# 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 = 0.0129 A Wavelength=1.54184

Cell: a=25.0842(6) b=25.0842(6) c=43.3591(10)
alpha=90 beta=90 gamma=120
Temperature: 150 K

| | Calculated | Reported |
|---|---|---|
| Volume | 23627.2(14) | 23627.1(10) |
| Space group | P 32 2 1 | P 32 2 1 |
| Hall group | P 32 2" | P 32 2" |
| Moiety formula | C244 H252 N6 O12 Ru6, 2(C H3) | C246 H258 N6 O12 Ru6, 6 (C F3 O3 S), 40( C H4 O) |
| Sum formula | C246 H258 N6 O12 Ru6 | C292 H418 F18 N6 O70 Ru6 S6 |
| Mr | 4097.02 | 6273.10 |
| Dx,g cm-3 | 0.864 | 1.323 |
| Z | 3 | 3 |
| Mu (mm-1) | 2.590 | 3.360 |
| F000 | 6408.0 | 9882.0 |
| F000' | 6424.20 | |
| h,k,lmax | 31,31,53 | 30,30,53 |
| Nref | 31427[ 16829] | 30698 |
| Tmin,Tmax | 0.355,0.353 | 0.063,1.000 |
| Tmin' | 0.268 | |

Correction method= # Reported T Limits: Tmin=0.063 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.82/0.98 Theta(max)= 72.880

R(reflections)= 0.0605( 19178) wR2(reflections)= 0.1956( 30698)

S = 0.965 Npar= 1203

---

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 3

From the CIF: _chemical_formula_weight 6273.10

TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 246.00 | 2954.71 |
| H | 1.01 | 258.00 | 260.06 |
| F | 19.00 | 0.00 | 0.00 |
| N | 14.01 | 6.00 | 84.04 |
| O | 16.00 | 12.00 | 191.99 |
| Ru | 101.07 | 6.00 | 606.42 |
| S | 32.07 | 0.00 | 0.00 |

Calculated formula weight 4097.22

**Author Response: The unit cell contains solvent and anions atoms which were not modelled but the corresponding scattering contribution were taken into account using SQUEEZE/PLATON procedure. The full composition (with triflates anions and methanol molecules) was included in the calculation of the empirical formula,molecular weight,density, linear absorption coefficient and F(000).**

---

## Alert level B

PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 7.3 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for O2 -- C108 .. 11.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for N1 -- C16 .. 8.6 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C38 -- C39 .. 8.2 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C44 -- C45 .. 11.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C55 -- C56 .. 8.6 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C57 -- C58 .. 10.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C59 -- C60 .. 12.2 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C71 -- C72 .. 21.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C90 -- C91 .. 8.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C91 -- C92 .. 14.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C94 -- C95 .. 9.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C100 -- C101 .. 9.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C101 -- C102 .. 9.7 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C102 -- C103 .. 8.4 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C107 -- C108 .. 10.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C107 -- C116 .. 7.8 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C112 -- C113 .. 8.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C114 -- C115 .. 10.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C116 -- C117 .. 8.4 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C119 -- C120 .. 8.7 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference C65 -- C66 .. 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C88 -- C89 .. 0.28 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C49 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C82 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C89 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C91 Check

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        C93 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C111 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C112 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C121 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C65 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C88 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C92 Check
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond   C61    -   C62    ..       1.27 Ang.
PLAT369_ALERT_2_B Long    C(sp2)-C(sp2) Bond  C78    -   C83    ..       1.58 Ang.
PLAT732_ALERT_1_B Angle   Calc     71.6(8), Rep   71.53(19) ......       4.21 s.u.-R
             C92  -C93  -RU3     1.555   1.555   1.555      #       437
PLAT732_ALERT_1_B Angle   Calc     37.7(6), Rep   37.68(10) ......       6.00 s.u.-R
             C93  -RU3  -C88     1.555   1.555   1.555      #       641
```

---

## Alert level C

```
PLAT213_ALERT_2_C Atom C87            has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom C91            has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom C94            has ADP max/min Ratio .....        3.6 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1  H Uiso(max)/Uiso(min) Range        7.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N2     --  C29     ..        5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C26    --  C30     ..        5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C45    --  C46     ..        6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C47    --  C48     ..        6.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C51    --  C52     ..        5.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C52    --  C53     ..        6.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C61    --  C62     ..        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C70    --  C71     ..        7.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C71    --  C74     ..        6.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C77    --  C78     ..        6.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ru1    --  C68     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ru2    --  C78     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ru3    --  C88     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ru3    --  C90     ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O3     --  C117    ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O5     --  C100    ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3     --  C41     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29    --  C30     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C53    --  C54     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C60    --  C61     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C68    --  C73     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C84    --  C85     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C97    --  C98     ..       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C98    --  C99     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C99    --  C103_a  ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C103   --  C99_a   ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C104   --  C105    ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C117   --  C118    ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C120   --  C121    ..       0.22 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C40 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C61 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        C72 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C73 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C78 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C79 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C83 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C119 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ru1 Check
```

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ru2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ru3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C45 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C52 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C57 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C60 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        C80 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C81 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        C95 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C98 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C101 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C104 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C106 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C110 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C113 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C114 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C117 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C118 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C122 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01286 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond   C48    -   C49    ..       1.36 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond   C47    -   C48    ..       1.71 Ang.
PLAT368_ALERT_2_C Short   C(sp2)-C(sp2) Bond  C119   -   C120   ..       1.19 Ang.
PLAT369_ALERT_2_C Long    C(sp2)-C(sp2) Bond  C72    -   C73    ..       1.56 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H22    ..  H59B    ..       1.98 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H34    ..  H47B    ..       1.96 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H87B   ..  H89     ..       1.87 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H90    ..  H94B    ..       1.85 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H23    ..  H94C    ..       2.02 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H92    ..  H96B    ..       2.14 Ang.
PLAT732_ALERT_1_C Angle   Calc     70.7(8), Rep     70.7(2) ......       4.00 s.u.-R
             C93  -C92  -RU3     1.555   1.555   1.555      #       431
PLAT732_ALERT_1_C Angle   Calc     71.9(7), Rep     71.9(2) ......       3.50 s.u.-R
             C88  -C93  -RU3     1.555   1.555   1.555      #       438
PLAT732_ALERT_1_C Angle   Calc     37.7(4), Rep   37.75(11) ......       3.64 s.u.-R
             C93  -RU3  -C92     1.555   1.555   1.555      #       637
PLAT732_ALERT_1_C Angle   Calc     67.8(5), Rep   67.84(15) ......       3.33 s.u.-R
             C92  -RU3  -C88     1.555   1.555   1.555      #       642
PLAT732_ALERT_1_C Angle   Calc     79.6(4), Rep   79.60(12) ......       3.33 s.u.-R
             C93  -RU3  -C90     1.555   1.555   1.555      #       659
PLAT732_ALERT_1_C Angle   Calc     67.1(5), Rep   67.15(13) ......       3.85 s.u.-R
             C92  -RU3  -C90     1.555   1.555   1.555      #       660
PLAT732_ALERT_1_C Angle   Calc     67.0(4), Rep   67.01(15) ......       2.67 s.u.-R
             C88  -RU3  -C90     1.555   1.555   1.555      #       661
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.196 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          9 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
```

