checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0151 A   Wavelength=1.54184

Cell: a=20.4323(8)   b=27.8575(11)   c=32.2485(11)
               alpha=74.192(3)   beta=88.216(3)   gamma=87.829(3)
Temperature: 150 K

	Calculated	Reported
Volume	17644.6(12)	17644.6(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C152 H136 Fe2 N4 P4 Pd2 S8 [+ solvent]	2(C152 H136 Fe2 N4 P4 Pd2 S8), 8(C F3 O3 S), 8 (C5 H12 O)
Sum formula	C152 H136 Fe2 N4 P4 Pd2 S8 [+ solvent]	C352 H368 F24 Fe4 N8 O32 P8 Pd4 S24
Mr	2723.52	7344.72
Dx,g cm-3	1.025	1.382
Z	4	2
Mu (mm-1)	4.446	5.192
F000	5632.0	7600.0
F000'	5650.78	
h,k,lmax	25,34,39	24,33,39
Nref	70545	66698
Tmin,Tmax	0.442,0.674	0.616,1.000
Tmin'	0.295	

Correction method= # Reported T Limits: Tmin=0.616 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.945   Theta(max)= 72.990

R(reflections)= 0.1257(22013)   wR2(reflections)= 0.3734(66698)

S = 0.914   Npar= 3061

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 A

```
CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.90 <> 1.10
            From the CIF: _cell_formula_units_Z                     2
            From the CIF: _chemical_formula_weight         7344.72
            TEST: Calculate formula weight from _atom_site_*
            atom      mass      num      sum
            C         12.01   304.00  3651.34
            H          1.01   272.00   274.18
            N         14.01     8.00   112.06
            O         16.00     0.00     0.00
            F         19.00     0.00     0.00
            P         30.97     8.00   247.79
            S         32.07    16.00   513.06
            Fe        55.85     4.00   223.39
            Pd       106.42     4.00   425.68
            Calculated formula weight                 5447.49
```

**Author Response: The unit cell contains 16 methyl tert-butyl ether and 16
triflates anions not found by Fourier difference map and which were not
modelled but the corresponding scattering contribution were taken into
account using SQUEEZE/ PLATON procedure. The new composition (16
MTBE + 16 CF3SO3 per unit cell) was included in the calculation of the
empirical formula, molecular weight, density, linear absorption coefficient
and F(000).**

```
PLAT241_ALERT_2_A High    'MainMol' Ueq as Compared to Neighbors of      C81 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_A High    'MainMol' Ueq as Compared to Neighbors of      C228 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT242_ALERT_2_A Low     'MainMol' Ueq as Compared to Neighbors of      C80 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

```
PLAT242_ALERT_2_A Low     'MainMol' Ueq as Compared to Neighbors of      C83 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_A Low     'MainMol' Ueq as Compared to Neighbors of      C227 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_A Low     'MainMol' Ueq as Compared to Neighbors of      C229 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

🔴 **Alert level B**
```
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..       33 %
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ...................     0.37 Report
PLAT213_ALERT_2_B Atom C94           has ADP max/min Ratio .....      4.4 prolat
PLAT213_ALERT_2_B Atom C150          has ADP max/min Ratio .....      4.1 prolat
PLAT213_ALERT_2_B Atom C230          has ADP max/min Ratio .....      4.8 prolat
PLAT220_ALERT_2_B Non-Solvent Resd 1  C   Ueq(max)/Ueq(min) Range     10.0 Ratio
PLAT220_ALERT_2_B Non-Solvent Resd 2  C   Ueq(max)/Ueq(min) Range     10.0 Ratio
PLAT241_ALERT_2_B High  'MainMol' Ueq as Compared to Neighbors of      C33 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High  'MainMol' Ueq as Compared to Neighbors of      C35 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High  'MainMol' Ueq as Compared to Neighbors of      C146 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High  'MainMol' Ueq as Compared to Neighbors of      C150 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C151 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C187 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C189 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C192 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C193 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C235 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C246 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C260 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C263 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_B High    'MainMol' Ueq as Compared to Neighbors of      C286 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of       C32 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of       C34 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of       C82 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C147 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C152 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C191 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C232 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C234 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C255 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C259 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_B Low     'MainMol' Ueq as Compared to Neighbors of      C278 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT330_ALERT_2_B Large Average Phenyl  C-C Dist.  C119   -C124          1.43 Ang.
PLAT331_ALERT_2_B Small Average Phenyl  C-C Dist. C289    -C294          1.36 Ang.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C186   -  C187   ..         1.32 Ang.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C187   -  C188   ..         1.27 Ang.
PLAT361_ALERT_2_B Long   C(sp3)-C(sp3) Bond   C83   -  C84    ..         1.75 Ang.
PLAT369_ALERT_2_B Long    C(sp2)-C(sp2) Bond  C144  -  C145   ..         1.59 Ang.
PLAT369_ALERT_2_B Long    C(sp2)-C(sp2) Bond  C263  -  C264   ..         1.61 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H80A   ..  H82B   ..        1.83 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H22F   ..  H22G   ..        1.88 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H22G   ..  H22J   ..        1.88 Ang.
PLAT973_ALERT_2_B Check Calcd Positive Residual Density on     Pd1       1.62 eA-3
PLAT973_ALERT_2_B Check Calcd Positive Residual Density on     Pd4       1.54 eA-3
PLAT990_ALERT_1_B Deprecated RES file style based SQUEEZE job ....        ! Note
```

