# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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```
Bond precision:   C-C = 0.0040 A          Wavelength=0.71073

Cell:             a=25.328(2)     b=5.7081(5)          c=24.491(2)
                  alpha=90        beta=118.384(4)      gamma=90
Temperature:      150 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 3115.1(5) | 3115.1(5) |
| Space group | C 2/c | C 2/c |
| Hall group | -C 2yc | -C 2yc |
| Moiety formula | C32 H40 F6 N6 | C32 H40 F6 N6 |
| Sum formula | C32 H40 F6 N6 | C32 H40 F6 N6 |
| Mr | 622.70 | 622.70 |
| Dx,g cm-3 | 1.328 | 1.328 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.105 | 0.105 |
| F000 | 1312.0 | 1312.0 |
| F000' | 1312.72 | |
| h,k,lmax | 32,7,31 | 32,7,31 |
| Nref | 3475 | 3475 |
| Tmin,Tmax | 0.987,0.994 | 0.987,0.994 |
| Tmin' | 0.981 | |

```
Correction method= # Reported T Limits: Tmin=0.987 Tmax=0.994
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 27.180

R(reflections)= 0.0642( 1977)                    wR2(reflections)=
                                                 0.1729( 3457)
S = 1.050                 Npar= 199
```

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 C

```
PLAT213_ALERT_2_C Atom F2              has ADP max/min Ratio .....        4.0 prolat
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F3       --C13      .        7.0 s.u.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.2 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     11.852 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.189 Check
```

## Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
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).          2 Note
               2  0  0,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         15 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
               0  0  2,   2  0  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.9 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       2.54 Note
             Predicted wR2: Based on SigI**2  6.81 or SHELX Weight 16.95
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

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

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**PLATON version of 13/12/2023; check.def file version of 13/12/2023**

**Datablock shelx** - ellipsoid plot