

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AX2882abs

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: AX2882abs

Bond precision: C-C = 0.0023 Å

Wavelength=1.54178

```
Cell:      a=10.4253(4)
           alpha=85.795(1)
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b=12.0534 (4) c=13.6573 (5)
beta=72.188 (1) gamma=78.129 (1)

Temperature: 150 K

	Calculated
Volume	1598.87 (10)
Space group	P -1
Hall group	-P 1
Moiety formula	C36 H36 N6 O8
Sum formula	C36 H36 N6 O8
Mr	680.71
Dx, g cm ⁻³	1.414
Z	2
Mu (mm ⁻¹)	0.842
F000	716.0
F000'	718.33
h, k, lmax	12, 14, 16
Nref	5665
Tmin, Tmax	0.941, 0.951
Tmin'	0.935

Reported
1598.87 (10)
P -1
-P 1
C36 H36 N6 O8
C36 H36 N6 O8
680.71
1.414
2
0.842
716.0

12,14,16
5598
0.627,0.753

```
Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.753
AbsCorr = MULTI-SCAN
```

Data completeness= 0.988

$$\text{Theta (max)} = 66.702$$

R(reflections)= 0.0428(4932)

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wR2 (reflections) =  
0.1241 ( 5598)
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$$S = 1.036$$

Npar= 453

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.40 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.596 66 Report
-1 1 0, -9 7 0, 4 10 0, -2 -1 1, 0 -1 1, 1 -1 1,
-2 0 1, -1 0 1, 2 0 1, -11 1 1, -2 1 1, -1 1 1,
1 1 1, -4 2 1, -2 4 1, -11 -3 2, -11 -1 2, -11 0 2,
0 1 2, 6 1 2, -4 2 2, -2 2 2, -4 3 2, 6 3 2,
-6 10 2, -6 1 3, -10 2 3, -10 3 3, -4 3 3, 4 9 3,
(36 More Missing: see the .ckf listing file)

● Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 81% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
2 0 1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.238 Note
Predicted wR2: Based on SigI**2 3.83 or SHELX Weight 11.98
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 8 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 3 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 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.

