COMPOUND 6

Supervisor Kumarasamy-bhisaini5

COMPOUND 6

**Current Data Parameters**
- **NAME**: 0901BE-6
- **EXPNO**: 31
- **PROCNO**: 1

**Acquisition Parameters**
- **DATE**: 08-25-11
- **DATE_d**: Sep 06 2009
- **DS**: 1
- **LOCN**: 2
- **NX**: 16
- **O1**: 1833.67 Hz
- **O2**: 1833.67 Hz
- **R2**: 545.0997 Hz
- **SFO2**: 300.173537 MHz
- **SOLVENT**: DMSO
- **SR**: 21544 ppm
- **TD**: 31760
- **TE**: 300 K

**Processing Parameters**
- **LB**: 0.30 Hz
- **PC**: 1.60
- **SP**: 300.173537 MHz
- **SI**: 16384

**ID FID Plot Parameters**
- **SR**: 21544 Hz
- **SOLVENT**: DMSO
COMPOUND 32
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vs3arepro

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: vs3arepro

Bond precision: C-C = 0.0150 Å Wavelength=0.71073

Cell: a=23.015(5) b=31.326(6) c=4.984(1)
    alpha=90 beta=90 gamma=90

Temperature: 100 K

| Calculated | Reported |
|------------|----------|
| Volume     | 3593.3(13) | 3593.3(12) |
| Space group| P 2 2ab   | P 2 2ab   |
| Hall group | P 2 21 2  | P 2 21 2  |
| Moiety formula | C35 H42 N4 O10 [+ solvent] | C35 H42 N4 O10 |
| Sum formula | C35 H42 N4 O10 [+ solvent] | C35 H42 N4 O10 |
| Mr         | 678.73    | 678.72    |
| Dx,g cm^{-3}| 1.255    | 1.255    |
| Z          | 4         | 4         |
| Mu (mm^{-1})| 0.093    | 0.093    |
| F000       | 1440.0    | 1440.0    |
| F000'      | 1440.75   |           |
| h,k,lmax   | 26,35,5   | 26,35,5   |
| Nref       | 5588[ 3284] | 5471     |
| Tmin,Tmax  | 0.999,0.999 | 0.999   |
| Tmin’      | 0.999     |           |

Correction method= Not given

Data completeness= 1.67/0.98 Theta(max)= 23.885

R(reflections)= 0.1380( 4913) wR2(reflections)= 0.3602( 5471)

