

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) HeliIm_chiral2

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: HeliIm_chiral2

Bond precision:	C-C = 0.0027 A	Wavelength=0.71075	
Cell:	a=5.60752(11)	b=14.3072(3)	c=13.7727(3)
	alpha=90	beta=90.014(6)	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	1104.96(4)	1104.96(4)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C31 H27 N O2	C31 H27 N O2	
Sum formula	C31 H27 N O2	C31 H27 N O2	
Mr	445.54	445.56	
Dx,g cm-3	1.339	1.339	
Z	2	2	
Mu (mm-1)	0.083	0.083	
F000	472.0	472.0	
F000'	472.19		
h,k,lmax	7,18,17	7,18,17	
Nref	5066[2636]	5062	
Tmin,Tmax	0.994,0.998	0.817,0.998	
Tmin'	0.979		

Correction method= # Reported T Limits: Tmin=0.817 Tmax=0.998
AbsCorr = MULTI-SCAN

Data completeness= 1.92/1.00 Theta(max)= 27.484

R(reflections)= 0.0315(4760) wR2(reflections)= 0.0767(5062)

S = 1.018 Npar= 309

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

PLAT411_ALERT_2_C Short Inter H...H Contact H17 .. H27A .. 2.14 Ang.

Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
_publ_requested_category classification of your compound;
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
FO or CO or EO for organic.
From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or
From the CIF: _chemical_formula_sum:C31 H27 N1 O2
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 4 Report

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT411_HeliIm_chiral2
;
PROBLEM: Short Inter H...H Contact H17 .. H27A .. 2.14 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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*, 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.

