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: Fe3

```
Bond precision:  C-C = 0.0044 A          Wavelength=1.54184

Cell:            a=32.4190(2)     b=32.4190(2)     c=31.8280(3)
                 alpha=90         beta=90          gamma=90
Temperature:     170 K
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	Calculated	Reported
Volume	33451.0(5)	33451.0(5)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C92 H91 Cl2 Fe N3 [+ solvent]	C92 H91 Cl2 Fe N3
Sum formula	C92 H91 Cl2 Fe N3 [+ solvent]	C92 H89 Cl2 Fe N3
Mr	1365.43	1363.41
Dx,g cm-3	1.084	1.083
Z	16	16
Mu (mm-1)	2.359	2.359
F000	11584.0	11552.0
F000’	11604.33	
h,k,lmax	40,40,39	36,40,39
Nref	17360	16088
Tmin,Tmax	0.753,0.889	0.743,1.000
Tmin’	0.702	

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Correction method= # Reported T Limits: Tmin=0.743 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.927          Theta(max)= 75.566

R(reflections)= 0.0531( 13594)    wR2(reflections)= 0.1417( 16088)

S = 1.026                 Npar= 967
```

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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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.965 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.85 Report
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
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C34      --C35      .        6.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30      --C31      .       0.19 Ang.
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        C37 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C38 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C51 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C69 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C70 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C75 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C76 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C78 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C68 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C71 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C74 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C77 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C28      --C33      .       1.36 Ang.
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C74      --C79      .       1.36 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range     C28       -C33      .       0.20 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range     C01J      -C02M     .       0.20 Ang.
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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:   C92 H89 Cl2 Fe1 N3
            Atom count from _chemical_formula_moiety:C92 H91 Cl2 Fe1 N3
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C92 H89 Cl2 Fe1 N3
            Atom count from the _atom_site data:  C92 H91 Cl2 Fe1 N3
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z   16
           From the CIF: _chemical_formula_sum  C92 H89 Cl2 Fe N3
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C       1472.00   1472.00    0.00
           H       1424.00   1456.00  -32.00
           Cl        32.00     32.00    0.00
           Fe        16.00     16.00    0.00
           N         48.00     48.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        107 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT013_ALERT_1_G N.O.K.   _shelx_hkl_checksum Found in CIF ......     Please Check
PLAT014_ALERT_1_G N.O.K.   _shelx_fab_checksum Found in CIF ......     Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      44.40 Why ?
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PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00030 Ang.
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C02S     --C10      .        7.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --Cl2      .       14.7 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         9% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H02D     ..H61B     .       2.13 Ang.
                                                     x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         20 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)      .       2.13 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        168 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.0 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           4 Units
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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
  23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  27 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
   8 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

Datablock: Fe5

Bond precision: C-C = 0.0185 A Wavelength=0.71073

Cell:	a=18.8805(6)	b=19.1069(5)	c=35.1775(10)
	alpha=90	beta=90	gamma=90
Temperature:	173 K		

	Calculated	Reported
Volume	12690.2(6)	12690.2(6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	2(C70 H75 Cl2 Fe N3), 3(C H2 Cl2)	2(C70 H75 Cl2 Fe N3), 3(C H2 Cl2)
Sum formula	C143 H156 Cl10 Fe2 N6	C143 H156 Cl10 Fe2 N6
Mr	2424.95	2424.93
Dx,g cm-3	1.269	1.269
Z	4	4
Mu (mm-1)	0.492	0.492
F000	5112.0	5112.0
F000'	5122.08	
h,k,lmax	22,22,41	22,22,41
Nref	22371[12106]	21892
Tmin,Tmax	0.913,0.970	0.644,1.000
Tmin'	0.913	

Correction method= # Reported T Limits: Tmin=0.644 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.81/0.98 Theta(max)= 25.000

R(reflections)= 0.0953(13352) wR2(reflections)= 0.2913(21892)

