Protones.
Current Data Parameters
NAME   usbrd569a
EXPNO  30
PROCNO  1

F2 - Acquisition Parameters
Date_  20110809
Time_  13.45
INSTRUM spec
PROBDH 5 mm TBI 1H-BB
FUPROG zgpg30
TD    65536
SOLVENT CDCl3
NS    256
DS    4
SWH   80645.164 Hz
FIDRES 1.230548 Hz
AQ    0.4063794 sec
RG    362
DW    6.200 usec
DE    6.00 usec
TE    296.2 K
D1    2.00000000 sec
d11   0.03000000 sec
DELTA 1.89999990 sec
TD0   1

======== CHANNEL f1 ========
NUC1   31P
FL1    17.25 usec
FL2    0.00 dB
SF01   202.4037100 MHz

======== CHANNEL f2 ========
CPDPKG2 waltz16
NUC2   1H
FCPD2  90.00 usec
FL2    0.00 dB
FL12   18.66 dB
FL13   18.66 dB
SF02   500.0020000 MHz

F2 - Processing parameters
SI    32768
SF    202.4037100 MHz
WDW   EM
SSB   0
LB    1.00 Hz
GB    0
PC    1.40
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) R,S-4

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 Interpreting this report

Datablock: R,S-4

Bond precision: C-C = 0.0034 Å  Wavelength=0.71073

Cell:

\begin{align*}
\text{a} &= 7.5632(2) \\
\text{b} &= 8.9693(2) \\
\text{c} &= 10.2710(3) \\
\text{alpha} &= 93.421(2) \\
\text{beta} &= 99.686(2) \\
\text{gamma} &= 99.738(2)
\end{align*}

Temperature: 160 K

\begin{tabular}{ll}
\text{Calculated} & \text{Reported} \\
\text{Volume} & 674.13(3) \\
\text{Space group} & P 1 \\
\text{Hall group} & P 1 \\
\text{Moiety formula} & C31 H27 N2 O P, C2 H3 N \\
\text{Sum formula} & C33 H30 N3 O P \\
\text{Mr} & 515.57 \\
\text{Dx,g cm}^{-3} & 1.270 \\
\text{Z} & 1 \\
\text{Mu (mm}^{-1}) & 0.133 \\
\text{F000} & 272.0 \\
\text{F000'} & 272.19 \\
\text{h,k,lmax} & 11,13,15 \\
\text{Nref} & 9732[4866] \\
\text{Tmin,Tmax} & 0.974,0.976 \\
\text{Tmin'} & 0.974 \\
\text{Correction method= #} & \text{Reported T Limits: Tmin=0.961 Tmax=1.000} \\
\text{AbsCorr = MULTI-SCAN} & \\
\text{Data completeness= 1.75/0.88} & \text{Theta(max)= 32.443} \\
\text{R(reflections)= 0.0369( 7816)} & \text{wr2(reflections)= 0.0902( 8519)} \\
\text{S = 1.021} & \text{Npar= 344}
\end{tabular}

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.
<table>
<thead>
<tr>
<th>Alert level C</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT244_ALERT_4_C</td>
</tr>
<tr>
<td>PLAT915_ALERT_3_C</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alert level G</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT154_ALERT_1_G</td>
</tr>
<tr>
<td>PLAT791_ALERT_4_G</td>
</tr>
<tr>
<td>PLAT910_ALERT_3_G</td>
</tr>
<tr>
<td>PLAT912_ALERT_4_G</td>
</tr>
</tbody>
</table>

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

1 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
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, 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 19/11/2015; check.def file version of 17/11/2015
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) S,S-4

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: S,S-4

Bond precision: C-C = 0.0030 Å  Wavelength=0.71073

Cell:
    a=7.94645(11)  b=16.7110(2)  c=18.5889(3)
    alpha=90  beta=90  gamma=90

Temperature: 160 K

Calculated  Reported
Volume  2468.48(6)  2468.47(6)
Space group  P 21 21 21  P 21 21 21
Hall group  P 2ac 2ab  P 2ac 2ab
MoIety formula  C31 H27 N2 O P  C31 H27 N2 O P
Sum formula  C31 H27 N2 O P  C31 H27 N2 O P
Mr  474.52  474.54
Dx, g cm⁻³  1.277  1.277
Z  4  4
Mu (mm⁻¹)  0.139  0.139
F000  1000.0  1000.0
F000’  1000.76
h,k,lmax  10,22,24  10,21,24
Nref  6272[ 3539]  5288
Tmin,Tmax  0.975,0.983  0.886,1.000
Tmin’  0.963

Correction method= # Reported T Limits: Tmin=0.886 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.49/0.84  Theta(max)= 28.510
R(reflections)= 0.0303( 4915)  wR2(reflections)= 0.0711( 5288)
S = 1.031  Npar= 317

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
PLAT915_ALERT_3_C Low Friedel Pair Coverage ....(No Flack x Check) 78 %

Alert level G
PLAT791_ALERT_4_G The Model has Chirality at C1 (Chiral SPGR) S Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 374 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
3 ALERT level G = General information/check it is not something unexpected

0 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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PLATON version of 19/11/2015; check.def file version of 17/11/2015
## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) R-5

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### Datablock: R-5

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0030 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=10.4501(4)</td>
<td>b=13.3950(5)</td>
</tr>
<tr>
<td></td>
<td>alpha=90</td>
<td>beta=90</td>
</tr>
<tr>
<td>Temperature:</td>
<td>100 K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>2404.32(15)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21 21 21</td>
</tr>
<tr>
<td>Hall group</td>
<td>P 2ac 2ab</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C31 H24 N O2 P</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C31 H24 N O2 P</td>
</tr>
<tr>
<td>Mr</td>
<td>473.48</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.308</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.144</td>
</tr>
<tr>
<td>F000</td>
<td>992.0</td>
</tr>
<tr>
<td>F000’</td>
<td>992.79</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>14,18,23</td>
</tr>
<tr>
<td>Nref</td>
<td>6773[3789]</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.945,0.983</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.944</td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.683 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 1.77/0.99

Theta(max)= 29.604

R(reflections)= 0.0349 (6402)

wr2(reflections)= 0.0824 (6714)

S = 1.049

Npar= 316

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.
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(R)-Spinol

$^1$H NMR spectrum (400 MHz, CDCl$_3$, 298 K):

$^{13}$C NMR spectrum (100 MHz, CDCl$_3$, 298 K):