

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ga601

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: ga601

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Bond precision:      C-C = 0.0046 Å

Wavelength=0.71073

Cell:                      a=11.6732 (5)                      b=16.7232 (7)                      c=17.6214 (8)  
                              alpha=98.987 (1)                      beta=96.472 (2)                      gamma=109.408 (1)  
Temperature:              150 K

|                        | Calculated  | Reported    |
|------------------------|-------------|-------------|
| Volume                 | 3154.2 (2)  | 3154.2 (2)  |
| Space group            | P -1        | P -1        |
| Hall group             | -P 1        | -P 1        |
| Moiety formula         | C80 H96 O4  | C80 H96 O4  |
| Sum formula            | C80 H96 O4  | C80 H96 O4  |
| Mr                     | 1121.57     | 1121.56     |
| Dx, g cm <sup>-3</sup> | 1.181       | 1.181       |
| Z                      | 2           | 2           |
| Mu (mm <sup>-1</sup> ) | 0.070       | 0.070       |
| F000                   | 1216.0      | 1216.0      |
| F000'                  | 1216.47     |             |
| h,k,lmax               | 14,20,22    | 14,20,22    |
| Nref                   | 12942       | 12821       |
| Tmin,Tmax              | 0.982,0.996 | 0.628,0.745 |
| Tmin'                  | 0.982       |             |

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.745  
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 26.416

R(reflections)= 0.0846 ( 8352)

wR2(reflections)=  
0.2170 ( 12821)

S = 1.057

Npar= 801

test-name\_ALERT\_alert-type\_alert-level.

● Alert level C

● Alert level G

|                   |  |        |        |
|-------------------|--|--------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 33     | Note   |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | 1      | Report |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 12     | Report |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records | 7      | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used | 0.0100 | Report |
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| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used | 0.0100 | Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used | 0.0100 | Report |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for C8 --C015 .              | 7.0    | s.u.   |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for C9 --C01K .              | 7.5    | s.u.   |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for C14 --C01Q .             | 7.0    | s.u.   |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for C15 --C015 .             | 5.5    | s.u.   |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for C01K --C023 .            | 6.0    | s.u.   |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C1 Constrained at         | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C7 Constrained at         | 0.75   | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C8 Constrained at         | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C9 Constrained at         | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C14 Constrained at        | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C15 Constrained at        | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C16 Constrained at        | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C01S Constrained at       | 0.75   | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C01U Constrained at       | 0.75   | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C01V Constrained at       | 0.5    | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C01W Constrained at       | 0.75   | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C01X Constrained at       | 0.75   | Check  |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C01Z Constrained at       | 0.75   | Check  |

[illegible]

|                   |  |                |       |       |
|-------------------|--|----------------|-------|-------|
| PLAT300_ALERT_4_G | Atom Site Occupancy of H020            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02A            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02B            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02C            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02D            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02E            | Constrained at | 0.7   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02F            | Constrained at | 0.7   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02G            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02H            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H026            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02I            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02J            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02K            | Constrained at | 0.7   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02L            | Constrained at | 0.7   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02M            | Constrained at | 0.7   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H029            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02N            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02O            | Constrained at | 0.5   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02P            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02Q            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02R            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02S            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H02T            | Constrained at | 0.75  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H2A             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H2B             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H3A             | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H3B             | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H4A             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H4B             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H5A             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H5B             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H6A             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H10A            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H10B            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H11A            | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H11B            | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H11C            | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H12A            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H12B            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H13A            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H13B            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H13C            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H17             | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H18A            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H18B            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H19A            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H19B            | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of He              | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hf              | Constrained at | 0.3   | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hl              | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hm              | Constrained at | 0.25  | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H021            | Constrained at | 0.25  | Check |
| PLAT301_ALERT_3_G | Main Residue Disorder ..... (Resd 1)   |                | 23%   | Note  |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C00G - C015 . |                | 1.53  | Ang.  |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C015 - C01C . |                | 1.53  | Ang.  |
| PLAT410_ALERT_2_G | Short Intra H...H Contact H00L ..H8B . |                | 2.08  | Ang.  |
|                   | x,y,z =                                |                | 1_555 | Check |

PLAT410\_ALERT\_2\_G Short Intra H...H Contact H000 ..H15B . 2.07 Ang.  
x,y,z = 1\_555 Check

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 170 Note

|      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|
| O001 | O002 | O003 | O004 | C005 | C006 | C007 | H007 |
| C008 | H008 | C009 | C00A | C00B | H00B | C00C | C00D |
| C00E | C00F | C00G | C00H | C00I | H00I | C00J | C00K |
| H00A | H00C | C00L | H00L | C00M | C00N | C00O | H00O |
| C00P | C00Q | C00R | C00S | H00S | C00T | H00T | C00U |
| C00V | C00W | H00D | H00E | C00X | H00F | H00G | C00Y |
| C00Z | H00H | H00J | C010 | H01A | H01B | C011 | H01C |
| H01D | C012 | H01E | H01F | C013 | H01G | H01H | C014 |
| H014 | C015 | C016 | C017 | H01I | H01J | C018 | H018 |
| C019 | H01K | H01L | C01A | H01M | C01B | H01N | H01O |
| C01C | H01P | H01Q | C01D | H01R | H01S | C01E | H01T |
| H01U | C01F | H01V | C01G | H01W | H01X | C01H | H01Y |
| C01I | H01Z | C01J | H01  | C01K | Ha   | C01L | Hb   |
| C01M | Hc   | C01N | Hd   | He   | Hf   | C01O | C01P |
| Hg   | C01Q | Hh   | Hi   | Hj   | C01R | C01S | C01T |
| Hk   | Hl   | Hm   | C01U | Hn   | C01V | Ho   | C01W |
| Hp   | C01X | Hq   | C01Y | C01Z | C020 | H020 | C021 |
| H021 | C022 | H02A | H02B | C023 | H02C | H02D | C024 |
| H02E | H02F | C025 | H02G | H02H | C026 | H026 | C027 |
| H02I | H02J | C028 | H02K | H02L | H02M | C029 | H029 |
| C02A | H02N | H02O | C02B | H02P | H02Q | C02C | H02R |
| H02S | H02T |      |      |      |      |      |      |

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 41 Note

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

0 1 0, 0 -1 1, 0 0 1,

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 41 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 2 Note

0 -1 1, -3 5 1,

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.3 Low

PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 3.04 Note

Predicted wR2: Based on SigI\*\*2 7.14 or SHELX Weight 21.21

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 5 Info

PLAT992\_ALERT\_5\_G Repd & Actual \_reflns\_number\_gt Values Differ by 5 Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
14 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  
127 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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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.