S = 1.024 Npar= 1376

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

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01846 Ang.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.122
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.122 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C87 --C88 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C89 --C90 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C89 --C94 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C95 --C99 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C118 --C119 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C118 --C122 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C124 --C129 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C132 --C133 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C8 --C9 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C14 . 0.17 Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference C15      --C16      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22      --C23      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C32      --C33      .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35      --C36      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C44      --C45      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C54      --C59      .       0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C60      --C65      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C66      --C67      .       0.17 Ang.
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        C85 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C87 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C90 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C94 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C97 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C99 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C120 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C121 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C128 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       C139 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        C15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C50 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C51 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C58 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C59 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C69 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        C86 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C89 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C95 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C119 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C129 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C130 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C54 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C66 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C142 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl5      0.149 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl7      0.132 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C71      -C76            1.37 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C139     - C140     .       1.41 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H9A      ..H11D     .       2.11 Ang.
                                      1-x,-1/2+y,1/2-z  =      4_645 Check
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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 Uij Restrained non-H Atoms ...        73 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......    Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      7.33 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 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         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe2      --Cl4      .      10.4 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        3% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3A     ..C87           3.01 Ang.
                                       -x,1/2+y,1/2-z  =      4_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl4A     ..C142          3.20 Ang.
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                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl4A     ..C37             3.23 Ang.
                                                    x,y,z  =      1_555 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1      (II)      .       1.92 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       447 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         3 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
  58 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  45 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  24 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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

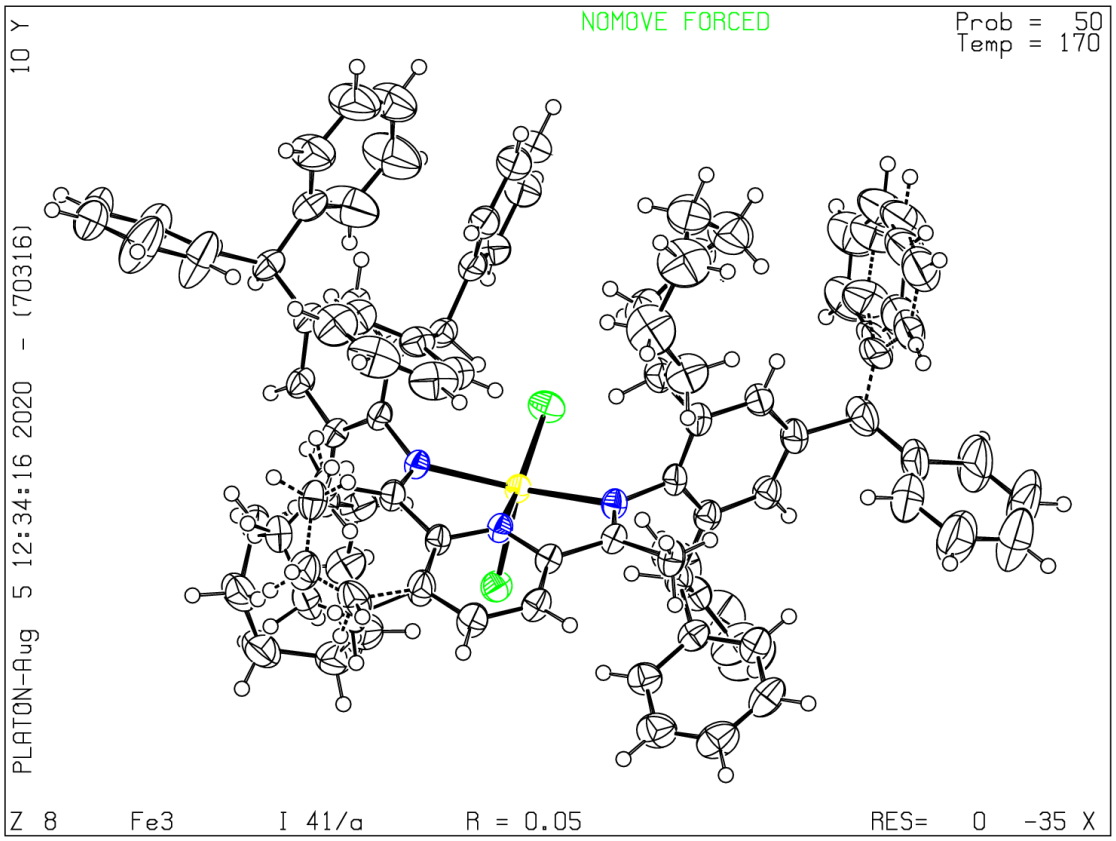
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 16/07/2020; check.def file version of 12/07/2020

Datablock Fe3 - ellipsoid plot



Datablock Fe5 - ellipsoid plot