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_d8v3276_0m

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Bond precision:    C-C = 0.0168 A              Wavelength=0.71073

Cell:            a=12.6928(15)      b=15.7124(19)      c=20.603(2)
                 alpha=90           beta=90            gamma=90
Temperature:     122 K

                   Calculated                Reported
Volume           4109.0(8)                 4109.0(8)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C30 H24 Cr F18 La O12     C30 H24 Cr F18 La O12
Sum formula      C30 H24 Cr F18 La O12     C30 H24 Cr F18 La O12
Mr               1109.40                   1109.40
Dx,g cm-3        1.793                     1.793
Z                4                         4
Mu (mm-1)        1.427                     1.427
F000             2172.0                    2172.0
F000'            2174.04
h,k,lmax         16,20,27                  16,20,27
Nref             10197[ 5628]              10186
Tmin,Tmax        0.859,0.900               0.643,0.746
Tmin'            0.780

Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00      Theta(max)= 28.282

R(reflections)= 0.0676( 8846)     wR2(reflections)= 0.1767( 10186)

S = 1.050                  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

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PLAT230_ALERT_2_B Hirshfeld Test Diff for   F6AA     --C8AA    .        8.3 s.u.
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Alert level C

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PLAT213_ALERT_2_C Atom F5              has ADP max/min Ratio .....        3.1 prolat
PLAT215_ALERT_3_C Disordered C6#       has ADP max/min Ratio .....        3.2 Note
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C    Ueq(max)/Ueq(min) Range       5.4 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 1  F    Ueq(max)/Ueq(min) Range       3.6 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H    Uiso(max)/Uiso(min) Range       4.9 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   F5AA     --C8AA    .          6.7 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4        --C7            0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O13       --C10           0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O13       --C5BA          0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O16       --C5            0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O16       --C0CA          0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O17       --C1BA          0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1AA      --C5AA          0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5        --C7AA          0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6        --C1BA          0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10       --C16           0.19 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O17 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.01675 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H3BB     ..H4BA          2.03 Ang.
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Alert level G

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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 ...         7 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     26.47 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         4 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C8AA     --C20     .          7.2 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C1AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C6 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C7 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      C16 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4AA     Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5AA     Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10      Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6AA     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 C2BA     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 C4BA     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 C18      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 C7BA     Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20      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 C0CA     Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AA     Constrained at       0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H2BA        Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18         Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4BA        Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6BA        Constrained at         0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )          15% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F7AA    ..C4BA                 2.95 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F11     ..C2                   2.89 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          48 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C7       --C8BA              1.75 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C7AA     --C0CA              1.87 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        201 Check
          C7  -C8BA -F4      1.555   1.555   1.555            42.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        210 Check
          C16 -C5BA -F13     1.555   1.555   1.555            44.50 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Cr2       (III)    .         3.19 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         66 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
  20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  47 ALERT level G = General information/check it is not something unexpected


   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  22 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
  39 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