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.145
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........      0.145 Report
PLAT082_ALERT_2_C High R1 Value ...................................      0.13 Report
PLAT213_ALERT_2_C Atom C82              has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom C84              has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom C95              has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C106             has ADP max/min Ratio .....       3.4 oblate
PLAT213_ALERT_2_C Atom C143             has ADP max/min Ratio .....       3.9 prolat
PLAT213_ALERT_2_C Atom C145             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C146             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C149             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom C151             has ADP max/min Ratio .....       4.0 prolat
PLAT213_ALERT_2_C Atom C186             has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C187             has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C188             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C231             has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom C247             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom C253             has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C258             has ADP max/min Ratio .....       3.1 oblate
PLAT213_ALERT_2_C Atom C259             has ADP max/min Ratio .....       3.2 oblate
PLAT213_ALERT_2_C Atom C260             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C265             has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C279             has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C287             has ADP max/min Ratio .....       3.1 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range      10.0 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 2   H Uiso(max)/Uiso(min) Range      10.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        S3 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C18 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C22 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C25 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C30 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C37 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C73 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C87 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C88 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C94 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C100 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C111 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C127 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C129 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C133 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C139 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C141 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C145 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      S14 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of     C172 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C179 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C183 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C214 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C216 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C219 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C231 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C250 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

```
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of    C253 Check
```

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is higher as compared with bonded neighbors.**

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C257 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C258 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C265 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C279 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C280 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C281 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C288 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C291 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C292 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C298 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is higher as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Fe2 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   P3 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C3 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C12 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C26 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C38 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C39 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C41 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C74 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C77 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C79 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C126 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C130 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C131 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of     C140 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      Fe3 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      Fe4 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      S12 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of       P5 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of     C171 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of     C178 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of     C184 Check
```

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C186 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C190 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C197 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C213 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C225 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C237 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C243 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C248 Check

Author Response: This terminal hexyl C atom is constrained at its position with ISOR and/or DFIX constraints, that is why its thermal anisotropic displacement is lower as compared with bonded neighbors.

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C249 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C254 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C266 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C282 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C283 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C285 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C287 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C289 Check

**Author Response: This terminal hexyl C atom is constrained at its position
with ISOR and/or DFIX constraints, that is why its thermal anisotropic
displacement is lower as compared with bonded neighbors.**

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PLAT332_ALERT_2_C Large Phenyl C-C Range                C277   -C282         0.16 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range                C283   -C288         0.23 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range                C289   -C294         0.20 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.01508 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C39    -  C40    ..      1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C185   -  C186   ..      1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C189   -  C190   ..      1.34 Ang.
PLAT362_ALERT_2_C Short   C(sp3)-C(sp2) Bond  C143   -  C147   ..      1.32 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C148   -  C152   ..      1.56 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C198   -  C210   ..      1.54 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H82B   ..  H83B   ..      1.96 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H18G   ..  H18J   ..      1.92 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H22C   ..  H22E   ..      1.99 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H22D   ..  H22F   ..      1.98 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H146   ..  H247   ..      2.00 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......  23.398 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......   6.111 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......   3.088 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600      891 Report
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on      Pd2    1.05 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.       0 Note
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⚪ **Alert level G**

```
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:C352 H368 F24 Fe4 N8 O32 P8 Pd
           Atom count from the _atom_site data:  C304 H272 Fe4 N8 P8 Pd4 S16
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    2
          From the CIF: _chemical_formula_sum  C352 H368 F24 Fe4 N8 O32 P8 Pd4
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        704.00    608.00   96.00
          H        736.00    544.00  192.00
          F         48.00      0.00   48.00
          Fe         8.00      8.00    0.00
          N         16.00     16.00    0.00
          O         64.00      0.00   64.00
          P         16.00     16.00    0.00
          Pd         8.00      8.00    0.00
          S         48.00     32.00   16.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         20 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         14 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF    Please Do !
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ   Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT044_ALERT_1_G Calculated and Reported Density Dx  Differ by ..   0.3567 Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     2.00 Check
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .    14.37 %
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large     0.15 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.003 Degree
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for     C33    Check
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for     C82    Check
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for     C83    Check
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for     C143   Check
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for     C189   Check
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PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C191    Check
PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C225    Check
PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C226    Check
PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C227    Check
PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C228    Check
PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C229    Check
PLAT343_ALERT_2_G Unusual sp3         Angle Range in Main Residue for      C235    Check
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C13    -    C17    ..        1.46 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C18    -    C19    ..        1.44 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C25    -    C26    ..        1.51 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C50    -    C66    ..        1.47 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C55    -    C59    ..        1.42 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C60    -    C61    ..        1.41 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C67    -    C68    ..        1.48 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C170   -    C171   ..        1.41 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C202   -    C218   ..        1.44 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C207   -    C211   ..        1.45 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C212   -    C213   ..        1.45 Ang.
PLAT371_ALERT_2_G Long    C(sp2)-C(sp1) Bond  C219   -    C220   ..        1.43 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure         ! Info
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C83    --   C84    .         1.75 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............           97 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed            ! Info
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .       71.20 %
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)             4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         2744 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
```

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  7 ALERT level A = Most likely a serious problem - resolve or explain
 45 ALERT level B = A potentially serious problem, consider carefully
123 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 46 ALERT level G = General information/check it is not something unexpected

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

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock I - ellipsoid plot