# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

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```
Bond precision:   C-C = 0.0032 A           Wavelength=1.54184

Cell:           a=8.9459(1)         b=17.2753(2)      c=21.8372(3)
                alpha=110.107(1)    beta=91.709(1)    gamma=93.859(1)
Temperature:    100 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 3156.86(7) | 3156.86(7) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C43 H61 N7 O9, C16 H32 O8 | C16 H32 O8, C43 H61 N7 O9 |
| Sum formula | C59 H93 N7 O17 | C59 H93 N7 O17 |
| Mr | 1172.40 | 1172.40 |
| Dx,g cm-3 | 1.233 | 1.233 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.744 | 0.744 |
| F000 | 1264.0 | 1264.0 |
| F000' | 1268.05 | |
| h,k,lmax | 11,21,27 | 11,21,27 |
| Nref | 13279 | 12687 |
| Tmin,Tmax | 0.875,0.915 | 0.297,1.000 |
| Tmin' | 0.824 | |

```
Correction method= # Reported T Limits: Tmin=0.297 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.955            Theta(max)= 76.544

R(reflections)= 0.0730( 10763)                    wR2(reflections)=
                                                  0.2149( 12687)
S = 1.062                  Npar= 820
```

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

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C43 H61 N7 O9, C16 H32 O8
             Rep.: C16 H32 O8, C43 H61 N7 O9
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.10 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       0.77 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N3       --N4       .        5.1 s.u.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.832 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         57 Report
             -10  4  0,  -8-12  1,  10 -3  1, -10  4  1,   2 16  1,  10 -2  2,
             -10  3  2, -10  4  2,   2 16  2, -10  2  3, -10  3  3, -10  4  3,
             -10  5  3, -10  6  3, -10  7  3,  10 -1  4, -10  3  4, -10  4  4,
             -10  5  4, -10  6  4, -10  7  4,   7-16  5,  -9-10  5,  10  0  5,
             -10  1  5,  10  1  5, -10  3  5, -10  4  5, -10  5  5, -10  6  5,
                  (   27 More Missing: see the .ckf listing file)
```

## Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         14 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         14 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
             H1
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par     0.0100 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par     0.0100 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         10% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H31      ..H34F     .       2.05 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H37      ..H42C     .       2.09 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H37      ..H35A     .       2.14 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H37      ..H42F     .       2.08 Ang.
                                                     x,y,z  =      1_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        120 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        535 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
              -8  5 12, -10  2  9, -10  1  5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.396 Note
             Predicted wR2: Based on SigI**2  6.33 or SHELX Weight 20.23
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          6 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
  7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 22 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
  3 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.

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**PLATON version of 04/06/2025; check.def file version of 30/05/2025**

**Datablock a** - ellipsoid plot