checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound1

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: Compound1

| Bond precision: C-C = 0.0083 Å | Wavelength=0.71073 |
|-------------------------------|-------------------|
| Cell:                         |                   |
| a=14.3488(9)                 | b=15.0188(9)      |
| alpha=97.162(5)              | c=15.2848(10)     |
| beta=92.241(4)               | gamma=101.857(4)  |
| Temperature: 140 K           |                   |
|                               |                   |
| Volume                        |                   |
| 3191.4(4)                     | 3191.4(4)         |
| Space group                   |                   |
| P -1                          | P -1              |
| Hall group                    |                   |
| P 1                           | -P 1              |
| Moiety formula                |                   |
| C24 H12 N4 O14, C H4 O       | 2(C24 H12 N4 O14), 2(C H4 solvent) |
| Sum formula                   |                   |
| C25 H16 N4 O15 [+ solvent]   | C50 H32 N8 O30    |
| Mr                            |                   |
| 612.42                        | 1224.83           |
| Dx, g cm⁻³                    |                   |
| 1.275                         | 1.275             |
| Z                              |                   |
| 4                             | 2                 |
| Mu (mm⁻¹)                     |                   |
| 0.108                         | 0.108             |
| F000                          |                   |
| 1256.0                        | 1256.0            |
| F000’                         |                   |
| 1256.86                       |                   |
| h,k,lmax max                  |                   |
| 17,17,18                      | 17,17,18          |
| Nref                          |                   |
| 11231                         | 11054             |
| Tmin,Tmax                     |                   |
| 0.974,0.992                  | 0.643,0.745       |
| Tmin’                         |                   |
| 0.968                         |                   |

Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 25.000
R(reflections)= 0.1041( 6294) wr2(reflections)= 0.3288( 11054)
S = 1.036 Npar= 799
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 B

| ALERT        | Test Name                  | Detail                                                   | Alert Level |
|--------------|----------------------------|----------------------------------------------------------|-------------|
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for O27 --N8 | 9.8 s.u.                                                 | B           |
| PLAT420_ALERT_2_B | D-H Bond Without Acceptor O19 --H19 | Please Check                                            | B           |
| PLAT420_ALERT_2_B | D-H Bond Without Acceptor O24 --H24A | Please Check                                            | B           |
| PLAT420_ALERT_2_B | D-H Bond Without Acceptor O33 --H33A | Please Check                                            | B           |

### Alert level C

| ALERT        | Test Name                  | Detail                                                   | Alert Level |
|--------------|----------------------------|----------------------------------------------------------|-------------|
| DIFMX02_ALERT_1_C | The maximum difference density is > 0.1*2MAX*0.75 | The relevant atom site should be identified. | C           |
| PLAT084_ALERT_3_C | High wR2 Value (i.e. > 0.25) | ................. 0.33 Report | C           |
| PLAT097_ALERT_2_C | Large Reported Max. (Positive) Residual Density | 0.70 eA-3 | C           |
| PLAT220_ALERT_2_C | NonSolvent Resd 2 O Ueq(max)/Ueq(min) Range | 3.3 Ratio | C           |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for O28 --N8 | 5.8 s.u.                                                 | C           |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of O2 | Check | C           |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of O18 | Check | C           |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of N1 | Check | C           |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of N4 | Check | C           |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of N5 | Check | C           |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of N8 | Check | C           |
| PLAT260_ALERT_2_C | Large Average Ueq of Residue Including O32 | 0.102 Check | C           |
| PLAT334_ALERT_2_C | Small Aver. Benzene C-C Dist C25 -C30 | 1.37 Ang. | C           |
| PLAT340_ALERT_3_C | Low Bond Precision on C-C Bonds | ................. 0.00829 Ang. | C           |
| PLAT415_ALERT_2_C | Short Inter D-H..H-X H19 ..H26 | 2.10 Ang. | C           |
| PLAT790_ALERT_4_C | Centre of Gravity not Within Unit Cell: Resd. | 1 Note | G           |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | 4.477 Check | G           |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | 2.332 Check | G           |
| PLAT720_ALERT_4_G | Solvent Accessible VOID(S) in Structure | ! Info | G           |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). | 3 Note | G           |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File | 23 Note | G           |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | ................. 2.7 Low | G           |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 0 Info | G           |
| PLAT992_ALERT_5_G | Repd & Actual _reflans_number_gt Values Differ by | 2 Check | G           |

### Alert level G

| ALERT        | Test Name                  | Detail                                                   | Alert Level |
|--------------|----------------------------|----------------------------------------------------------|-------------|
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms | ................. 6 Report | G           |
| PLAT042_ALERT_1_G | Calc. and Reported Moiety Formula Strings Differ | Please Check | G           |
| PLAT045_ALERT_1_G | Calculated and Reported Z Differ by a Factor ... | 2.00 Check | G           |
| PLAT072_ALERT_2_G | SHEXL First Parameter in WGHT Unusually Large | 0.19 Report | G           |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact C21 ..C26 | 3.17 Ang. | G           |
| PLAT606_ALERT_4_G | Solvent Accessible VOID(S) in Structure | ! Info | G           |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | 1 Note | G           |
| PLAT790_ALERT_3_G | Centre of Gravity not Within Unit Cell: Resd. | 3 Note | G           |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). | 3 Note | G           |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File | 23 Note | G           |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | ................. 2.7 Low | G           |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 0 Info | G           |
| PLAT992_ALERT_5_G | Repd & Actual _reflans_number_gt Values Differ by | 2 Check | G           |

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

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