



Supporting Information

for

Indium-mediated C-allylation of melibiose

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Cif-report of compound 2-syn

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: chde_mehle_p21

Bond precision: C-C = 0.0033 Å Wavelength=0.71073
 Cell: a=14.1418(6) b=9.0704(3) c=29.6461(12)
 alpha=90 beta=91.8306(15) gamma=90
 Temperature: 100 K

| | Calculated | Reported |
|------------------------|---------------------------------|----------------------------------|
| Volume | 3800.8(3) | 3800.8(3) |
| Space group | P 21 | P 21 |
| Hall group | P 2yb | P 2yb |
| Moiety formula | C33 H46 O20 | 1(C33 H46 O20) |
| Sum formula | C33 H46 O20 | C33 H46 O20 |
| Mr | 762.70 | 762.70 |
| Dx, g cm ⁻³ | 1.333 | 1.333 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 0.111 | 0.111 |
| F000 | 1616.0 | 1616.0 |
| F000' | 1617.12 | |
| h,k,lmax | 19,12,41 | 19,12,41 |
| Nref | 22306[11803] | 22249 |
| Tmin, Tmax | 0.970,0.977 | 0.719,0.746 |
| Tmin' | 0.962 | |
| Correction method= | # Reported T Limits: Tmin=0.719 | |
| Tmax=0.746 | AbsCorr = MULTI-SCAN | |
| Data completeness= | 1.89/1.00 | Theta(max)= 30.062 |
| R(reflections)= | 0.0384(19783) | wR2(reflections)= 0.1031(22249) |
| S = 1.093 | Npar= 1051 | |

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](#) Non-Solvent Resd 2 O Ueq(max)/Ueq(min) Range 3.1 Ratio

Alert level G

| | | |
|-----------------------------------|--|-----------------|
| PLAT002 ALERT 2 G | Number of Distance or Angle Restraints on AtSite | 9 Note |
| PLAT012 ALERT 1 G | No _shelx_res_checksum Found in CIF | Please Check |
| PLAT042 ALERT 1 G | Calc. and Reported MoietyFormula Strings Differ | Please Check |
| PLAT171 ALERT 4 G | The CIF-Embedded .res File Contains EADP Records | 1 Report |
| PLAT176 ALERT 4 G | The CIF-Embedded .res File Contains SADI Records | 4 Report |
| PLAT301 ALERT 3 G | Main Residue Disorder(Resd 1) | 9% Note |
| PLAT301 ALERT 3 G | Main Residue Disorder(Resd 2) | 8% Note |
| PLAT380 ALERT 4 G | Incorrectly? Oriented X(sp2)-Methyl Moiety | C27A Check |
| PLAT398 ALERT 2 G | Deviating C-O-C Angle From 120 for O2B | 109.7 Degree |
| PLAT432 ALERT 2 G | Short Inter X...Y Contact O10Y ..C29B x,y,z = 1_555 | 2.79 Ang. Check |
| PLAT720 ALERT 4 G | Number of Unusual/Non-Standard Labels | 4 Note |
| PLAT791 ALERT 4 G | Model has Chirality at C1A (Chiral SPGR) | S Verify |

And 14 other [PLAT791 Alerts](#)

| | | |
|-----------------------------------|--|----------|
| PLAT791 ALERT 4 G | Model has Chirality at C1B (Chiral SPGR) | S Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C2A (Chiral SPGR) | R Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C2B (Chiral SPGR) | R Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C3A (Chiral SPGR) | S Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C3B (Chiral SPGR) | S Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C4A (Chiral SPGR) | S Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C4B (Chiral SPGR) | S Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C7A (Chiral SPGR) | R Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C7B (Chiral SPGR) | R Verify |
| PLAT791 ALERT 4 G | Model has Chirality at C8A (Chiral SPGR) | R Verify |

| | | | |
|--------------------------|--|---------------|----------|
| <u>PLAT791 ALERT 4 G</u> | Model has Chirality at C8B | (Chiral SPGR) | R Verify |
| <u>PLAT791 ALERT 4 G</u> | Model has Chirality at C9A | (Chiral SPGR) | R Verify |
| <u>PLAT791 ALERT 4 G</u> | Model has Chirality at C10A | (Chiral SPGR) | S Verify |
| <u>PLAT791 ALERT 4 G</u> | Model has Chirality at C11A | (Chiral SPGR) | R Verify |
| <u>PLAT860 ALERT 3 G</u> | Number of Least-Squares Restraints | | 5 Note |

