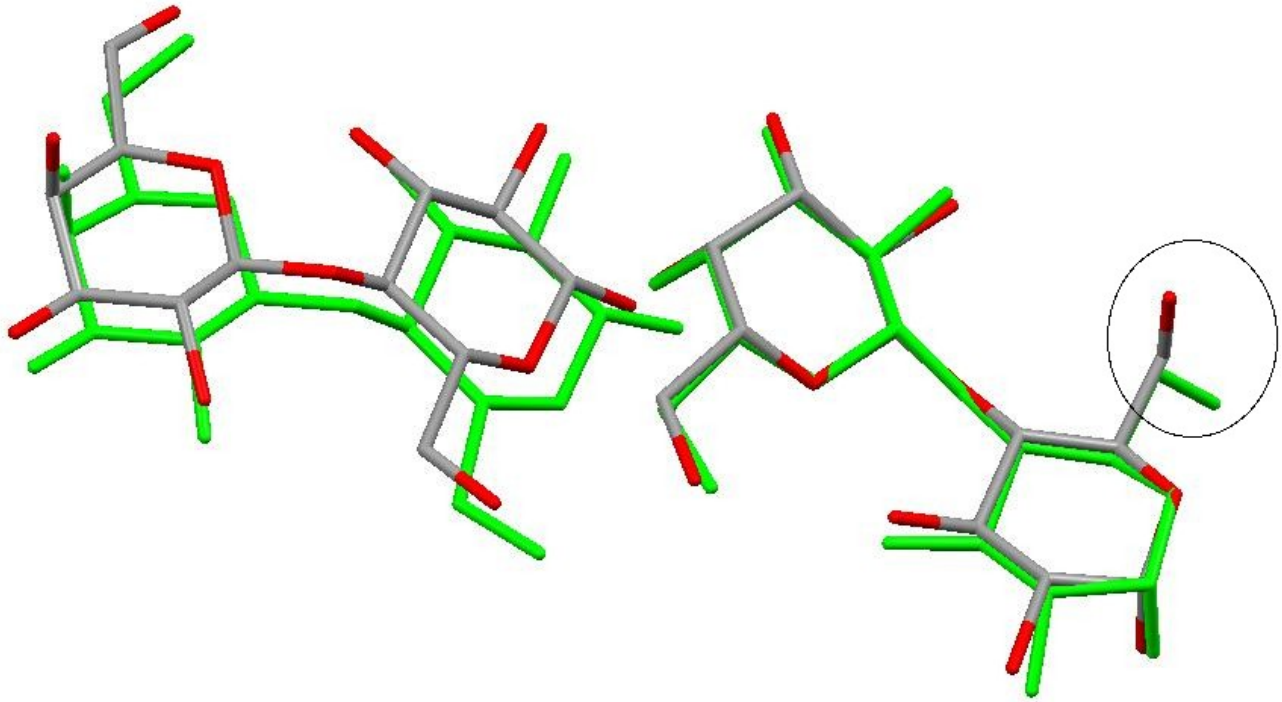
**SUPPORTING INFO**

XPac comparison of the single crystal analysis of αβ-D-lactose with that obtained from powder data (green). Note the difference in orientation of the oxygen of the $CH_2OH$ group on the glucose ring of the α anomer (circled).



CHECK CIF OUTPUT from IUCr for both structures. Note ORTEPs at end.

# checkCIF/PLATON report (publication check)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

## Datablock: 1-deoxy-D-lactose

---

Bond precision: C-C = 0.0030 A Wavelength=0.71073
Cell: a=4.6930(1) b=19.9373(4) c=7.5503(2)
alpha=90 beta=103.159(1) gamma=90

| | Calculated | Reported |
|---|---|---|
| Volume | 687.90(3) | 687.90(3) |
| Space group | P 21 | P 21 |
| Hall group | P 2yb | P 2yb |
| Moiety formula | C12 H22 O10 | C12 H22 O10 |
| Sum formula | C12 H22 O10 | C12 H22 O10 |

| | | |
|---|---|---|
| Mr | 326.30 | 326.30 |
| Dx,g cm-3 | 1.575 | 1.575 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.139 | 0.139 |
| F000 | 348.0 | 348.0 |
| F000' | 348.26 | |
| h,k,lmax | 6,25,9 | 6,25,9 |
| Nref | 1616( 3141) | 1614 |
| Tmin,Tmax | 0.953,0.986 | 0.953,0.986 |
| Tmin' | 0.953 | |

