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: 2-open

```
Bond precision:    C-C = 0.0183 A            Wavelength=0.71073

Cell:              a=28.340(4)      b=12.5017(16)         c=26.031(3)
                   alpha=90         beta=112.042(1)       gamma=90
Temperature:       93 K

                   Calculated                 Reported
Volume             8548.6(19)                 8548.7(18)
Space group        C 2/c                      C 2/c
Hall group         -C 2yc                     -C 2yc
                   C65 H34 Dy2 F36 N4 O12 S2, ?
Moiety formula     C5 H11, 2(C H2.50)
Sum formula        C72 H50 Dy2 F36 N4 O12 S2  C72 H50 Dy2 F36 N4 O12 S2
Mr                 2236.28                    2236.28
Dx,g cm-3          1.738                      1.738
Z                  4                          4
Mu (mm-1)          1.921                      1.921
F000               4376.0                     4376.0
F000'              4378.96
h,k,lmax           32,14,29                   32,14,29
Nref               6659                       6583
Tmin,Tmax          0.955,0.962                0.750,1.000
Tmin'              0.681

Correction method= # Reported T Limits: Tmin=0.750 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.989         Theta(max)= 23.925

R(reflections)= 0.0784( 4881)     wR2(reflections)= 0.2358( 6583)

S = 1.033                   Npar= 709
```

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

```
PLAT213_ALERT_2_A Atom F17A              has ADP max/min Ratio .....        9.4 prolat
PLAT213_ALERT_2_A Atom C31A              has ADP max/min Ratio .....        6.3 prolat
PLAT234_ALERT_4_A Large Hirshfeld Difference F13B      -- C29B            0.35 Ang.
```

___

🟠 Alert level B

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
          Calculated sin(theta_max)/wavelength =     0.5706
PLAT213_ALERT_2_B Atom O6A               has ADP max/min Ratio .....        4.3 prolat
PLAT213_ALERT_2_B Atom C32A              has ADP max/min Ratio .....        5.0 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 1  F   Ueq(max)/Ueq(min) Range        10.0 Ratio
PLAT234_ALERT_4_B Large Hirshfeld Difference F5        -- C23_b           0.28 Ang.
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set   Please Do !
```

___

🟡 Alert level C

```
REFNR01_ALERT_3_C  Ratio of reflections to parameters is < 10 for a
          centrosymmetric structure
          sine(theta)/lambda               0.5706
          Proportion of unique data used   1.0000
          Ratio reflections to parameters  9.2849
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....................        9.39 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....        2.23 Report
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C50 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C50 Check
PLAT213_ALERT_2_C Atom F4                has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom F10               has ADP max/min Ratio .....        3.9 prolat
PLAT213_ALERT_2_C Atom F12               has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom F16B              has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom F17B              has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C21               has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom C29B              has ADP max/min Ratio .....        3.5 prolat
PLAT213_ALERT_2_C Atom C33B              has ADP max/min Ratio .....        3.5 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1  O   Ueq(max)/Ueq(min) Range         3.2 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        4.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy2A      -- O4             0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy2A      -- N1             0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2        -- C6             0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30B      -- C31B           0.24 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C17 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C20 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.01831 Ang.
```

___

⚪ Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         26 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     202.54 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          7 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          6 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy1A      --O1        .        7.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy2A      --O2        .        5.7 s.u.
```

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy2A      --O3        .        11.2 s.u.
PLAT242_ALERT_2_G Low      'MainMol' Ueq as Compared to Neighbors of      C19 Check
PLAT242_ALERT_2_G Low      'MainMol' Ueq as Compared to Neighbors of      C23 Check
PLAT242_ALERT_2_G Low      'MainMol' Ueq as Compared to Neighbors of      C24 Check
PLAT242_ALERT_2_G Low      'MainMol' Ueq as Compared to Neighbors of      C28 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C50          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C51          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C52          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C53          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C54          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50C         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C55          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C56          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56B         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56C         Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       23% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )      100% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C15 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F17B     ..C51          2.20 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F17B     ..C52          2.92 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C50      ..C50          0.85 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C50      ..C51          2.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C53      ..C55          2.62 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C54      ..C55          1.55 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C54      ..C56          2.50 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      125 Check
            O1   -C20  -DY2A    1.555   1.555   1.555          31.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      132 Check
            O2   -C22  -DY2A    1.555   1.555   1.555          34.00 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....       ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       44 Note
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  36 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
  40 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

Datablock: 2-close

Bond precision: C-C = 0.0121 A   Wavelength=0.71073

Cell: a=11.7047(3)   b=19.6164(1)   c=20.8522(2)
               alpha=71.022(8)   beta=79.601(9)   gamma=70.806(7)
Temperature: 96 K

	Calculated	Reported
Volume	4261.3(3)	4261.3(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C65 H34 Dy2 F36 N4 O12 S2, C7 H16	?
Sum formula	C72 H50 Dy2 F36 N4 O12 S2	C72 H50 Dy2 F36 N4 O12 S2
Mr	2236.28	2236.28
Dx,g cm-3	1.743	1.743
Z	2	2
Mu (mm-1)	1.926	1.926
F000	2188.0	2188.0
F000'	2189.48	
h,k,lmax	13,22,23	12,22,22
Nref	13593	10338
Tmin,Tmax	0.955,0.962	0.737,1.000
Tmin'	0.680	

Correction method= # Reported T Limits: Tmin=0.737 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.761   Theta(max)= 24.133

R(reflections)= 0.0365(8283)   wR2(reflections)= 0.0963(10338)

S = 0.978   Npar= 1191

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
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .   0.760 Why?
PLAT213_ALERT_2_A Atom F1   has ADP max/min Ratio .....   5.6 prolat
PLAT213_ALERT_2_A Atom F3   has ADP max/min Ratio .....   5.4 prolat
PLAT234_ALERT_4_A Large Hirshfeld Difference C69   -- C70   0.37 Ang.

