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: 1_c

```
Bond precision:   C-C = 0.0258 A          Wavelength=1.54178

Cell:             a=37.098(2)    b=29.5954(16)       c=23.5807(13)
                  alpha=90       beta=102.756(3)     gamma=90
Temperature:      193 K
```

	Calculated	Reported
Volume	25251(2)	25251(2)
Space group	C 2	C 2
Hall group	C 2y	C 2y
Moiety formula	C168 H108 Cl4 Fe3 N12 O20 Zr6, C168 H108 Cl2 Fe3 N12 O20 Zr6, 8	C168 H114 N12 O20 Zr6 Fe3 Cl3, 4(C3 H7 N O), 5(O), 2(Cl)
Sum formula	C360 H272 Cl10 Fe6 N32 O58 Zr12 [+ solvent]	C360 H272 Cl10 Fe6 N32 O58 Zr12
Mr	7758.35	7758.32
Dx,g cm-3	1.020	1.020
Z	2	2
Mu (mm-1)	4.196	4.196
F000	7852.0	7852.0
F000'	7860.93	
h,k,lmax	44,35,28	44,35,28
Nref	46446[23711]	45636
Tmin,Tmax	0.403,0.414	0.365,0.420
Tmin'	0.305	

```
Correction method= # Reported T Limits: Tmin=0.365 Tmax=0.420
AbsCorr = MULTI-SCAN

Data completeness= 1.92/0.98        Theta(max)= 68.423
```

R(reflections)= 0.0754(30760)

wR2(reflections)= 0.2253(45636)

S = 0.983 Npar= 2131

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.

[IMAGE] **Alert level B**

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PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C152 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        Fe1 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C147 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including       O25      0.373 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including       O24      0.351 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O21 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O22 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O23 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O24 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O27 Check
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.02576 Ang.
PLAT368_ALERT_2_B Short  C(sp2)-C(sp2) Bond  C76      - C76_a    .       1.12 Ang.
PLAT369_ALERT_2_B Long   C(sp2)-C(sp2) Bond  C153     - C153_b   .       1.60 Ang.
PLAT369_ALERT_2_B Long   C(sp2)-C(sp2) Bond  C1       - C2       .       1.57 Ang.
PLAT369_ALERT_2_B Long   C(sp2)-C(sp2) Bond  C33      - C50      .       1.58 Ang.
PLAT369_ALERT_2_B Long   C(sp2)-C(sp2) Bond  C74      - C79      .       1.64 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O7       ..O301     .       2.69 Ang.
                                                      x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O13      ..O26      .       2.70 Ang.
                                                 1-x,1+y,1-z  =      2_666 Check
PLAT987_ALERT_1_B The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ...          ! Note
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[IMAGE] **Alert level C**

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STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.449
          From the CIF: _refine_ls_abs_structure_Flack_su    0.012
PLAT214_ALERT_2_C Atom O24       (Anion/Solvent) ADP max/min Ratio        4.4 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Fe4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C02U Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C03S Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C03W Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C056 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C91 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C92 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C101 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C114 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C122 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C135 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C137 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C142 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C146 Check
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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C151 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C167 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C35 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C41 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C60 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C65 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C80 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C82 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zr4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zr5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zr6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N14 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C02L Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C90 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C136 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zr1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zr3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C61 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C63 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C77 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C81 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        N18 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        N15 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        N16 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C160 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        N17 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O28      0.280 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O301      0.126 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O21      0.246 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O22      0.266 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O23      0.279 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O27      0.278 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .....           O25 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .....           O28 Check
PLAT317_ALERT_2_C Too many H on C in C=N Moiety in Solvent/Ion ...      C166 Check
PLAT332_ALERT_2_C Large Phenyl C-C Range     C50       -C55      .      0.23 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range     C56       -C61      .      0.21 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C047     - C167     .      1.55 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C056     - C05E     .      1.56 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C108     - C125     .      1.54 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C128     - C131     .      1.56 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C136     - C139     .      1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C146     - C154     .      1.56 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C6       - C10      .      1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C26      - C27      .      1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C28      - C43      .      1.55 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C62      - C63      .      1.54 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H15G     ..H15J     .      1.89 Ang.
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                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H02L     ..H16I     .       2.03 Ang.
                                               1-x,1+y,1-z  =      2_666 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H13      ..H15L     .       2.06 Ang.
                                                    x,y,z  =      1_555 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C168 H108 Cl4 Fe3 N12 O20 Zr6
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[IMAGE] **Alert level G**

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C360 H272 Cl10 Fe6 N32 O58 Zr
           Atom count from _chemical_formula_moiety:C180 H142 Cl5 Fe3 N16 O29 Zr6
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         12 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        219 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * Sigma from Zero .      0.449 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
            Calc: C168 H108 Cl4 Fe3 N12 O20 Zr6, C168 H108 Cl2 F
                  e3 N12 O20 Zr6, 8(C3 H7 N O), 4(Cl), 10(O)
            Rep.: C168 H114 N12 O20 Zr6 Fe3 Cl3, 4(C3 H7 N O), 5
                  (O), 2(Cl)
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         13 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C87      -C92            0.16 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C43      -C48            0.15 Ang.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C155 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C157 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C164 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C166 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C158 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C159 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C161 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C162 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl4      ..O2       .       3.06 Ang.
                                                    x,y,z  =      1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl4      ..O14      .       3.07 Ang.
                                                  1-x,-1+y,1-z  =      2_646 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl5      ..O8       .       2.96 Ang.
                                                    x,y,z  =      1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl5      ..O12      .       2.99 Ang.
                                                  1-x,-1+y,1-z  =      2_646 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2      ..C157     .       2.91 Ang.
                                               1/2-x,1/2+y,1-z  =      4_556 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         26 Note
            C01W    H01W    C028    H028    C02L    H02L    C02U    H02U
            C03P    H03P    C03S    H03S    C03W    H03W    C047    H047
            C04F    H04F    C04T    H04T    C056    H056    C05E    H05E
            C05G    H05G
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
            C3 H7 N O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          9 Note
            O
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PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         10 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         11 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         12 Note
             O
PLAT794_ALERT_5_G Tentative Bond Valency for Zr1       (IV)      .       4.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr2       (IV)      .       4.26 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr3       (IV)      .       3.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr4       (IV)      .       3.92 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr5       (IV)      .       4.45 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zr6       (IV)      .       3.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)      .       1.98 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (II)      .       2.35 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe3       (III)     .       2.79 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe4       (III)     .       3.19 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1424 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated   and Succeeded by SHELXL     2019/3 Note
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  0 ALERT level A = Most likely a serious problem - resolve or explain
 20 ALERT level B = A potentially serious problem, consider carefully
 79 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

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 96 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
 30 ALERT type 4 Improvement, methodology, query or suggestion
 10 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 1_c - ellipsoid plot