checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ov_pmf_auto

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: ov_pmf_auto

Bond precision: C-C = 0.0108 A   Wavelength=1.54184

Cell: a=41.6176(10)   b=10.7884(2)   c=22.8010(6)
                   alpha=90   beta=99.547(2)   gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	10095.6(4)	10095.6(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	3(C24 H26 Cl4 Fe2 N6), 5(C H2 Cl2)	1.5(C24 H26 Cl4 Fe2 N6), 2.5(C H2 Cl2)
Sum formula	C77 H88 Cl22 Fe6 N18	C38.50 H44 Cl11 Fe3 N9
Mr	2380.66	1190.32
Dx,g cm-3	1.566	1.566
Z	4	8
Mu (mm-1)	12.496	12.496
F000	4824.0	4824.0
F000'	4837.90	
h,k,lmax	52,13,28	52,13,28
Nref	10624	10116
Tmin,Tmax	0.156,0.287	0.189,0.368
Tmin'	0.043	

Correction method= # Reported T Limits: Tmin=0.189 Tmax=0.368
AbsCorr = MULTI-SCAN

Data completeness= 0.952   Theta(max)= 76.545

R(reflections)= 0.0696(6413)   wR2(reflections)= 0.2304(10116)

S = 1.039   Npar= 636

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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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
              a literature citation. This should be contained in the
              _exptl_absorpt_process_details field.
              Absorption correction given as multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ      Please Check
              Calc: C77 H88 Cl22 Fe6 N18
              Rep.: C38.50 H44 Cl11 Fe3 N9
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ      Please Check
              Calc: 3(C24 H26 Cl4 Fe2 N6), 5(C H2 Cl2)
              Rep.: 1.5(C24 H26 Cl4 Fe2 N6), 2.5(C H2 Cl2)
PLAT234_ALERT_4_C Large Hirshfeld Difference C26      --C27      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31      --C42      .       0.23 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Fe03 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of      Cl18 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C37 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl8    0.197 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl1    0.169 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl7    0.157 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.01075 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N7      --H7      .      Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    2.562 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       43 Report
              16 12  0,  35  9  0, -35  9  1, -16 12  1, -14 12  1, -35  9  2,
             -14 12  2, -14 12  3,  19  3  3,  21  3  3,  18  4  4, -38  8  6,
             -38  8  7, -36  8  7,   4 12  7, -34  8  8, -30 10  8, -28 10  8,
              42  4  8, -30  8  9, -28 10  9, -26 10  9, -28 10 10,  40  4 10,
               3 11 11,   3 11 12, -44  4 13,  -9 11 14,  31  5 14,  32  4 14,
             -32  8 15, -30  8 15, -27  9 15,  32  4 15,  35  3 15,  29  5 16,
              34  2 16, -10 10 17,  30  4 17, -13  7 22, -11  7 22,   7  5 23,
               5  5 24,
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        5 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms       18 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        3 Report
              H1     H4     H7
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   15.84 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        7 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used   0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used   0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par   0.0010 Report
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PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0020 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used      0.0400 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for      C7      --C46      .      9.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for      C7      --C8      .      5.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for      C31      --C32      .      5.1 s.u.
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............      0.5 Check
          H38A      H38B
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)       33% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    2)       17% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       67% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H7BC     ..H6B     .      2.11 Ang.
                                             x,y,z =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H6B      ..H7AB    .      2.10 Ang.
                                             x,y,z =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H30A     ..H31A    .      2.14 Ang.
                                             x,y,z =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H30A     ..H31D    .      2.12 Ang.
                                             x,y,z =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H1       ..H7BD    .      2.05 Ang.
                                             x,y,z =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H1       ..H7AA    .      2.04 Ang.
                                             x,y,z =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H7       ..H31B    .      2.09 Ang.
                                             x,y,z =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H7       ..H31C    .      2.07 Ang.
                                             x,y,z =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2      ..Cl2     .      3.27 Ang.
                                   3/2-x,-1/2-y,1-z =      7_646 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       13 Note
          Fe01      Fe02      Fe03      H7BC      H7BD      H7AA      H7AB      N0
          C0        H0        C01R      H01A      H01B
PLAT721_ALERT_1_G Bond    Calc    0.96000, Rep    0.97000 Dev...       0.01 Ang.
          C39      -H39A        1_555  1_555 ........    #  124 Check
PLAT722_ALERT_1_G Angle   Calc    107.00, Rep    108.10 Dev...       1.10 Degree
          CL10     -C39     -H39B     1_555  1_555  1_555  #  248 Check
PLAT793_ALERT_4_G Model has Chirality at N1        (Centro SpGr)        R Verify
PLAT793_ALERT_4_G Model has Chirality at N4        (Centro SpGr)        R Verify
PLAT793_ALERT_4_G Model has Chirality at N7        (Centro SpGr)        S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Fe01     (II)     .      1.91 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      350 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
            2  0  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      464 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........      3.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    4.640 Note
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                  Predicted wR2: Based on SigI**2  4.97 or SHELX Weight 22.18
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
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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
  17 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

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 ALERT type 2 Indicator that the structure model may be wrong or deficient
  25 ALERT type 3 Indicator that the structure quality may be low
  16 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 02/02/2025; check.def file version of 02/02/2025

Datablock ov_pmf_auto - ellipsoid plot

NOMOVE FORCED

Prob = 50%
Temp = 298K

23 Y

PLATON-Mar 24 7:20:22 2025 - (20225)

Z -41   ov_pmf_auto   C 1 2/c 1   R = 0.07   RES= 0   18 X