# wwPDB X-ray Structure Validation Summary Report (i)

Apr 3, 2024 – 03:10 am BST

| | | |
|---|---|---|
| PDB ID | : | 7NSN |
| Title | : | Multi-domain GH92 alpha-1,2-mannosidase from Neobacillus novalis: mannoimidazole complex |
| Authors | : | Kolaczkowski, B.M.; Moroz, O.V.; Blagova, E.; Davies, G.J.; Wilson, K.S.; Moeler, M.S.; Meyer, A.S.; Westh, P.; Jensen, K.; Krogh, K.B.R.M. |
| Deposited on | : | 2021-03-08 |
| Resolution | : | 2.29 Å(reported) |

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

---

The following versions of software and data (see references (i)) were used in the production of this report:

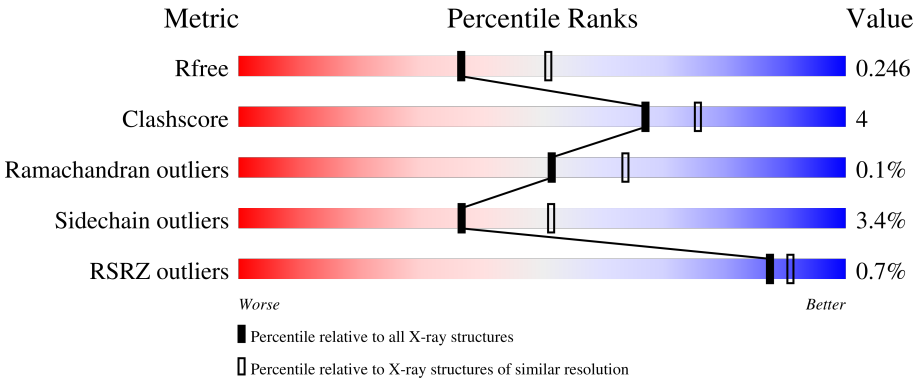
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 5042 (2.30-2.30) |
| Clashscore | 141614 | 5643 (2.30-2.30) |
| Ramachandran outliers | 138981 | 5575 (2.30-2.30) |
| Sidechain outliers | 138945 | 5575 (2.30-2.30) |
| RSRZ outliers | 127900 | 4938 (2.30-2.30) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1411 | 87% 9% |
| 1 | B | 1411 | % 78% 8% 13% |

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

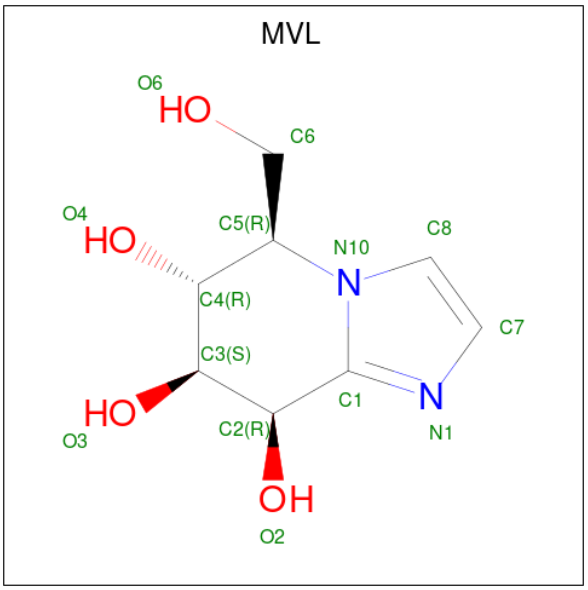
- Molecule 1 is a protein called GH92 alpha-1,2-mannosidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1371 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10648 | 6716 | 1789 | 2118 | 25 | | | |
| 1 | B | 1224 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9492 | 5987 | 1597 | 1884 | 24 | | | |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

