

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) BocPiperazineBenzoxdiazole_red_0m

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](#)

Please wait while processing [Interpreting this report](#)

[Structure factor report](#)

Datablock: BocPiperazineBenzoxdiazole_red_0m

Bond precision: C-C = 0.0039 Å Wavelength=0.71073

Cell: a=33.438(5) b=6.4498(9) c=7.6136(10)

alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1642.0(4)	1642.0(4)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C15 H19 N5 O5	?
Sum formula	C15 H19 N5 O5	C15 H19 N5 O5
Mr	349.35	349.35
Dx, g cm ⁻³	1.413	1.413
Z	4	4
Mu (mm ⁻¹)	0.108	0.108
F000	736.0	736.0
F000'	736.36	
h,k,lmax	44,8,10	44,8,10
Nref	4089[2198]	3813
Tmin,Tmax	0.977,0.995	0.663,0.746
Tmin'	0.971	

Correction method= # Reported T Limits: Tmin=0.663 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.93 Theta(max)= 28.326

R(reflections)= 0.0392(3206) wR2(reflections)= 0.0893(3813)

S = 1.052 Npar= 229

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 test results are meaningless.

From the CIF: _refine_ls_abs_structure_Flack 0.000

From the CIF: _refine_ls_abs_structure_Flack_su 0.600

[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

● Alert level G

PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.600	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact O4 ..C9 .	3.02	Ang.
	x,1+y,z = 1_565	Check	
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 with s.u.	0.60	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	35	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	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
 6 **ALERT level G** = General information/check it is not something unexpected

- 0 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
2 ALERT type 3 Indicator that the structure quality may be low
4 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

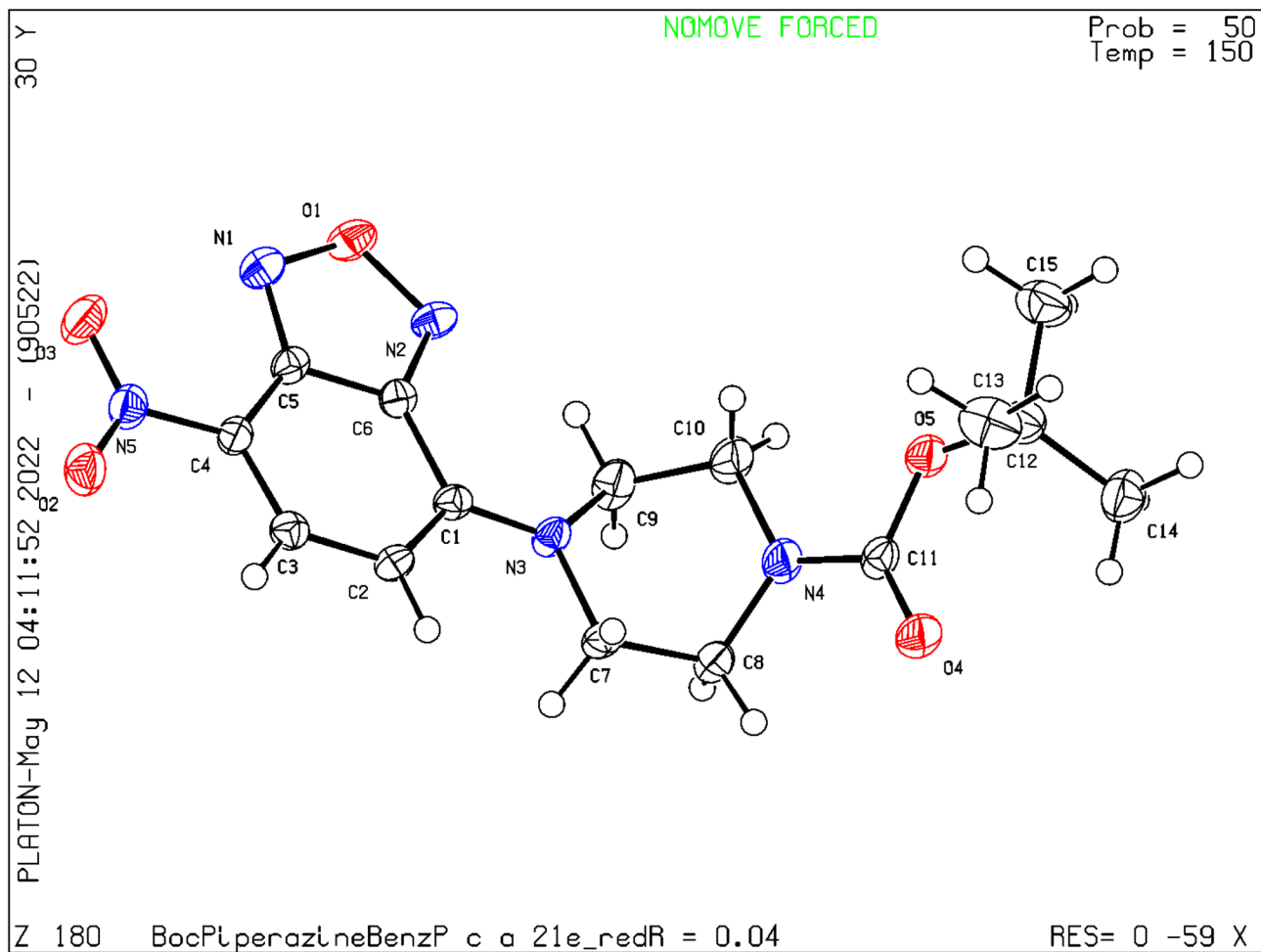
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 09/05/2022; check.def file version of 21/03/2022

Datablock BocPiperazineBenzoxdiazole_red_0m - ellipsoid
plot



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