

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) bmk1820c

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.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

[Structure factor report](#)

Datablock: bmk1820c

Bond precision: C-C = 0.0074 Å Wavelength=1.54184
Cell: a=18.4634(11) b=12.0289(8) c=7.7553(5)
alpha=90 beta=101.401(6) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1688.42(19)	1688.42(19)
Space group	Pc	Pc
Hall group	: P -2yc	P -2yc
Moiety formula	C18 H17 N5 O2	C18 H17 N5 O2
Sum formula	C18 H17 N5 O2	C18 H17 N5 O2
Mr	335.37	335.36
Dx, g cm ⁻³	1.319	1.319
Z	4	4
Mu (mm ⁻¹)	0.735	0.735
F000	704.0	704.0
F000'	706.15	
h, k, l max	23, 15, 9	22, 14, 9
Nref	6883[3449]	5379
Tmin, Tmax	0.957, 0.978	0.852, 1.000
Tmin'	0.885	

Correction method= # Reported T Limits: Tmin=0.852 Tmax=1.000 AbsCorr = GAUSSIAN

Data completeness= 1.56/0.78 Theta(max)= 74.298

R(reflections)= 0.0544(4293) wR2(reflections)= 0.1478(5379)

S = 1.065

Npar= 455

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

[STRVA01_ALERT_4_C](#)

Flack parameter is too small

From the CIF: _refine_ls_abs_structure_Flack -0.600

From the CIF: _refine_ls_abs_structure_Flack_su 0.300

[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00737 Ang.

[PLAT480_ALERT_4_C](#) Long H...A H-Bond Reported H2 ..O2 . 2.81 Ang.

[PLAT915_ALERT_3_C](#) No Flack x Check Done: Low Friedel Pair Coverage 57 %

[PLAT978_ALERT_2_C](#) Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms 2 Report

[PLAT012_ALERT_1_G](#) N.O.K. _shelx_res_checksum Found in CIF Please Check

[PLAT032_ALERT_4_G](#) Std. Uncertainty on Flack Parameter Value High . 0.300 Report

[PLAT910_ALERT_3_G](#) Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

[PLAT912_ALERT_4_G](#) Missing # of FCF Reflections Above STh/L= 0.600 34 Note

[PLAT916_ALERT_2_G](#) Hooft y and Flack x Parameter Values Differ by . 0.16 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **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

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
3 ALERT type 3 Indicator that the structure quality may be low
4 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

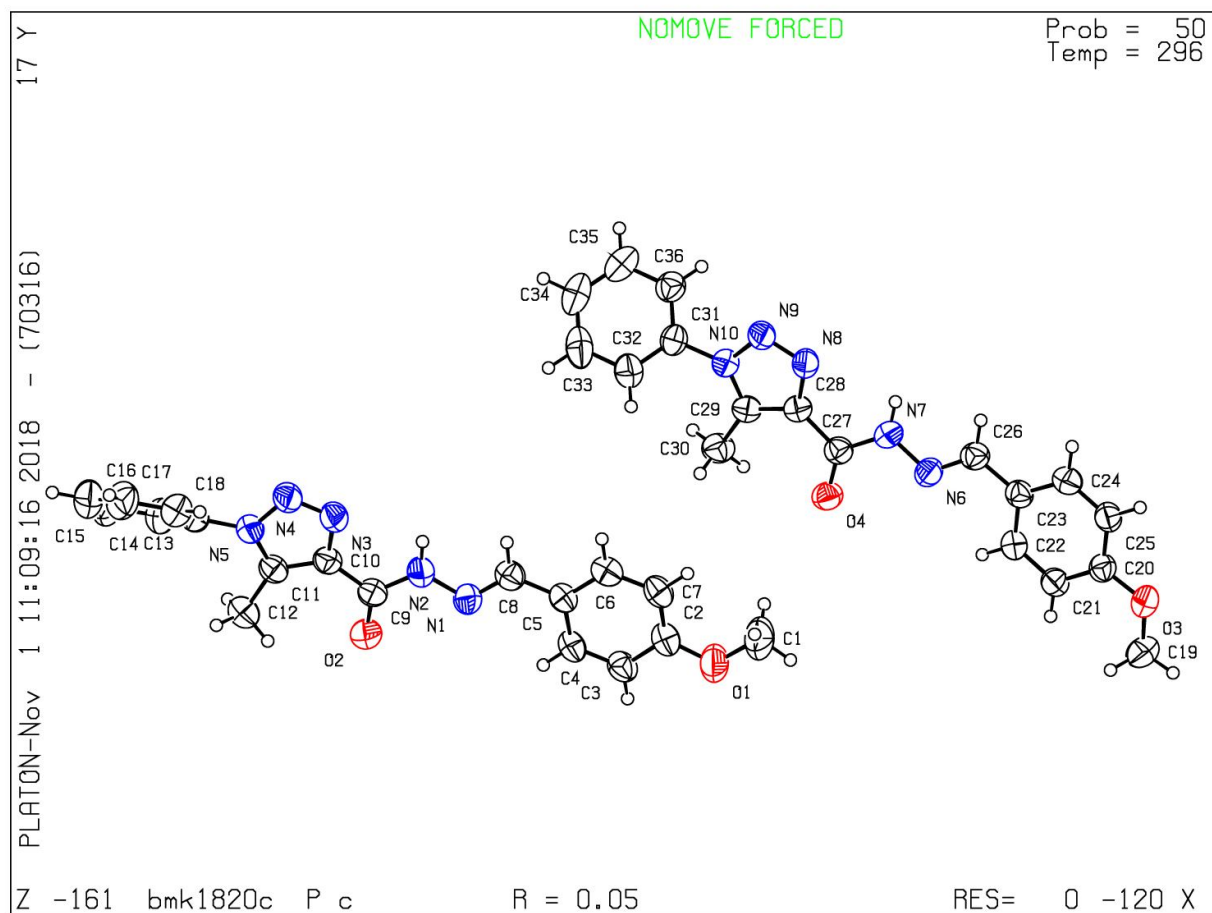
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 19/10/2018; check.def file version of 15/10/2018

Datablock bmk1820c - ellipsoid plot



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