---

## 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:C292 H418 F18 N6 O70 Ru6 S6
           Atom count from the _atom_site data:  C246 H258 N6 O12 Ru6
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    3
```

From the CIF: _chemical_formula_sum  C292 H418 F18 N6 O70 Ru6 S6
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|---|---|---|---|
| C | 876.00 | 738.00 | 138.00 |
| H | 1254.00 | 774.00 | 480.00 |
| F | 54.00 | 0.00 | 54.00 |
| N | 18.00 | 18.00 | 0.00 |
| O | 210.00 | 36.00 | 174.00 |
| Ru | 18.00 | 18.00 | 0.00 |
| S | 18.00 | 0.00 | 18.00 |

| | | | |
|---|---|---|---|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 7 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 11 | Report |
| PLAT005_ALERT_5_G | No Embedded Refinement Details found  in the CIF | Please | Do ! |
| PLAT033_ALERT_4_G | Flack x Value Deviates > 3.0 * sigma from Zero . | 0.204 | Note |
| 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 .. | 0.4592 | Check |
| PLAT051_ALERT_1_G | Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . | 22.92 | % |
| PLAT068_ALERT_1_G | Reported F000 Differs from Calcd (or Missing)... | Please | Check |
| PLAT072_ALERT_2_G | SHELXL First  Parameter in WGHT  Unusually Large | 0.11 | Report |
| PLAT152_ALERT_1_G | The Supplied and Calc. Volume s.u. Differ by ... | 4 | Units |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)  Ru1  --  C69  .. | 10.0 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)  Ru1  --  C72  .. | 5.2 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)  Ru1  --  O2_a  .. | 6.0 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)  Ru2  --  C79  .. | 6.3 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)  Ru3  --  O3  .. | 5.6 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)  Ru3  --  O4  .. | 24.5 | s.u. |
| PLAT333_ALERT_2_G | Check Large Av C6-Ring C-C Dist. C99  -C103_a | 1.45 | Ang. |
| PLAT333_ALERT_2_G | Check Large Av C6-Ring C-C Dist. C101  -C101_a | 1.45 | Ang. |
| PLAT333_ALERT_2_G | Check Large Av C6-Ring C-C Dist. C106  -C123 | 1.44 | Ang. |
| PLAT333_ALERT_2_G | Check Large Av C6-Ring C-C Dist. C107  -C116 | 1.45 | Ang. |
| PLAT335_ALERT_2_G | Check Large C6 Ring  C-C Range C68  -C73 | 0.22 | Ang. |
| PLAT335_ALERT_2_G | Check Large C6 Ring  C-C Range C78  -C83 | 0.25 | Ang. |
| PLAT335_ALERT_2_G | Check Large C6 Ring  C-C Range C118  -C123 | 0.31 | Ang. |
| PLAT343_ALERT_2_G | Unusual sp?  Angle Range in Main Residue for | C95 | Check |
| PLAT344_ALERT_2_G | Unusual sp?  Angle Range in Solvent/Ion for . | C96 | Check |
| PLAT367_ALERT_2_G | Long?  C(sp?)-C(sp?) Bond  C91  -  C95  .. | 1.70 | Ang. |
| PLAT367_ALERT_2_G | Long?  C(sp?)-C(sp?) Bond  C94  -  C95  .. | 1.69 | Ang. |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact  C35  ..  C73  .. | 3.17 | Ang. |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact  C91  ..  C96  .. | 2.65 | Ang. |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact  C92  ..  C96  .. | 2.99 | Ang. |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact  C95  ..  C96  .. | 1.81 | 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: C47  --  C48  . | 1.71 | Ang. |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C91  --  C95  . | 1.70 | Ang. |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C95  --  C96  . | 1.80 | Ang. |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints ..... | 39 | Note |
| PLAT869_ALERT_4_G | ALERTS Related to the use of SQUEEZE Suppressed | ! | Info |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min) | 2 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L=  0.600 | 227 | Note |
| PLAT961_ALERT_5_G | Dataset Contains no Negative Intensities ..... | Please | Check |

---

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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
120 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
 25 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 06/05/2016; check.def file version of 05/05/2016**

**Datablock I** - ellipsoid plot