  3 10,  -1  4 10,
                0  4 10,    1  4 10,   0  5 10,   1  5 10,   2  5 10,   2  6 10,
                3  6 10,    0  3 11,   1  3 11,   2  4 11,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.77Ang From K4A              1.81 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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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.74Ang From K2A              1.63 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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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.83Ang From K3A              1.55 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.  0.68Ang From Mo1A            -2.15 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Mo1A        1.17 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From N1A     .        0.73 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From O1A     .        0.65 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.94Ang From N7A     .        0.60 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O1A     .        0.59 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.
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.84 Why ?
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)       0.67 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.67 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
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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).          1 Note
                0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        400 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        3.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........      1.992 Note
             Predicted wR2: Based on SigI**2 10.26 or SHELX Weight 19.08
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
  3 ALERT level B = A potentially serious problem, consider carefully
 16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 22 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
  5 ALERT type 3 Indicator that the structure quality may be low
 10 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. 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 19/12/2024; check.def file version of 19/12/2024

Datablock 2_cr1_pristine_a - ellipsoid plot