S = 1.571 Npar= 446
The following ALERTS were generated. Each ALERT has the format

```
test-name_ALERT_alert-type_alert-level.
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Click on the hyperlinks for more details of the test.

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**Alert level B**

THETM01_ALERT_3_B The value of \(\sin(\theta_{\text{max}})/\text{wavelength}\) is less than 0.575

\[
\text{Calculated } \sin(\theta_{\text{max}})/\text{wavelength} = 0.5697
\]

PLAT084_ALERT_3_B High \(wR2\) Value (i.e. > 0.25) ........................ 0.36 Report

**Author Response:** Crystals were ultra thin and could be only measured for
diffraction at Australian Synchrotron. Even with the synchrotron radiation
they diffracted only to lower angles. So, the alerts arising at level B below
are due to weak diffraction, disordered L-leu moieties and possible presence
of partially occupied water molecule in the crystal lattice.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 0.81 e\(\text{A}^{-3}\)

**Author Response:** as explained above

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ............... 0.01504 Ang.

**Author Response:** as explained above

PLAT369_ALERT_2_B Long \(C(\text{sp2})-C(\text{sp2})\) Bond C9B - C10B . 1.57 Ang.

**Author Response:** as explained above

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**Alert level C**

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

RINTE01_ALERT_3_C The value of \(R_{\text{int}}\) is greater than 0.12

\[
R_{\text{int}} \text{ given } 0.120
\]

STRVA01_ALERT_4_C Flack test results are meaningless.

\[
\text{From the CIF: } _\text{refine}_ls_abs_structure_Flack 0.300
\]

\[
\text{From the CIF: } _\text{refine}_ls_abs_structure_Flack_su 0.700
\]

PLAT082_ALERT_2_C High \(R_{\text{1}}\) Value ........................................... 0.14 Report

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........ 7.23 Note

PLAT213_ALERT_2_C Atom C13B has ADP max/min Ratio ...... 3.3 prolat

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.1 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 6.4 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference O3A --C10A . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference O4A --C12A . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C5A --C6A . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C11A --C12A . 0.19 Ang.

PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of C7B Check

PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of C14A Check

PLAT242_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of O5B Check

PLAT242_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of N1B Check

PLAT242_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of C7A Check

PLAT242_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of C11A Check

PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ............ C14B Check

PLAT369_ALERT_2_C Long \(C(\text{sp2})-C(\text{sp2})\) Bond C9A - C10A . 1.53 Ang.
Author Response: as explained above

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ...... 2.950 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.570 55 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ..... 7 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.90A From O3A 0.78 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15B -0.31 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ............ 4 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.700 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 9 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 17 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C15’ Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16’ Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17’ Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15’ Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16E Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16F Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16G Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16H Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16I Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16J Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16K Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16L Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17E Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17F Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17G Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17H Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17I Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17J Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17K Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17L  Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ..............(Resd 1 ) 10% Note
PLAT343_ALERT_2_G Unusual sp?Angle Range in Main Residue for C11A Check
PLAT367_ALERT_2_G Long? C(sp?) C(sp?) Bond C11A - C12A 1.56 Ang.
PLAT412_ALERT_2_G Short Intra XH3 .. Xh  H14B ..H17C 2.09 Ang.
PLAT413_ALERT_2_G Short Inter XH3 .. Xh  H14A ..H17K 2.14 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O3A ..C12A 2.88 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 56 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ........... 8 Note
PLAT791_ALERT_4_G Model has Chirality at C11B (Chiral SPGR) R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............. 29 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 7 Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
25 ALERT type 2 Indicator that the structure model may be wrong or deficient
14 ALERT type 3 Indicator that the structure quality may be low
55 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

# start Validation Reply Form
_vrf_THETM01_vs3arepro
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.575
RESPONSE: ...
;
# end Validation Reply Form
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 07/08/2019; check.def file version of 30/07/2019
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vs4repro