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 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
 19 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

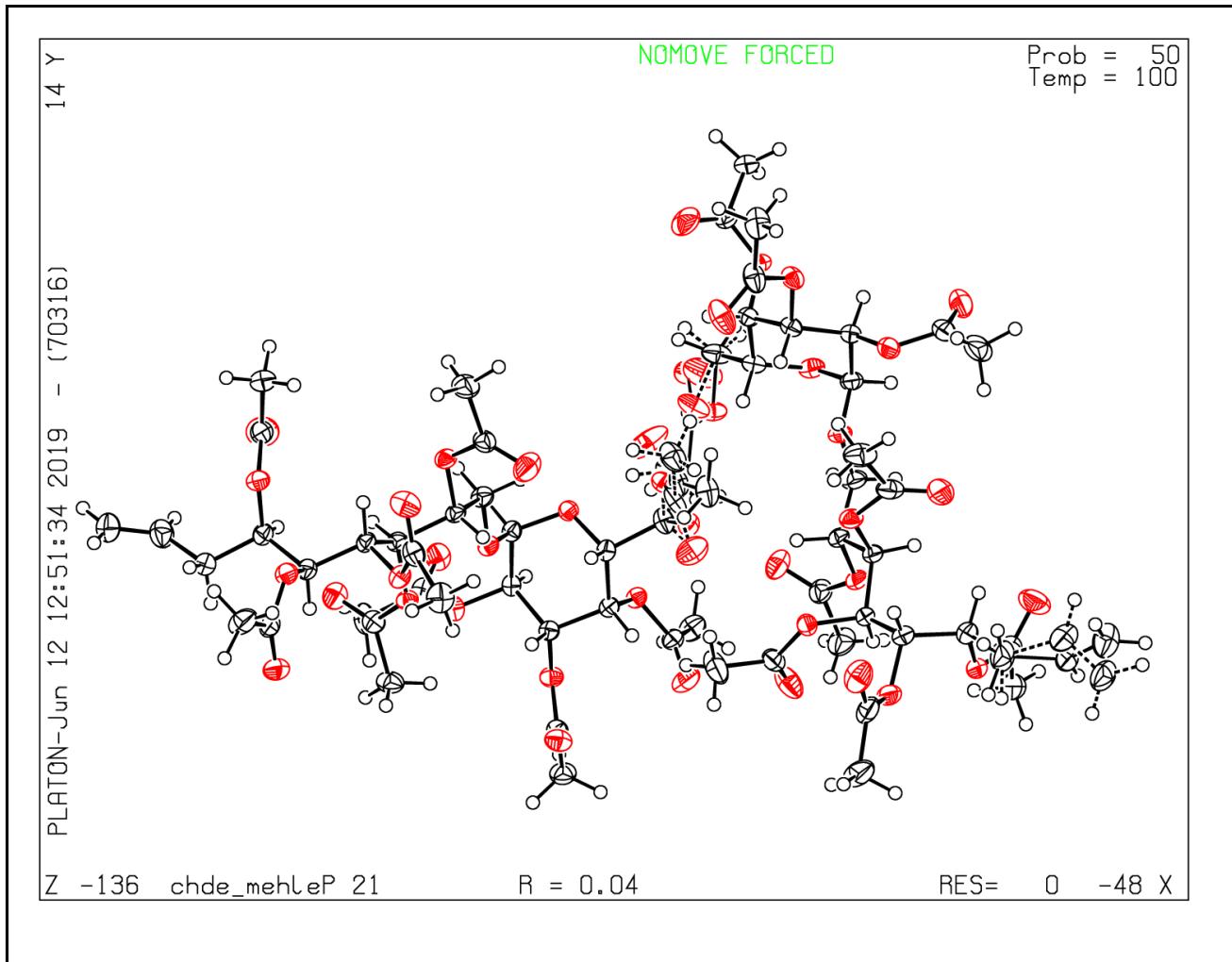
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/05/2019; check.def file version of 29/04/2019

Datablock chde_mehle_p21 - ellipsoid plot



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