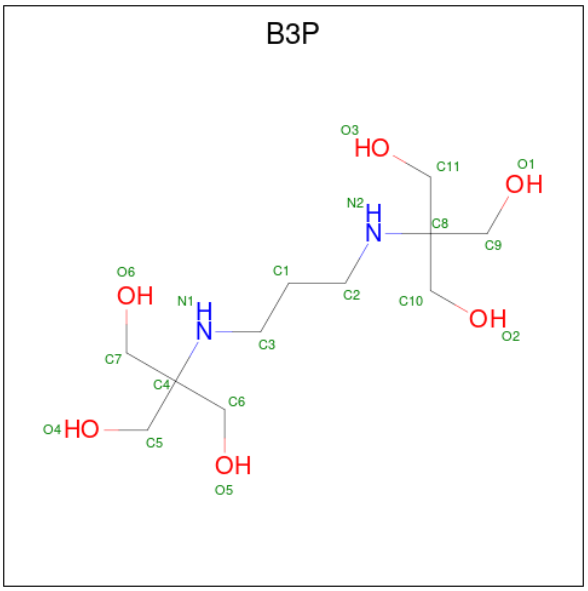
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 5 | Total | Ca | 0 | 0 |
| | | | 5 | 5 | | |
| 2 | B | 4 | Total | Ca | 0 | 0 |
| | | | 4 | 4 | | |

- Molecule 3 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (three-letter code: MVL) (formula: $C_8H_{12}N_2O_4$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total C N O<br>14 8 2 4 | 0 | 0 |
| 3 | A | 1 | Total C N O<br>14 8 2 4 | 0 | 0 |
| 3 | B | 1 | Total C N O<br>14 8 2 4 | 0 | 0 |

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 1 | Total C N O<br>19 11 2 6 | 0 | 0 |
| 4 | B | 1 | Total C N O<br>19 11 2 6 | 0 | 0 |

- Molecule 5 is water.

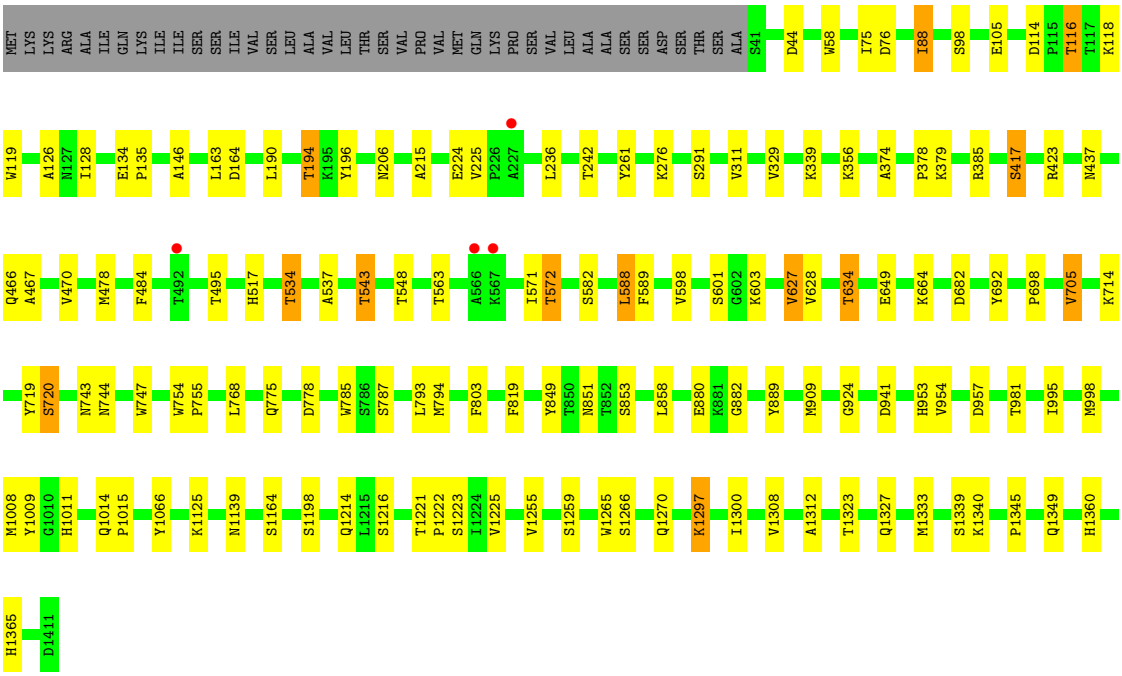
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | A | 318 | Total O<br>318 318 | 0 | 0 |
| 5 | B | 243 | Total O<br>243 243 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