Correction method= AbsCorr=MULTI-SCAN

Data completeness= 1.00(0.51)  Theta(max)= 27.470

R(reflections)= 0.0269( 1528)  wR2(reflections)= 0.0676( 1614)

S = 1.066  Npar= 207

---

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  -0.300
From the CIF: _refine_ls_abs_structure_Flack_su  0.900

PLAT032_ALERT_4_C Std. Uncertainty in Flack Parameter too High ...  0.90
PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical .  ?
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax .LT. 18) .....  7.80
PLAT720_ALERT_4_C Number of Unusual/Non-Standard Label(s) ........  5

---

## Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max  27.47
From the CIF: _reflns_number_total  1614
Count of symmetry unique reflns  1616
Completeness (_total/calc)  99.88%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured  0
Fraction of Friedel pairs measured  0.000
Are heavy atom types Z>Si present  no

PLAT791_ALERT_1_G Confirm the Absolute Configuration of C1'  = .  S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C2  = .  S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C2'  = .  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C3  = .  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C3'  = .  S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C4  = .  S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C4'  = .  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C5  = .  R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C5'  = .  R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .....  1

---

0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
5 **ALERT level C** = Check and explain
11 **ALERT level G** = General alerts; check

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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

# Datablock: alpha-beta-lactose

Bond precision: C-C = 0.0072 A Wavelength=0.69110

Cell: a=5.030(3) b=7.593(5) c=19.374(12)
alpha=81.026(10) beta=85.044(9) gamma=74.247(9)

| | Calculated | Reported |
|---|---|---|
| Volume | 702.7(8) | 702.7(8) |
| Space group | P 1 | P 1 |
| Hall group | P 1 | P 1 |
| Moiety formula | C12 H22 O11 | C12 H22 O11 |
| Sum formula | C12 H22 O11 | C12 H22 O11 |
| Mr | 342.30 | 342.30 |
| Dx,g cm-3 | 1.618 | 1.618 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.161 | 0.145 |
| F000 | 364.0 | 364.0 |
| F000' | 363.97 | |
| h,k,lmax | 7,10,27 | 7,10,27 |
| Nref | 4309( 8618) | 4678 |
| Tmin,Tmax | 0.953,0.986 | 0.953,0.986 |
| Tmin' | 0.953 | |

Correction method= AbsCorr=MULTI-SCAN

Data completeness= 1.09(0.54) Theta(max)= 29.620

R(reflections)= 0.0746( 4292) wR2(reflections)= 0.2067( 4678)

S = 1.046 Npar= 432

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 A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.81

## Alert level B

DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
_refine_diff_density_max given = 0.915
Test value = 0.800

PLAT024_ALERT_4_B Merging of Friedel Pairs is STRONGLY Indicated . !
PLAT097_ALERT_2_B Maximum (Positive) Residual Density ..... 0.92 e/A**
PLAT222_ALERT_3_B Large Non-Solvent H Ueq(max)/Ueq(min) ... 4.37 Ratio
PLAT415_ALERT_2_B Short Inter D-H..H-X H6C .. H11A .. 1.99 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D H3B .. H6' .. 1.54 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D H12B .. H16' .. 1.50 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor O1 - H1A ... ?

## Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
STRVA01_ALERT_4_C Flack test results are meaningless.
From the CIF: _refine_ls_abs_structure_Flack 0.100
From the CIF: _refine_ls_abs_structure_Flack_su 1.400

PLAT032_ALERT_4_C Std. Uncertainty in Flack Parameter too High ... 1.40
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.14
PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ... 3.26 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O11 - C11 .. 5.24 su
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ... 7
PLAT414_ALERT_2_C Short Intra D-H..H-X H1A .. H5 .. 1.98 Ang.

