checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Kcryptofix_MoCN6_293K

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.

Datablock: Kcryptofix_MoCN6_293K

```
C-C = 0.0169 A
Bond precision:
                                           Wavelength=0.71073
Cell:
                  a=18.4282(14)
                                    b=20.1869(18)
                                                        c=43.971(4)
                                     beta=90
                  alpha=90
                                                       gamma=90
                  293 K
Temperature:
                Calculated
                                            Reported
                16358(2)
Volume
                                            16358(2)
Space group
               Pbca
                                            Pbca
Hall group
                -P 2ac 2ab
                                            -P 2ac 2ab
                3(C18 H36 K N2 O6), C6 Mo
Moiety formula
                N6, 2 (C2 H3 N)
Sum formula
                C64 H114 K3 Mo N14 O18
                                            C64 H114 K3 Mo N14 O18
                1580.93
                                            1580.93
Dx,g cm-3
                1.284
                                            1.284
                8
                                            8
                0.382
                                            0.382
Mu (mm-1)
                                            6712.0
F000
                6712.0
F000'
                6705.75
h,k,lmax
               22,24,52
                                            22,24,52
Nref
                15001
                                            14756
                                            0.656,0.745
Tmin, Tmax
                0.888,0.963
Tmin'
                0.872
Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.745
AbsCorr = MULTI-SCAN
Data completeness= 0.984
                                   Theta(max) = 25.358
                                                      wR2 (reflections) =
R(reflections) = 0.0810(8517)
                                                      0.1866( 14756)
S = 1.049
                          Npar= 903
```

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for O9 --C38 . 10.3 s.u.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT230_ALERT_2_B Hirshfeld Test Diff for 010 --C40 . 12.1 s.u.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT230_ALERT_2_B Hirshfeld Test Diff for 010 --C41 . 13.5 s.u.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C33 --C34 . 7.4 s.u.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C35 --C36 . 7.3 s.u.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT230_ALERT_2_B Hirshfeld Test Diff for C37 --C38 . 10.0 s.u.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O9 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O10 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C25 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C36 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C37 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of K2 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT410_ALERT_2_B Short Intra H...H Contact H02S ...H35A . 1.87 Ang. $x,y,z = 1_{555}$ Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT410_ALERT_2_B Short Intra H...H Contact H02I ...H037 . 1.86 Ang. $x,y,z = 1_{555}$ Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT410_ALERT_2_B Short Intra H...H Contact H31A ...H38A . 1.86 Ang. $x,y,z=1_{555}$ Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

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Alert level C
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
            Rint given 0.132
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ......
                                                                             0.132 Report
PLAT213_ALERT_2_C Atom C30
                                        has ADP max/min Ratio .....
                                                                               3.9 prolat
PLAT230_ALERT_2_C Hirshfeld Test Diff for
                                                         --C34
                                                                               5.2 s.u.
                                                08
                 Author Response: At room temperature, the crystal begins to lose its
                 crystallization so resulting in a deterioration of structural parameters.
PLAT230_ALERT_2_C Hirshfeld Test Diff for
                                                09
                                                          --C39
                                                                               5.7 s.u.
                 Author Response: At room temperature, the crystal begins to lose its
                 crystallization so resulting in a deterioration of structural parameters.
PLAT230_ALERT_2_C Hirshfeld Test Diff for
                                                          --c37
                                                                               6.3 s.u.
                 Author Response: At room temperature, the crystal begins to lose its
                 crystallization so resulting in a deterioration of structural parameters.
PLAT230_ALERT_2_C Hirshfeld Test Diff for
                                                          --C36
                                                N10
                                                                               5.5 s.u.
                 Author Response: At room temperature, the crystal begins to lose its
                 crystallization so resulting in a deterioration of structural parameters.
PLAT230_ALERT_2_C Hirshfeld Test Diff for
                                                N10
                                                          --C42
                                                                               6.6 s.u.
                 Author Response: At room temperature, the crystal begins to lose its
                 crystallization so resulting in a deterioration of structural parameters.
PLAT234_ALERT_4_C Large Hirshfeld Difference N7
                                                          --C19
                                                                              0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference 07
                                                          --C33
                                                                              0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31
                                                          --C32
                                                                              0.22 Ang.
                                                          --C42
PLAT234_ALERT_4_C Large Hirshfeld Difference C41
                                                                              0.20 Ang.
                                                          --C46
PLAT234_ALERT_4_C Large Hirshfeld Difference 014
                                                                              0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O18
                                                          --C59
                                                                              0.23 Ang.
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--C54

'MainMol' Ueg as Compared to Neighbors of

--C60 .

