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) Ghosalin_auto

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: Ghosalin_auto

Bond precision: C-C = 0.0058 A Wavelength=1.54184

Cell: a=8.7363(5) b=9.2403(8) c=10.9458(5)
alpha=81.948(6) beta=89.824(5) gamma=72.572(7)

Temperature: 293 K

	Calculated	Reported
Volume	834.03(10)	834.03(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H20 O6	C17 H20 O6
Sum formula	C17 H20 O6	C17 H20 O6
Mr	320.33	320.33
Dx,g cm-3	1.276	1.276
Z	2	2
Mu (mm-1)	0.807	0.807
F000	340.0	340.0
F000'	341.17	
h,k,lmax	10,11,13	10,11,13
Nref	3305	3233
Tmin,Tmax	0.865,0.908	0.744,1.000
Tmin'	0.865	

Correction method= # Reported T Limits: Tmin=0.744 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.978 Theta(max)= 72.400

R(reflections)= 0.0854(2247) wR2(reflections)= 0.2514(3233)

S = 1.186 Npar= 212

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

PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O00N --C00B . 6.5 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C00B Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C00F Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds..... 0.0058 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H00B ..H00D . 1.83 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H00H ..H00A . 2.09 Ang.
1-x,2-y,1-z = 2_676 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance..... 11.819 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance..... 2.447 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 23 Report
0 1 0, 10 3 0, -10 -3 1, 9 -2 1, 10 3 1, -5 -2 2,
-5 0 2, -7 -9 3, -1 -7 3, 3 -2 4, -7 3 4, 4 9 4,
4 10 4, -7 3 5, 1 -8 6, -9 0 6, 0 7 6, -4 -7 7,
-8 1 7, -6 -4 8, -5 5 9, 4 1 11, -4 0 12,
PLAT977_ALERT_2_C Check Negative Difference Density on H00B . -0.42 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H00A . -0.37 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
H00R
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C00B Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C008 - C00B . 1.50 Ang.
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O002 . 108.5 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O003 . 109.1 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 43 Note
O001 O002 O003 O004 O005 C006 C007 H007
C008 H008 C009 C00A C00B H00B C00C C00D
C00E H00E C00F C00G H00G C00H H00H C00I
H00I C00J H00A H00C H00D C00K H00F H00J
H00K C00L H00L H00M H00N C00M H00O H00P
H00Q O00N H00R
PLAT793_ALERT_4_G Model has Chirality at C007 (Centro SpGr) S Verify
PLAT793_ALERT_4_G Model has Chirality at C008 (Centro SpGr) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 49 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity..... 2.5 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value..... 3.203 Note
Predicted wR2: Based on SigI**2 7.85 or SHELX Weight 21.20
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 4 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
3 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

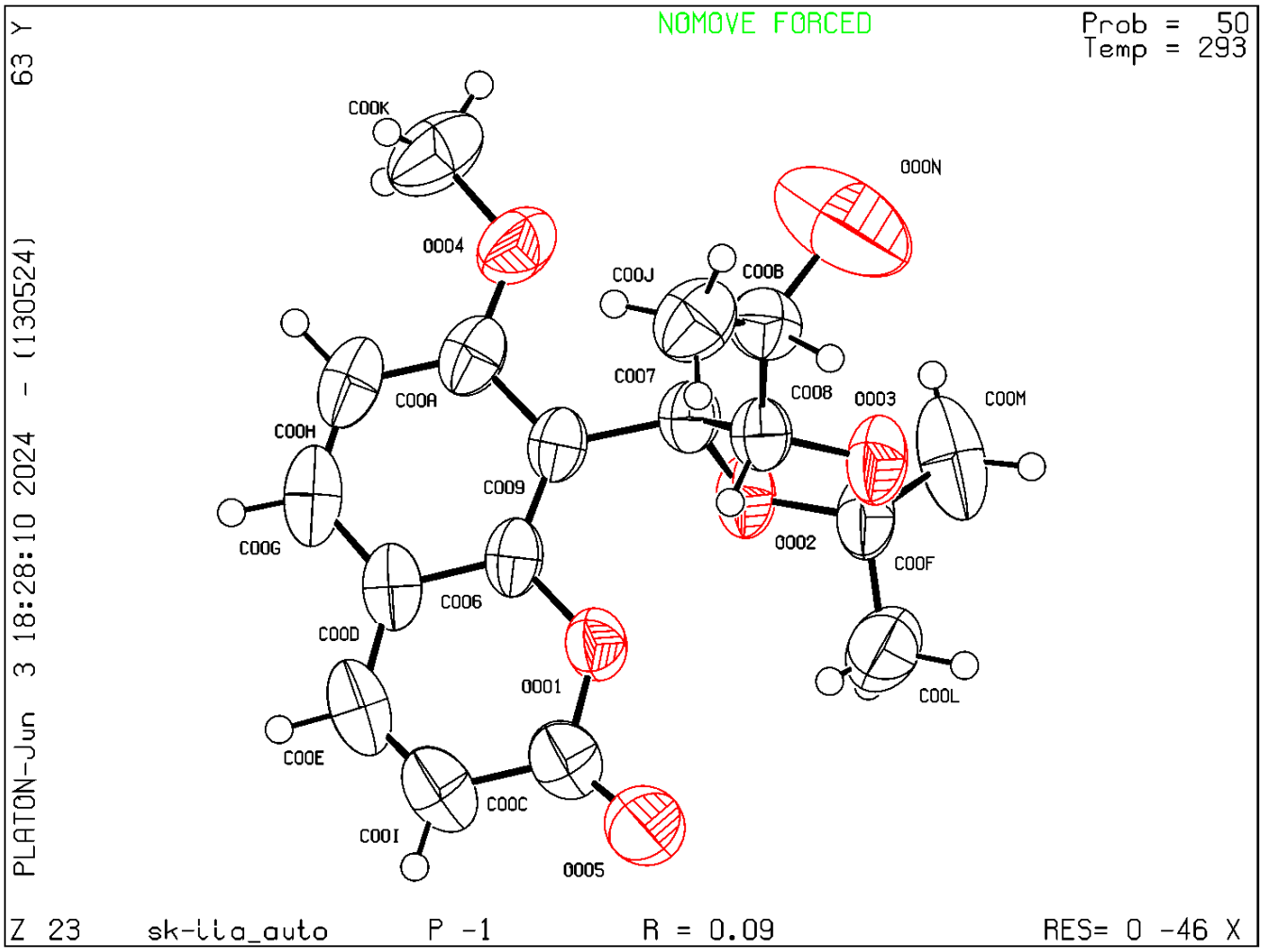
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/05/2024; check.def file version of 04/05/2024

Datablock Ghosalin_auto - ellipsoid plot



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