

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) r20200519c

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: r20200519c

Bond precision:	C-C = 0.0030 Å	Wavelength=0.71073
Cell:	a=9.7732(4)	b=14.8171(7)
	alpha=90	beta=90
		gamma=90
Temperature: 113 K		
	Calculated	Reported
Volume	2654.49(19)	2654.49(19)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C28 H44 N2 O2	C28 H44 N2 O2
Sum formula	C28 H44 N2 O2	C28 H44 N2 O2
Mr	440.65	440.65
Dx, g cm ⁻³	1.103	1.103
Z	4	4
Mu (mm ⁻¹)	0.068	0.068
F000	968.0	968.0
F000'	968.36	
h, k, lmax	12, 18, 22	12, 18, 22
Nref	5415[3060]	5364
Tmin, Tmax	0.986, 0.989	0.598, 1.000
Tmin'	0.986	
Correction method= # Reported T Limits: Tmin=0.598 Tmax=1.000 AbsCorr = MULTI-SCAN		
Data completeness= 1.75/0.99	Theta(max)= 26.371	
R(reflections)= 0.0378(4871)	wR2(reflections)= 0.0907(5364)	
S = 1.026	Npar= 297	

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` -0.400
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.500
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 31 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 28 Note

●Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.500 Report
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1 109.0 Degree
PLAT791_ALERT_4_G Model has Chirality at C11 (Sohnke SpGr) R Verify
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 15 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 15 Info

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- 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
 - 5 **ALERT level G** = General information/check it is not something unexpected
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- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 3 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
 - 3 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

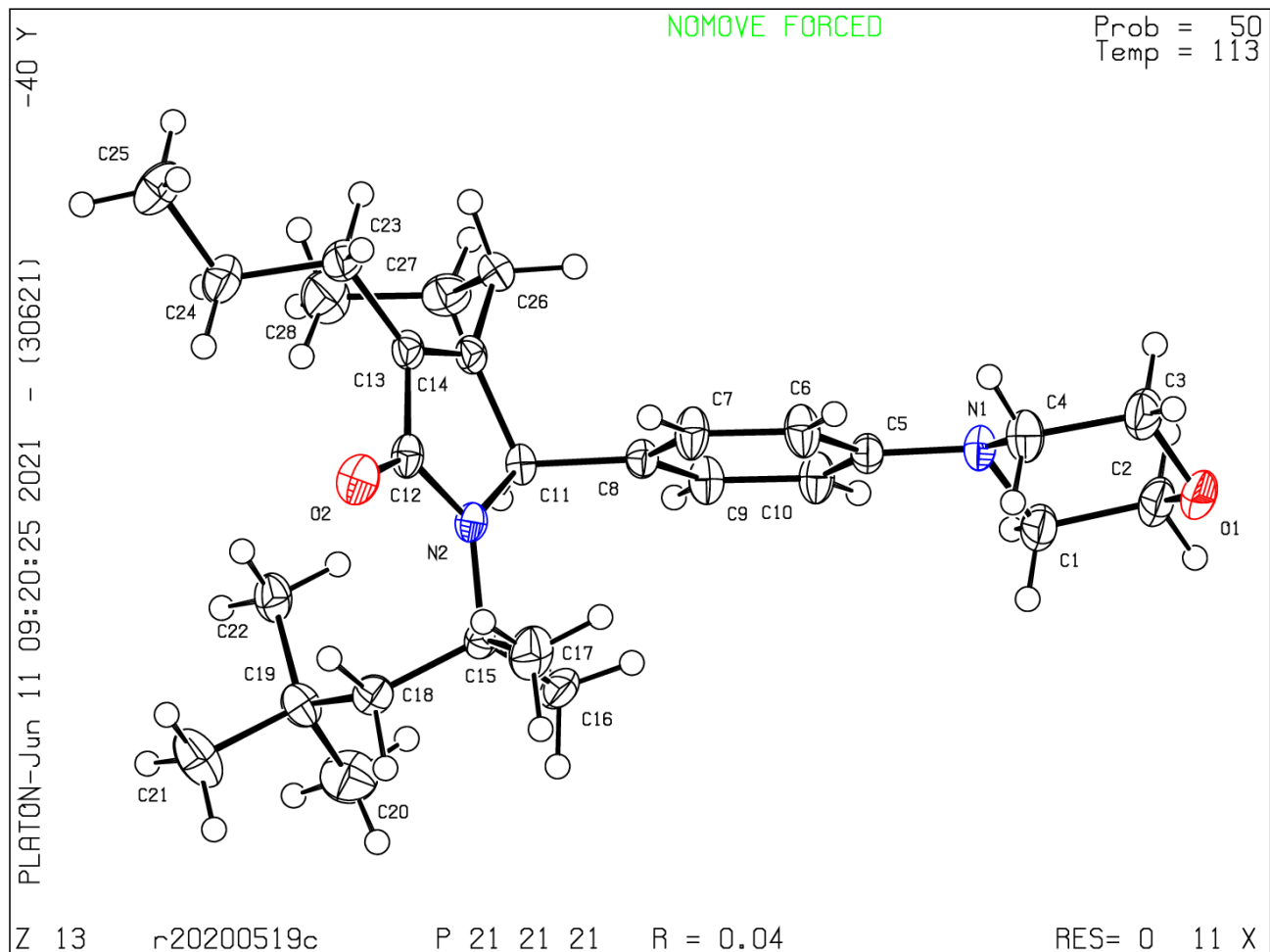
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/06/2021; check.def file version of 02/06/2021

Datablock r20200519c - ellipsoid plot



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