

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) 8

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: 8

Bond precision: C-C = 0.0030 Å Wavelength=0.71073
Cell: a=10.1782(2) b=12.5203(3) c=19.0389(5)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	2426.21(10)	2426.21(10)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C27 H38 O4	C27 H38 O4
Sum formula	C27 H38 O4	C27 H38 O4
Mr	426.57	426.57
Dx, g cm ⁻³	1.168	1.168
Z	4	4
Mu (mm ⁻¹)	0.077	0.077
F000	928.0	928.0
F000'	928.42	
h, k, lmax	13, 16, 25	13, 16, 25
Nref	6056 [3405]	5467
Tmin, Tmax	0.956, 0.975	0.964, 0.981
Tmin'	0.951	

Correction method= # Reported T Limits: Tmin=0.964 Tmax=0.981
AbsCorr = ANALYTICAL
Data completeness= 1.61/0.90 Theta(max)= 28.326
R(reflections)= 0.0384(4792) wR2(reflections)= 0.0846(5467)
S = 1.038 Npar= 287

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 G

[PLAT032_ALERT_4_G](#) Std. Uncertainty on Flack Parameter Value High . 0.400 Report
[PLAT063_ALERT_4_G](#) Crystal Size Possibly too Large for Beam Size .. 0.65 mm
[PLAT398_ALERT_2_G](#) Deviating C-O-C Angle From 120 for O1 . 105.8 Degree
[PLAT791_ALERT_4_G](#) Model has Chirality at C3 (Sohnke SpGr) R Verify

And 2 other PLAT791 Alerts

[Less ...](#)

[PLAT791_ALERT_4_G](#) Model has Chirality at C6 (Sohnke SpGr) S Verify
[PLAT791_ALERT_4_G](#) Model has Chirality at C13 (Sohnke SpGr) S Verify

PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	232 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	15 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **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
1 ALERT type 3 Indicator that the structure quality may be low
6 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

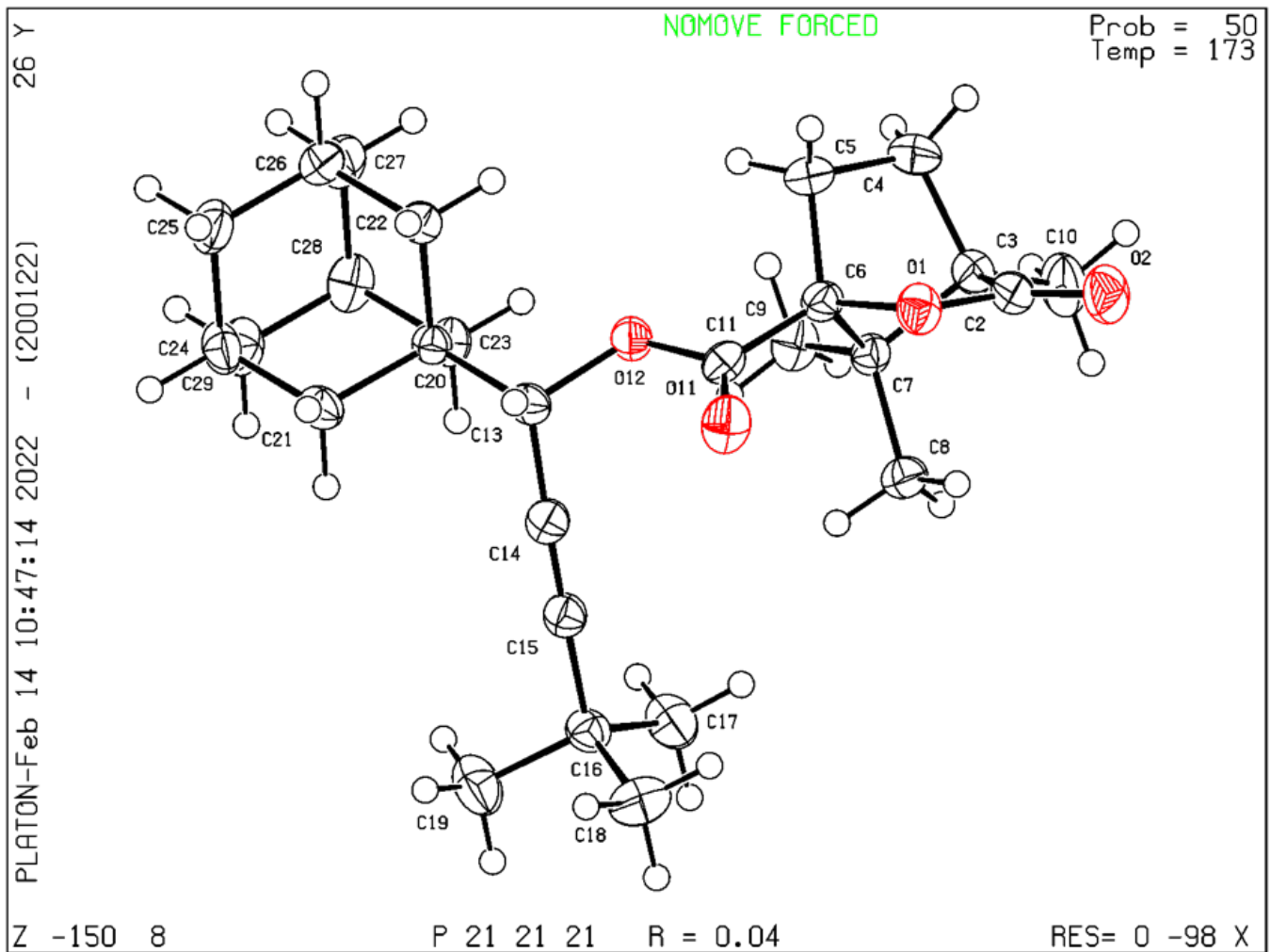
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 20/01/2022; check.def file version of 19/01/2022

Datablock 8 - ellipsoid plot



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