checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kv908

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: kv908

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Bond precision:   C-C = 0.0062 A            Wavelength=0.71073

Cell:           a=15.9891(18)     b=27.544(3)           c=21.779(2)
                alpha=90          beta=108.762(4)       gamma=90
Temperature:    200 K

                Calculated                Reported
Volume          9081.9(17)                9081.7(17)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
                4(C20 H23 Mn N3 O5), 4(C18 C20 H23 Mn N3 O5, C18 H22
Moiety formula  H22 Mn N2 O6), 8(C24 H20  Mn N2 O6, 5(C2 H3 N),
                B), 19(C2 H                2(C24 H20 B)
Sum formula     C384 H400 B8 Mn8 N40 O44   C96 H100 B2 Mn2 N10 O11
Mr              6805.44                   1701.35
Dx,g cm-3       1.244                     1.244
Z               1                         4
Mu (mm-1)       0.342                     0.342
F000            3576.0                    3576.0
F000'           3580.05
h,k,lmax        19,32,25                  19,32,25
Nref            16022                     16018
Tmin,Tmax       0.968,0.973               0.699,0.745
Tmin'           0.893

Correction method= # Reported T Limits: Tmin=0.699 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.000        Theta(max)= 25.027

R(reflections)= 0.0563( 9349)     wR2(reflections)= 0.1556( 16018)

S = 1.021                 Npar= 1143
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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 C

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.10 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C217    --  C218    ..     6.5 s.u.
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      N13 Check
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C217 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of     C130 Check
PLAT244_ALERT_4_C Low     'Solvent' Ueq as Compared to Neighbors of     C12S Check
PLAT244_ALERT_4_C Low     'Solvent' Ueq as Compared to Neighbors of     C22S Check
PLAT244_ALERT_4_C Low     'Solvent' Ueq as Compared to Neighbors of     C32S Check
PLAT244_ALERT_4_C Low     'Solvent' Ueq as Compared to Neighbors of     C42S Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00624 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond   C217   -   C218    ..     1.43 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.595        4 Report
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        4 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        6 Report
PLAT012_ALERT_1_G No     _shelx_res_checksum found in CIF ........ Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.25 Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records        3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for     N13    --  C130    ..     5.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of N71S    is Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C72S    is Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C73S    is Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73A    is Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73B    is Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73C    is Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N51S    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52S    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C53S    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53A    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53B    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53C    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N61S    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C62S    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C63S    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H63B    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H63A    is Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H63C    is Constrained at     0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..        7 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13)..      100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.50) in Resd. #       10 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.25) in Resd. #       11 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.25) in Resd. #       12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #       13 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.25) in Resd. #       14 Check
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PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.25) in Resd. #      15 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      14 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)        2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        2 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  45 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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
  37 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 27/03/2017; check.def file version of 24/03/2017