

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ans7

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: ans7

Bond precision: C-C = 0.0028 Å

Wavelength=0.71073

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Cell:      a=8.2055(17)
           alpha=90.431(7)
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b=10.582 (2) c=10.910 (2)
beta=99.280 (7) gamma=105.860 (7)

Temperature: 165 K

	Calculated
Volume	898.0(3)
Space group	P -1
Hall group	-P 1
Moiety formula	C19 H18 Cl N O4
Sum formula	C19 H18 Cl N O4
Mr	359.79
Dx, g cm ⁻³	1.331
Z	2
Mu (mm ⁻¹)	0.235
F000	376.0
F000'	376.47
h, k, lmax	10, 13, 13
Nref	3869
Tmin, Tmax	0.994, 0.998
Tmin'	0.984

Reported
898.0 (3)
P -1
-P 1
C19 H18 Cl N O4
C19 H18 Cl N O4
359.79
1.331
2
0.235
376.0

10,13,13
3596
0.441,0.745

```
Correction method= # Reported T Limits: Tmin=0.441 Tmax=0.745
AbsCorr = MULTI-SCAN
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Data completeness= 0.929

$$\Theta(\max) = 26.830$$

R(reflections)= 0.0427(2774)

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wR2 (reflections)=  
0.1130 ( 3596)
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$$S = 1.033$$

Npar= 233

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 184 Report

8	0	0,	-9	1	0,	2	1	0,	7	1	0,	-1	2	0,	0	2	0,
2	2	0,	4	2	0,	1	3	0,	1	4	0,	1	6	0,	6	6	0,
-7	11	0,	8	-8	1,	-6	-5	1,	-6	-3	1,	-4	-3	1,	9	-3	1,
-8	-2	1,	-7	-2	1,	0	-2	1,	8	-2	1,	9	-2	1,	-9	-1	1,
-2	-1	1,	-1	-1	1,	1	-1	1,	2	-1	1,	7	-1	1,	-2	0	1,
-1	0	1,	1	0	1,	6	0	1,	-2	1	1,	1	1	1,	2	1	1,
0	2	1,	-1	3	1,	0	3	1,	7	3	1,	0	4	1,	1	6	1,
5	6	1,	6	6	1,	5	7	1,	6	7	1,	-2	12	1,	6	-10	2,
8	-8	2,	8	-7	2,	8	-6	2,	8	-5	2,	-6	-4	2,	7	-4	2,
-8	-3	2,	-1	-1	2,	0	-1	2,	1	-1	2,	-3	0	2,	-2	0	2,
-1	0	2,	-7	1	2,	0	1	2,	-1	2	2,	0	5	2,	2	6	2,
3	6	2,	5	6	2,	6	6	2,	2	7	2,	4	7	2,	5	7	2,
4	8	2,	5	8	2,	-3	12	2,	-1	-10	3,	7	-7	3,	-2	0	3,
0	0	3,	-4	1	3,	-3	3	3,	-2	3	3,	-3	4	3,	4	6	3,
-8	7	3,	2	7	3,	3	7	3,	4	7	3,	5	7	3,	2	8	3,
3	8	3,	4	8	3,	2	9	3,	3	9	3,	-3	10	3,	1	10	3,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 17 Note

2	1	0,	0	2	0,	4	2	0,	0	-2	1,	-2	-1	1,	-2	0	1,
-2	1	1,	1	1	1,	2	1	1,	0	-1	2,	1	-1	2,	-2	0	2,
0	1	2,	-3	3	3,	-2	3	3,	-1	-1	4,	0	0	4,			

Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.007 Degree

PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 43 Note

C101	O002	O003	O004	N005	O006	C007	C008
H008	C009	C00A	H00A	C00B	C00C	H00C	C00D
C00E	C00F	C00G	H00G	C00H	C00I	C00J	H00B
H00D	H00E	C00K	H00K	C00L	H00L	C00M	H00M
C00N	H00F	H00H	H00I	C00O	H00O	C00P	H00J
H00N	H00P	H005					

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

1	0	0,	0	1	0,	0	0	1,
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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 87 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note

-1	0	2,	1	-1	1,	-3	4	3,
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PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.7 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 1.726 Note

Predicted wR2: Based on SigI**2 6.55 or SHELX Weight 10.94

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

- 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

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

2 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
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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 13/05/2024; check.def file version of 04/05/2024