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: vs4repro**

| Bond precision:  | C-C = 0.0056 A | Wavelength=0.71073 |
|------------------|----------------|-------------------|
| Cell:            | a=25.705(5) b=5.020(1) c=30.114(6) | alpha=90 beta=113.79(3) gamma=90 |
| Temperature:     | 100 K          |                   |

| Calculated       | Reported       |
|------------------|----------------|
| Volume           | 3555.7(15)     | 3555.7(14)       |
| Space group      | C 2            | C 1 2 1          |
| Hall group       | C 2y           | C 2y             |
| Moiety formula   | C33 H40 N4 O10 S2 | 0.5(C33 H40 N4 O10 S2) |
| Sum formula      | C33 H40 N4 O10 S2 | C16.50 H20 N2 O5 S |
| Mr               | 716.81         | 358.40           |
| Dx,g cm-3        | 1.339          | 1.339            |
| Z                | 4              | 8                |
| Mu (mm-1)        | 0.211          | 0.211            |
| F000             | 1512.0         | 1512.0           |
| F000’            | 1513.73        |                   |
| h,k,lmax         | 28,5,34        | 28,5,34          |
| Nref             | 5495[ 3108]    | 5460             |
| Tmin,Tmax        | 0.996,0.997    |                   |
| Tmin’            | 0.996          |                   |

Correction method= Not given

Data completeness= 1.76/0.99 Theta(max)= 23.858

R(reflections)= 0.0366( 4781) wR2(reflections)= 0.0862( 5460)

S = 1.038 Npar= 450
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 B**
THETM01_ALERT_3_B  The value of sin(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5691

Author Response: Crystals were ultrathin which diffracted very weakly at high angles even in the synchrotron beam at Australian MX1 beam line.

**Alert level C**
PLAT089_ALERT_3_C  Poor Data / Parameter Ratio (Zmax < 18) ........... 6.88 Note
PLAT340_ALERT_3_C  Low Bond Precision on C-C Bonds ................. 0.00564 Ang.
PLAT369_ALERT_2_C  Long C(sp2)-C(sp2) Bond C9A - C10A . 1.55 Ang.
PLAT369_ALERT_2_C  Long C(sp2)-C(sp2) Bond C9B - C10B . 1.54 Ang.
PLAT911_ALERT_3_C  Missing FCF Refl Between Thmin & STth/L= 0.569 10 Report
PLAT913_ALERT_3_C  Missing # of Very Strong Reflections in FCF ....... 4 Note

**Alert level G**
PLAT007_ALERT_5_G  Number of Unrefined Donor-H Atoms ............. 4 Report
PLAT042_ALERT_1_G  Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G  Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT300_ALERT_4_G  Atom Site Occupancy of H1NA Constrained at 0.5 Check
PLAT300_ALERT_4_G  Atom Site Occupancy of H1MB Constrained at 0.5 Check
PLAT367_ALERT_2_G  Long C(sp2)-C(sp2) Bond C1M - C4A . 1.52 Ang.
PLAT367_ALERT_2_G  Long C(sp2)-C(sp2) Bond C1M - C4A_a . 1.52 Ang.
PLAT367_ALERT_2_G  Long C(sp2)-C(sp2) Bond C1N - C4B . 1.51 Ang.
PLAT367_ALERT_2_G  Long C(sp2)-C(sp2) Bond C1N - C4B_b . 1.51 Ang.
PLAT720_ALERT_4_G  Number of Unusual/Non-Standard Labels ........... 10 Note
PLAT791_ALERT_4_G  Model has Chirality at C11A (Chiral SPGR) S Verify
PLAT791_ALERT_4_G  Model has Chirality at C11B (Chiral SPGR) S Verify
PLAT883_ALERT_1_G  No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G  Percentage of I>2sig(I) Data at Theta(Max) Still 74% Note
PLAT910_ALERT_3_G  Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G  Number of OMIT Records in Embedded .res File ... 7 Note
PLAT978_ALERT_2_G  Number C-C Bonds with Positive Residual Density. 4 Info

0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
6 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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
7 ALERT type 4 Improvement, methodology, query or suggestion
1 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 07/08/2019; check.def file version of 30/07/2019
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vs5repro

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: vs5repro

Bond precision:  C-C = 0.0145 A  Wavelength=0.71073

Cell:  
  a=32.369(7)  b=4.869(1)  c=26.474(5)  
  alpha=90  beta=127.16(3)  gamma=90  

Temperature:  100 K

Calculated Reported
Volume  3325.2(18)  3325.3(16)
Space group  C 2  C 2 1
Hall group  C 2y  C 2y
Moiety formula  C33 H34 N4 O10, C33 H38 N4 O10
Sum formula  C66 H72 N8 O20  C33 H36 N4 O10
Mr  1297.32  648.66
Dx,g cm-3  1.296  1.296
Z  2  4
Mu (mm-1)  0.097  0.097
F000  1368.0  1368.0
F000’  1368.73
h,k,lmax  36,5,30  36,5,30
Nref  5143[ 2919]  4904
Tmin,Tmax  0.998,0.999  0.998
Tmin’  0.998

Correction method= Not given

Data completeness= 1.68/0.95  Theta(max)= 23.836
R(reflections)= 0.1237( 4712)  wr2(reflections)= 0.3870( 4904)

S = 2.026  Npar= 384
The following ALERTS were generated. Each ALERT has the format
\textit{test-name_ALERT_alert-type_alert-level}.
Click on the hyperlinks for more details of the test.

\begin{tabular}{|l|}
\hline
\textbf{Alert level B} \\
\textbf{DIFMN02_ALERT_2_B} The minimum difference density is \(< -0.1*ZMAX*1.00 \\
\_refine\_diff\_density\_min\ given = -1.141 \\
Test value = -0.800 \\
\textbf{THETM01_ALERT_3_B} The value of sine(\theta_{max})/wavelength is less than 0.575 \\
Calculated sin(\theta_{max})/wavelength = 0.5686 \\
\hline
\end{tabular}

Author Response: All the crystals were ultrathin and could only be measured at Australian synchrotron. Crystals diffracted only to lower values of \theta.

\begin{tabular}{|l|}
\hline
\textbf{PLAT029_ALERT_3_B} \_diffrn\_measured\_fraction\_theta\_full value Low . 0.955 Why? \\
\textbf{Author Response:} same as above \\
\hline
\textbf{PLAT084_ALERT_3_B} High wR2 Value (i.e. > 0.25) .................. 0.39 Report \\
\textbf{Author Response:} As a result of weak diffraction with asymmetric unit containing two molecules with disorders reflecting in higher values of wR2. One of the molecules takes two orientations which are very slightly displaced from each other. The limitation of data (not much of high angle data) and as a result inadequate modelling of disorder resulted in residual densities, low bond precisions and also inability to refine this molecule anisotropically. \\
\hline
\textbf{PLAT097_ALERT_2_B} Large Reported Max. (Positive) Residual Density 0.96 eA-3 \\