## Alert level G

```
  ABSMU_01  Radiation type not identified. Calculation of
            _exptl_absorpt_correction_mu not performed.
REFLT03_ALERT_4_G  ALERT: MoKa measured Friedel data cannot be used to
                   determine absolute structure in a light-atom
                   study EXCEPT under VERY special conditions.
                   It is preferred that Friedel data is merged in such cases.
            From the CIF: _diffrn_reflns_theta_max           29.62
            From the CIF: _reflns_number_total               4678
            Count of symmetry unique reflns         4309
            Completeness (_total/calc)            108.56%
            TEST3: Check Friedels for noncentro structure
            Estimate of Friedel pairs measured       369
            Fraction of Friedel pairs measured     0.086
            Are heavy atom types Z>Si present          no
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C1     = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C1'    = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C2     = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C2'    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C3     = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C3'    = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C4     = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C4'    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C5     = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C5'    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C11    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C11'   = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C12    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C12'   = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C13    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C13'   = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C14    = .          S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C14'   = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C15    = .          R
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C15'   = .          R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .....            3
```

```
   1 ALERT level A = In general: serious problem
   8 ALERT level B = Potentially serious problem
   8 ALERT level C = Check and explain
  22 ALERT level G = General alerts; check

  21 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 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
```

# checkCIF publication errors

## Alert level A

```
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

## Alert level G

```
PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
            missing. This is required for a full paper submission (but is
            optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   2 ALERT level A = Data missing that is essential or data in wrong format
   2 ALERT level G = General alerts. Data that may be required is missing
```

---

**Publication of your CIF**

You should always 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 nature of your study may justify the reported deviations from the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT029_alpha-beta-lactose
;
PROBLEM: _diffrn_measured_fraction_theta_full Low .......       0.81
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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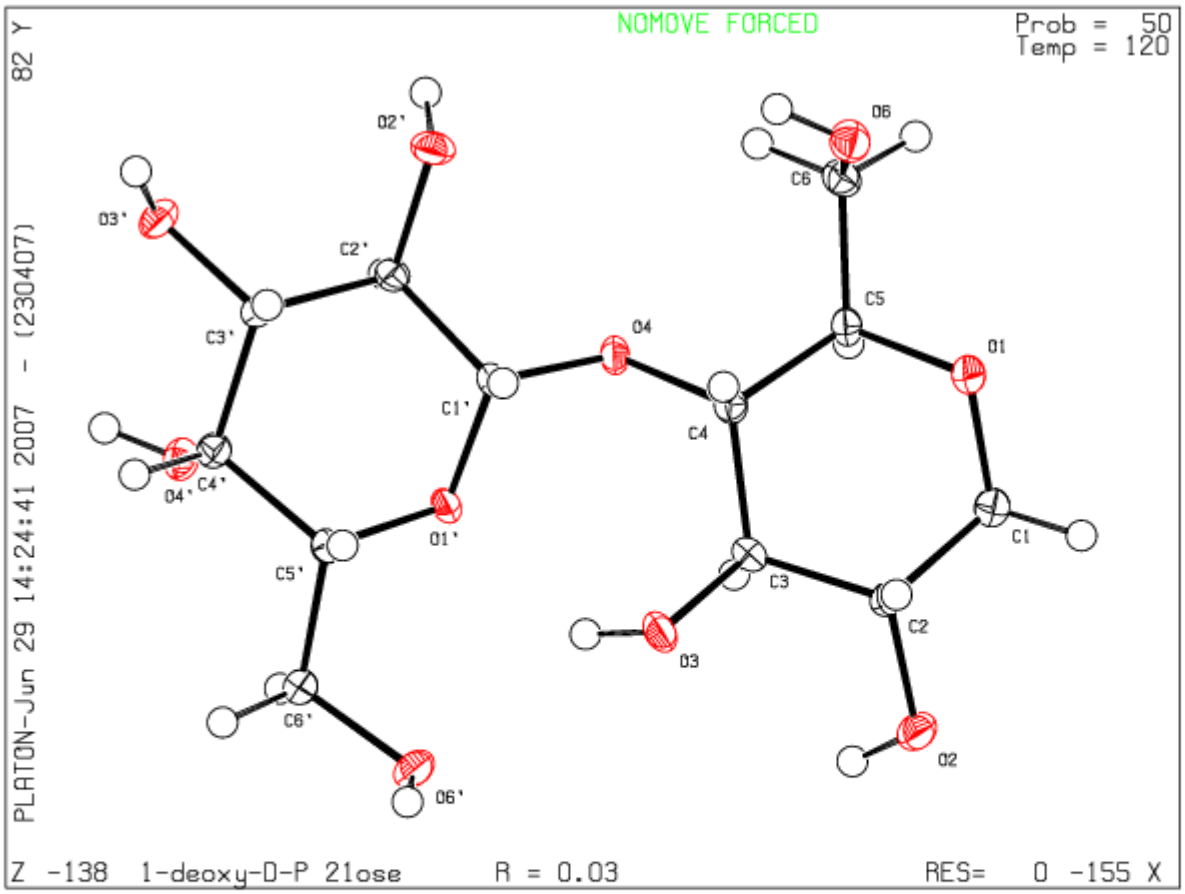
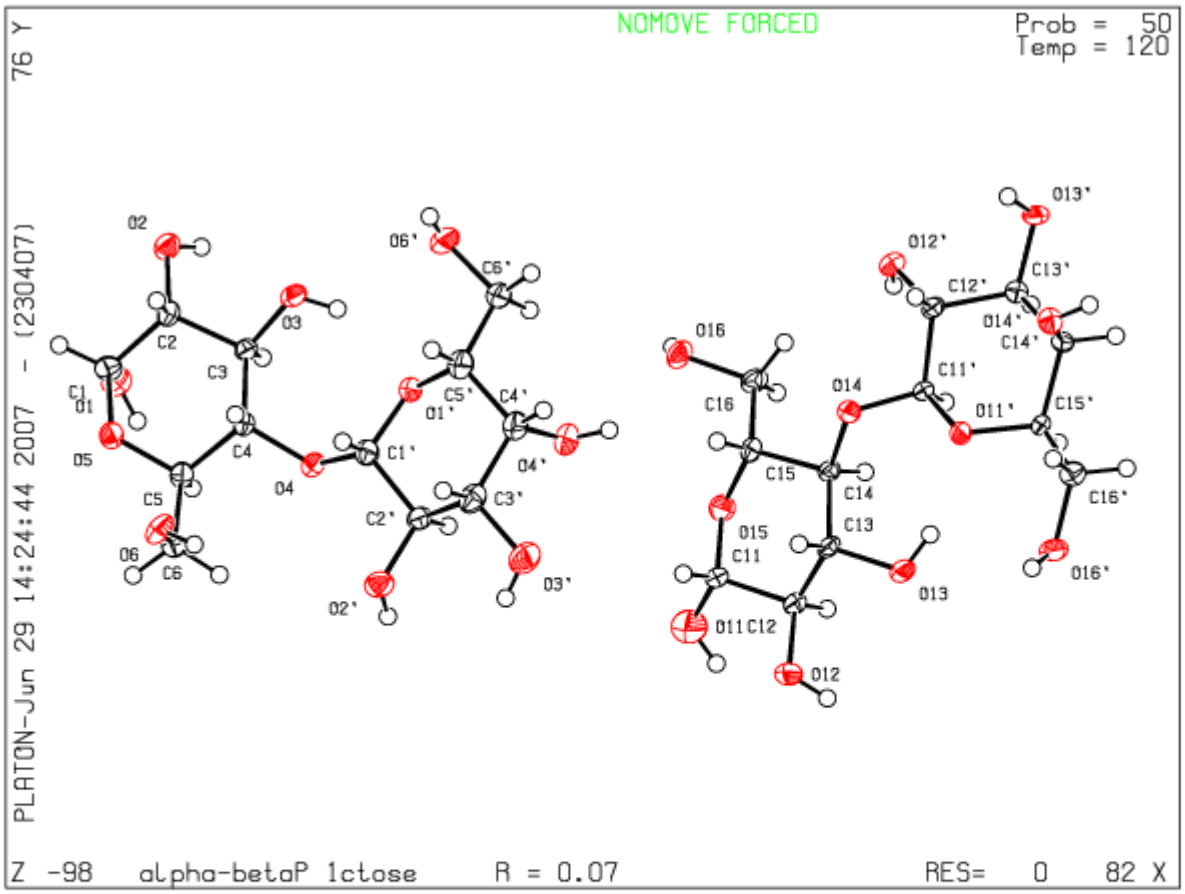
**PLATON version of 23/04/2007; check.def file version of 23/04/2007**

# **Datablock 1-deoxy-D-lactose** - ellipsoid plot




**Datablock alpha-beta-lactose** - ellipsoid plot


NOMOVE FORCED
Prob = 50
Temp = 120
76 Y
PLATON-Jun 29 14:24:44 2007 - (230407)
Z -98 alpha-betaP 1ctose R = 0.07 RES= 0 82 X
O2
O6'
C6'
O3
C2
C3
C1
O1
O5
C4
C5
O6
C6
O4
C1'
O1'
C5'
C4'
O4'
C3'
C2'
O2'
O3'
O13'
O12'
C12'
C13'
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C14'
O16
C16
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C13
C11
O13
O16'
O11
C12
O12