checkCIF/PLATON report

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

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: mo_d8v3172_1_0m_morten

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Bond precision:  C-C = 0.0172 A          Wavelength=0.71073

Cell:            a=12.6186(6)     b=15.7588(8)     c=20.5581(9)
                 alpha=90         beta=90          gamma=90
Temperature:     122 K
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	Calculated	Reported
Volume	4088.1(3)	4088.1(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C30 H24 Cr F18 O12 Pr	C30 H24 Cr F18 O12 Pr
Sum formula	C30 H24 Cr F18 O12 Pr	C30 H24 Cr F18 O12 Pr
Mr	1111.40	1111.40
Dx,g cm-3	1.806	1.806
Z	4	4
Mu (mm-1)	1.581	1.581
F000	2180.0	2180.0
F000’	2182.32	
h,k,lmax	15,18,24	15,18,24
Nref	7478[4170]	7465
Tmin,Tmax	0.846,0.887	0.584,0.745
Tmin’	0.822	

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Correction method= # Reported T Limits: Tmin=0.584 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.79/1.00      Theta(max)= 25.349

R(reflections)= 0.0555( 6993)     wR2(reflections)= 0.1433( 7465)

S = 1.073                 Npar= 646
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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 B

PLAT234_ALERT_4_B Large Hirshfeld Difference F12 --C2AA 0.26 Ang.

Alert level C

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 6.46 Note
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for F11 --C7AA . 6.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F1 --C4AA 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F0AA --C7AA 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F3AA --C3 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F2AA --C3 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F15 --C7AA 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O0AA --C4BA 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2 --C9BA 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O13 --C8BA 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O17 --C5BA 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7AA --C3BA 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7AA --C8BA 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O0AA Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01725 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H5AB ..H7BA 2.01 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 22.48 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C4AA Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C2AA Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C7AA Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C8AA Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0CA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2CA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1CA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3CA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0CA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BA Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H2CA       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        15% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         46 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.21 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4AA     --C9BA            1.73 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C8AA     --C3AA            1.79 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C6BA     --C0CA            2.01 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2BA     --C3AA            2.01 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         89 Check
              C6BA -O31  -C8      1.555   1.555   1.555             41.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        137 Check
              C8   -C10  -C6BA    1.555   1.555   1.555             32.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        168 Check
              C9AA -C8AA -C3AA    1.555   1.555   1.555             37.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        191 Check
              C8   -C6BA -C0CA    1.555   1.555   1.555             37.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        193 Check
              C9AA -C2BA -C3AA    1.555   1.555   1.555             30.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        214 Check
              C4BA -C3   -C3CA    1.555   1.555   1.555             42.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        224 Check
              C8   -C0CA -C6BA    1.555   1.555   1.555             22.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        233 Check
              C9AA -C3AA -C2BA    1.555   1.555   1.555             40.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        253 Check
              C4AA -C9BA -F13     1.555   1.555   1.555             40.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        265 Check
              C2AA -C1CA -F20     1.555   1.555   1.555             40.90 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         36 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cr2       (III)     .       3.23 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         78 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  57 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  19 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  51 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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock mo_d8v3172_1_0m_morten - ellipsoid plot