\textbf{Author Response:} reasons as given above. \\
\hline
\textbf{PLAT098_ALERT_2_B} Large Reported Min. (Negative) Residual Density -1.14 eA-3 \\
\textbf{Author Response:} reasons as given above \\
\hline
\textbf{PLAT201_ALERT_2_B} Isotropic non-H Atoms in Main Residue(s) ........ 4 Report \\
C1N C11B C13B C14B \\
\textbf{Author Response:} reasons as given above \\
\hline
\textbf{PLAT340_ALERT_3_B} Low Bond Precision on C-C Bonds ............... 0.0145 Ang. \\
\textbf{Author Response:} reasons as given above \\
\hline
\textbf{PLAT430_ALERT_2_B} Short Inter D...A Contact O3A ..N2A . 2.73 Ang. \\
x,1+y,z = 1.565 Check \\
\textbf{PLAT934_ALERT_3_B} Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check \\
\hline
\end{tabular}
Alert level C

DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies outside the range 0.80 < 2.00
Goodness of fit given = 2.026
STRVA01_ALERT_2_C  Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 0.900
From the CIF: _refine_ls_abs_structure_Flack_su 0.300
PLAT082_ALERT_2_C High R1 Value .................................. 0.12 Report
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) ............ 2.03 Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ....... 7.26 Note
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.6 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT222_ALERT_2_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O5A’ --C12A . 0.17 Ang.
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of C1N Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of C11B Check
PLAT242_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of C11A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .......... O4” Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .......... O2AA Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .......... C13B Check
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C9A - C10A . 1.54 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C33 H34 N4 O10
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.90 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.569 131 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 34 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 5 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 13.02 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ............. 3 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.30 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFTX Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O0AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N0AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1” Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6" Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1NB Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1NA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1NC Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1ND Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8BA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8BB Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8BC Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8"A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8"B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15E Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15F Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8"C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16E Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16F Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15' Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13E Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13F Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15G Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15H Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15I Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15J Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15K Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15L Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16G Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16H Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16I Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16J Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16K Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16L Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ..................(Resd 1 ) 85% Note
PLAT301_ALERT_3_G Main Residue Disorder ..................(Resd 2 ) 21% Note
PLAT309_ALERT_2_G Single Bonded Oxygen (C-O > 1.3 Ang) .......... 02" Check
PLAT367_ALERT_2_G Long? C(sp?)=C(sp?) Bond C11B - C14B . 1.53 Ang.
PLAT367_ALERT_2_G Long? C(sp?)=C(sp?) Bond C1M - C4A . 1.51 Ang.
PLAT367_ALERT_2_G Long? C(sp?)=C(sp?) Bond C1M - C4A_b . 1.51 Ang.
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5" 108.1 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5B 101.3 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ........... 22 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C11B --C12B 1.74 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 43 Check
  C4B -=C1N -=C4"
  2.453 1.555 2.453
  27.50 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
  C33 H38 N4 O10
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............. 4 Note
PLAT909_ALERT_3_G Percentage of I>2sigma(I) Data at Theta(Max) Still 90% Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
15 ALERT type 3 Indicator that the structure quality may be low
116 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Validation response form
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

# start Validation Reply Form
_vrf_DIFMN02_vs5repro
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*1.00
RESPONSE: ...
;
_vrf_PLAT430_vs5repro
;
PROBLEM: Short Inter D...A Contact O3A . .N2A . 2.73 Ang.
RESPONSE: ...
;
_vrf_PLAT934_vs5repro
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers . 2 Check
RESPONSE: ...
;
# end Validation Reply Form

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 07/08/2019; check.def file version of 30/07/2019
