checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sggrb3

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: sggrb3

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Bond precision:  C-C = 0.0122 A          Wavelength=0.71073

Cell:            a=19.454(2)     b=13.2430(11)       c=21.905(2)
                 alpha=90        beta=94.494(4)      gamma=90
Temperature:     150 K

                Calculated                Reported
Volume          5626.0(9)                 5626.2(9)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C24 H34 B4 Cr Mo2 O4      C24 H38 B4 Cr Mo2 O4
Sum formula     C24 H34 B4 Cr Mo2 O4      C24 H38 B4 Cr Mo2 O4
Mr              673.63                    677.66
Dx,g cm-3       1.591                     1.600
Z               8                         8
Mu (mm-1)       1.285                     1.285
F000            2704.0                    2736.0
F000'           2679.72
h,k,lmax        25,17,28                  25,17,28
Nref            12920                     12768
Tmin,Tmax       0.781,0.914               0.672,0.874
Tmin'           0.475

Correction method= # Reported T Limits: Tmin=0.672 Tmax=0.874
AbsCorr = MULTI-SCAN

Data completeness= 0.988          Theta(max)= 27.484

R(reflections)= 0.0810( 10014)    wR2(reflections)= 0.2013( 12768)

S = 1.018                 Npar= 651
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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. 0.86A From Mo3 6.70 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.71A From Mo4 5.89 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.84A From Mo1 4.90 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.75A From Mo3 -6.10 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.81A From Mo4 -4.01 eA-3

Author Response: same as above

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -6.070
Test value = -4.200

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density   7.10 eA-3

Author Response: same as above

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density   -6.07 eA-3

Author Response: same as above

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).   17 Note

Author Response: These reflections are cut by the beam-stop

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.72A   From Mo2   3.48 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.20A   From Mo3   3.03 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

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Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   4.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT213_ALERT_2_C Atom B82   has ADP max/min Ratio .....   3.8 prolat
PLAT230_ALERT_2_C Hirshfeld Test Diff for   B81   --B82   .   7.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference B83   --B84   .   0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   B82 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   B83 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01215 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   4.723 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   97 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.28A   From Mo4   2.32 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.37A   From B81   2.23 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.00A   From B83   1.72 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.38A   From Mo3   -2.36 eA-3

Author Response: same as above

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.49A   From Mo3   -1.94 eA-3

Author Response: same as above

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.64A   From Mo1   -1.64 eA-3

Author Response: same as above

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.67A   From Mo4   -1.62 eA-3

Author Response: same as above

PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on   Mo1   1.10 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8A   -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19C   -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H31   -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H67C   -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H81   -0.53 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C24 H38 B4 Cr1 Mo2 O4
           Atom count from the _atom_site data: C24 H34 B4 Cr1 Mo2 O4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z   8
          From the CIF: _chemical_formula_sum C24 H38 B4 Cr Mo2 O4
          TEST: Compare cell contents of formula and atom_site data

          atom   Z*formula cif sites diff
          C   192.00   192.00   0.00

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           H        304.00    272.00   32.00
           B         32.00     32.00    0.00
           Cr         8.00      8.00    0.00
           Mo        16.00     16.00    0.00
           O         32.00     32.00    0.00
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     133.36 Why ?
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C21 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C18 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         40 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  27 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  31 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.

PLATON version of 06/01/2019; check.def file version of 19/12/2018

Datablock sggrb3 - ellipsoid plot