checkCIF/PLATON report

Structure factors have been supplied for datablock(s) structure6

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: structure6

```
Bond precision:  C-C = 0.0085 A          Wavelength=0.71073

Cell:            a=12.962(3)     b=16.979(3)         c=13.317(3)
                 alpha=90        beta=104.16(3)      gamma=90
Temperature:     292 K
```

	Calculated	Reported
Volume	2841.8(11)	2841.8(11)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	2(C36 H70 O16 Ti4), 4(C1.75 H2), 4(H)	Ti4 O4 4(C5 H9 O2) 4(C4 H9 O1); 0.5(C7 H8)
Sum formula	C79 H152 O32 Ti8	C39.50 H76 O16 Ti4
Mr	1996.97	998.60
Dx,g cm-3	1.167	1.167
Z	1	2
Mu (mm-1)	0.596	0.596
F000	1058.0	1058.0
F000’	1060.72	
h,k,lmax	16,21,16	16,21,16
Nref	6022	6013
Tmin,Tmax	0.751,0.888	0.647,0.890
Tmin’	0.621	

```
Correction method= NUMERICAL

Data completeness= 0.999          Theta(max)= 26.372

R(reflections)= 0.0761( 4840)     wR2(reflections)= 0.2399( 6013)

S = 1.077                  Npar= Npar = 352
```

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 C9B             has ADP max/min Ratio .....        5.1 prolat
```

Author Response: Atom C9B already occurs with partial occupancy and further position splitting is not justified by the data quality.

Alert level B

```
            Crystal system given = monoclinic
PLAT220_ALERT_2_B Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        6.5 Ratio
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....         C7 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....        C11 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....        C15 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....        C18 Check
```

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.02 Why ?
PLAT213_ALERT_2_C Atom C8              has ADP max/min Ratio .....        3.1 prolat
```

Author Response: Atom C9B already occurs with partial occupancy and further position splitting is not justified by the data quality.

```
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.4 prolat
```

Author Response: Atom C9B already occurs with partial occupancy and further position splitting is not justified by the data quality.

```
PLAT213_ALERT_2_C Atom C8B             has ADP max/min Ratio .....        3.4 prolat
```

Author Response: Atom C9B already occurs with partial occupancy and further position splitting is not justified by the data quality.

```
PLAT213_ALERT_2_C Atom C19             has ADP max/min Ratio .....        3.3 oblate
```

Author Response: Atom C9B already occurs with partial occupancy and further position splitting is not justified by the data quality.

```
PLAT213_ALERT_2_C Atom C20B            has ADP max/min Ratio .....        3.3 prolat
```

Author Response: Atom C9B already occurs with partial occupancy and further position splitting is not justified by the data quality.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference C7     --  C10     ..       0.24 Ang.
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0085 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         33 Ang3
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      6.380 Check
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) .....          5 Why ?
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          4 Why ?
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) .          2 Check
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on     Ti2       1.36 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on     Ti1       1.31 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on     Ti3       1.07 eA-3
```

Alert level G

```
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:   C39.5 H76 O16 Ti4
            Atom count from _chemical_formula_moiety:C2000 H3600 O18800 Ti1600
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 ...         20 Why ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.80 mm
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.17 Why ?
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =         15 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ............ Percentage =        100 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          6 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.11 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
              H
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        136 Note
```

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

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

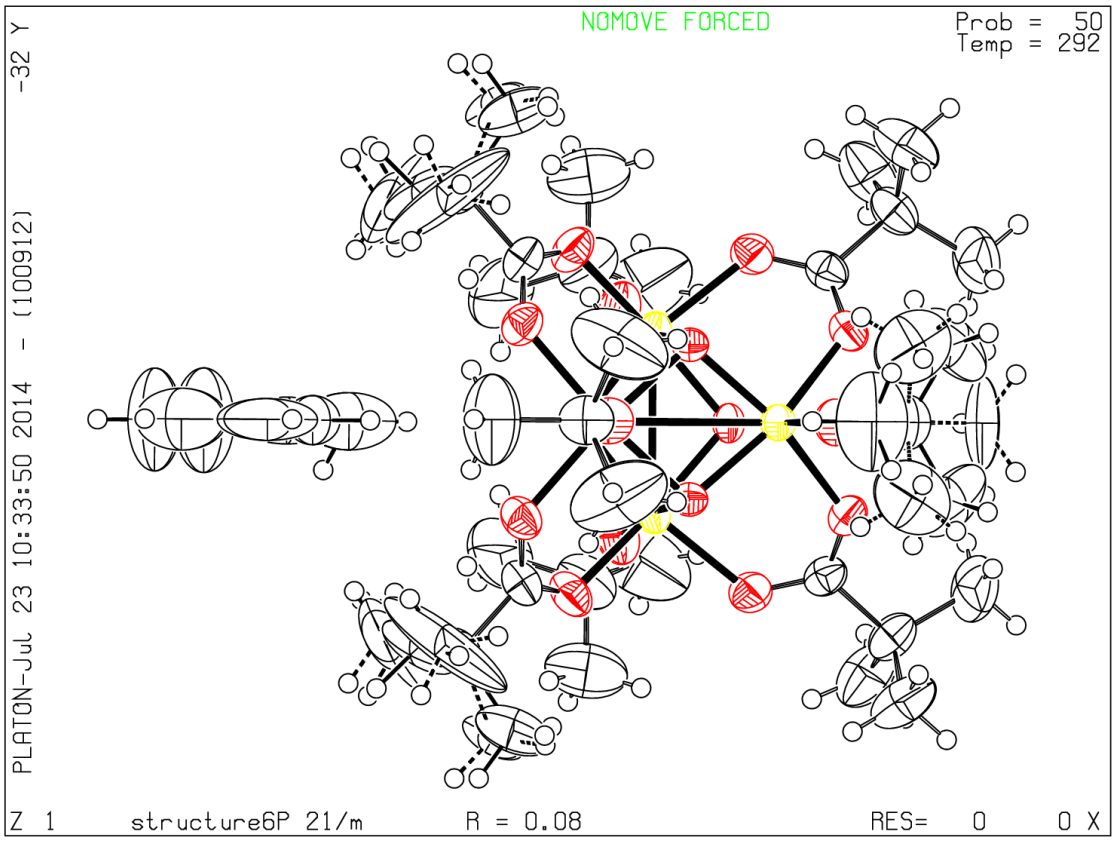
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock structure6 - ellipsoid plot