checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sh449

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: sh449

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

Cell:               a=28.4221(9)      b=5.9548(2)      c=25.7279(9)
                    alpha=90          beta=90          gamma=90
Temperature:        100 K
```

	Calculated	Reported
Volume	4354.4(3)	4354.4(3)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C5 H10 Cl2 N8 O8	C5 H10 Cl2 N8 O8
Sum formula	C5 H10 Cl2 N8 O8	C5 H10 Cl2 N8 O8
Mr	381.11	381.11
Dx,g cm-3	1.744	1.744
Z	12	12
Mu (mm-1)	0.506	0.506
F000	2328.0	2328.0
F000'	2332.75	
h,k,lmax	35,7,31	35,7,31
Nref	4314	4304
Tmin,Tmax	0.976,0.990	0.941,0.990
Tmin'	0.904	

```
Correction method= # Reported T Limits: Tmin=0.941 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 26.072

R(reflections)= 0.0569( 3615)                    wR2(reflections)=
                                                 0.1029( 4304)
S = 1.192                  Npar= 312
```

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

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O4'      ..O7       .       2.87 Ang.
                                          -x,2-y,1-z  =      5_576 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O6       ..N6       .       2.88 Ang.
                                         1/2-x,-1/2+y,z  =      8_655 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     10.433 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.158 Check
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       9.92 Why ?
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          5 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
```

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

0 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
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock sh449 - ellipsoid plot