🟠 Alert level B
PLAT213_ALERT_2_B Atom F2   has ADP max/min Ratio .....   5.0 prolat

```
PLAT213_ALERT_2_B Atom F8              has ADP max/min Ratio .....      4.1 prolat
PLAT213_ALERT_2_B Atom F20             has ADP max/min Ratio .....      4.7 prolat
PLAT234_ALERT_4_B Large Hirshfeld Difference C66      -- C67          0.30 Ang.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C69      - C70      .    1.27 Ang.
```

🟡 Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as Multi-scan
REFNR01_ALERT_3_C  Ratio of reflections to parameters is < 10 for a
            centrosymmetric structure
            sine(theta)/lambda               0.5753
            Proportion of unique data used   1.0000
            Ratio reflections to parameters  8.6801
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =     0.5753
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced ..........   Please Do !
PLAT220_ALERT_2_C Non-Solvent Resd 1  C   Ueq(max)/Ueq(min) Range      3.3 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1  F   Ueq(max)/Ueq(min) Range      5.9 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for  O1        --C37       ..    5.5 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) C68       --C69       ..    7.3 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) C71       --C72       ..    8.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F2       -- C36          0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F20      -- C51          0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F21      -- C51          0.18 Ang.
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of      C68 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of      C70 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C67 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C69 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C71 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      3.3 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.01213 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C67      - C68      .    1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C68      - C69      .    1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C70      - C71      .    1.34 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H44       ..H46       .    1.96 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H45       ..H47       .    1.96 Ang.
```

⚪ Alert level G

```
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C36 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C40 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C41 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C45 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C46 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C50 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C51 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C55 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C56 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C60 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C61 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C65 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      3% Note
PLAT344_ALERT_2_G Unusual sp3      Angle Range in Solvent/Ion for       C67 Check
PLAT344_ALERT_2_G Unusual sp3      Angle Range in Solvent/Ion for       C68 Check
PLAT344_ALERT_2_G Unusual sp3      Angle Range in Solvent/Ion for       C71 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5       ..F30           2.80 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F9       ..F32           2.84 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F13      ..F36           2.68 Ang.
```

```
PLAT793_ALERT_4_G Model has Chirality at C14A          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C22A          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C14B          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C22B          (Centro SPGR)          R Verify
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  33 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
  17 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.
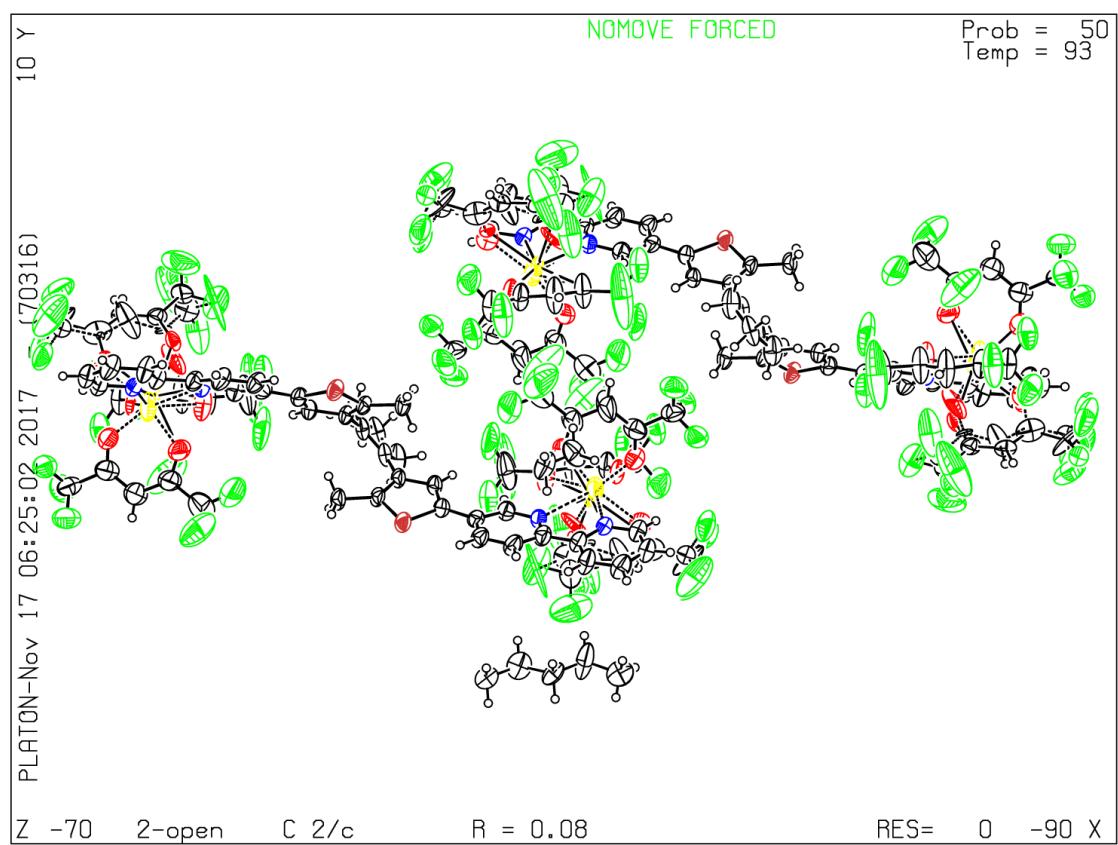
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 09/11/2017; check.def file version of 08/11/2017