0.17 Ang.

0.23 Ang.

C13 Check

PLAT234_ALERT_4_C Large Hirshfeld Difference N12

PLAT234_ALERT_4_C Large Hirshfeld Difference C59

PLAT241_ALERT_2_C High

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O8 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C30 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C31 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C33 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C35 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C43 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C44 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C46 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C47 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C48 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C49 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C54 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C55 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C58 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C59 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C60 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of K1 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N9 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C26 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C34 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C38 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C39 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N11 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N12 Check

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

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PLAT410_ALERT_2_C Short Intra H...H Contact H31B ..H029 . 1.95 Ang. x,y,z = 1_{555} Check
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Author Response: At room temperature, the crystal begins to lose its crystallization so resulting in a deterioration of structural parameters.

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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....
                                                            25.314 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....
                                                             3.219 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=
                                                   0.600
                                                                 79 Report
             18 14 0, 2 24 0, 18 14 1, 11 21 1,
                                                   9 22 1, 1 24 1,
              2 24 1, 18 14 2, 9 22 2, 0 24 2, 1 24 2, 2 24 2,
             22 2 3, 18 14 3, 9 22 3, 0 24 3, 1 24 3, 2 24 3,
                               0 24 4,
              2 4 4,
                      9 22 4,
                                         1 24 4,
                                                    2 24 4,
                                                            9 22 5,
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1 24 5,
                   2 24 5,
                             1 1 6, 6 23 6, 0 24 6,
0 24 5,
1 24 6, 12 20 7,
                   6 23 7,
                            0 24 7,
                                       1 2 8, 17 15 8,
12 20 8,
         6 23 8, 16 16 10, 13 19 10, 10 21 10,
5 23 10,
         20 9 11, 15 17 11, 14 18 11, 10 21 11,
                                                8 22 11,
5 23 11,
         4 23 13, 11 20 14,
                            7 22 14,
                                       3 23 14,
                                                9 21 15,
2 23 15,
        18 12 16,
                   16 15 16,
                             6 22 16,
                                       1 23 16, 14 17 17,
         5 22 18,
                             13 17 21,
                                       2 22 21, 10 19 22,
                   7 21 20,
8 21 18,
                            3 21 25, 10 18 26,
                                                6 20 26,
6 21 22,
          0 22 22,
                   5 21 23,
1 21 26,
         5 20 27,
                   9 18 28,
                              7 19 28,
                                       4 20 28,
                                                10 17 29,
7 18 31,
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Alert level G
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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite
                                                                     8 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms
                                                                    11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large
                                                                  57.34 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records
                                                                     4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records
                                                                     2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature .... (K)
                                                                    293 Check
PLAT200_ALERT_1_G Reported __diffrn_ambient_temperature .... (K)
                                                                    293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....
                                                                     80 Note
             H01M
                   H01N H014
                                 H015
                                         H01Q
                                                H01R H02S
             H02I
                   H02J
                         H03A H03B
                                         H01I
                                               H01J
                                                       H02E
                                                                H02F
             H03I
                   H03J
                         HO3M HO3N HO1W HO1X HO1D
                                                              H01E
                                                       H026
                   H01G
                         H01H H01O
                                        H01P H025
            H01F
                                                              H02K
                                                              H01S
                  H023
                         H024 H01Y H01Z H03K H03L
             H02L
                                H018
                                                       H01U
                    H032
                         Н033
                                         H019 H020
                                                              H01V
             H01T
                                 H017
             H01K
                    H01L
                           H016
                                          H021
                                                 H022
                                                        H010
                                                                H011
             H02C
                    H02D
                           H02G
                                  H02H
                                          H020
                                                 H02P
                                                        H020
             H013
                    H036
                           H037
                                  H029
                                          H030
                                                 H02Y
                                                        H02Z
                                                                H02V
                           H035 H038
                                                 H02B H03G
                                        H039
            H02W
                   H034
                                                                нозн
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...
                                                                44.10 Deg.
            010 -C40 -K2 1_555 1_555 1_555 .....
                                                                223 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...
                                                                 43.30 Deg.
            07 -C33 -K2 1_555 1_555 .....
                                                                438 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...
                                                                 43.70 Deg.
            09 -C39 -K2
                           1_555 1_555 1_555 .....
                                                             # 567 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
                                                                     3 Note
            C18 H36 K N2 O6
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters
                                                                    16 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                    70 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..
                                                                 Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL
                                                                 2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
                                                                   153 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File
                                                                      3 Note
              1 2 8, 1 1 6, 2 4 4,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged
                                                                 Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ......
                                                                5.204 Note
            Predicted wR2: Based on SigI**2 3.59 or SHELX Weight 17.79
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.
                                                                      0 Info
```

⁰ ALERT level A = Most likely a serious problem - resolve or explain

¹⁶ **ALERT level B** = A potentially serious problem, consider carefully

⁶⁵ ALERT level C = Check. Ensure it is not caused by an omission or oversight

²¹ **ALERT level G** = General information/check it is not something unexpected

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3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
71 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
19 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