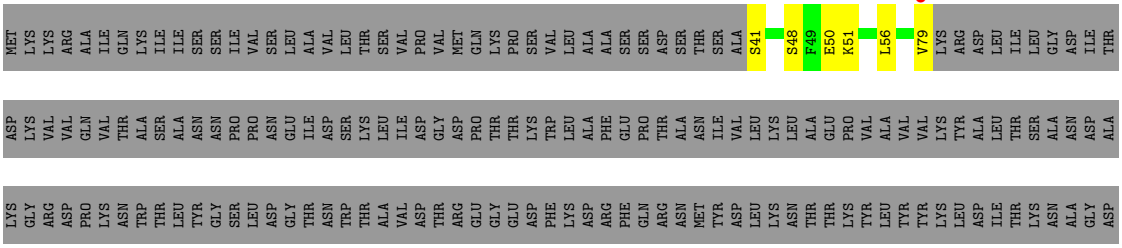
• Molecule 1: GH92 alpha-1,2-mannosidase

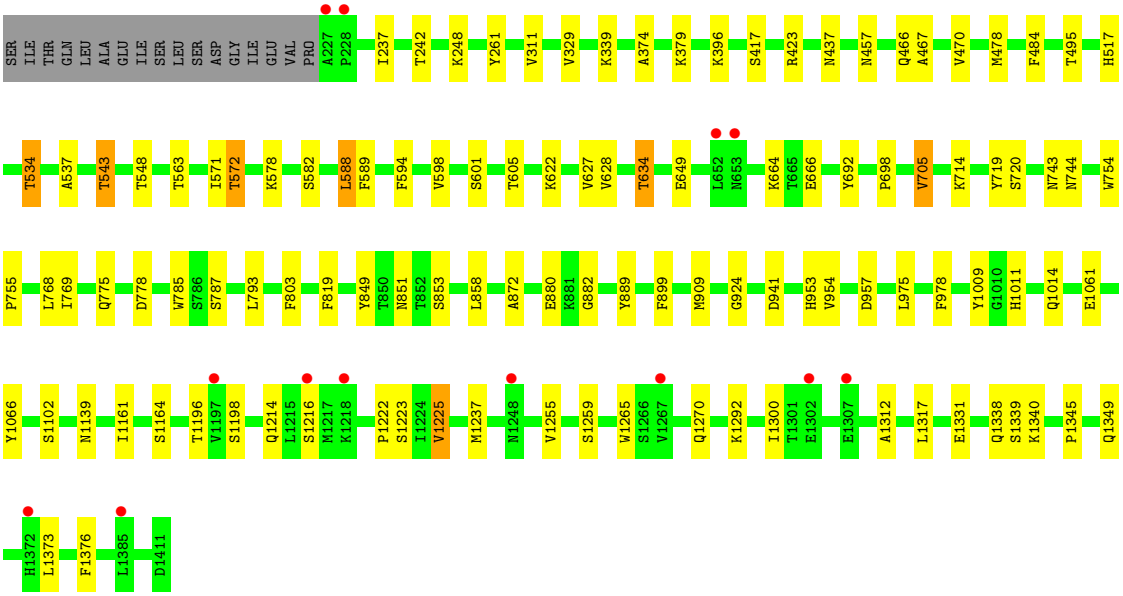
Chain A:


• Molecule 1: GH92 alpha-1,2-mannosidase

Chain B:


SER ILE THR GLN LEU ALA GLU ILE SER LEU SER ASP GLY ILE GLU VAL PRO A227 P228 I237 T242 K248 Y261 V311 V329 K339 A374 K379 K396 S417 R423 N437 M457 Q466 A467 V470 M478 F484 T495 H517
T534 A537 T543 T548 T563 I571 T572 K578 S582 L588 F589 F594 V598 S601 T605 K622 V627 V628 T634 E649 L652 M653 K664 T665 E666 Y692 P698 V706 K714 Y719 S720 N743 N744 W754
P755 L768 I769 Q775 D778 W785 S786 S787 L793 F803 F819 Y849 T850 N851 T852 S853 L858 A872 E880 K881 G882 Y889 F899 M909 G924 D941 H953 V954 D957 L975 F978 Y1009 G1010 H1011 Q1014 E1061
Y1066 S1102 N1139 I1161 S1164 T1196 V1197 S1198 Q1214 L1215 S1216 M1217 K1218 P1222 S1223 I1224 V1225 M1237 N1248 V1255 S1259 W1265 S1266 V1267 Q1270 K1292 I1300 T1301 E1302 E1307 A1312 L1317 E1331 Q1338 S1339 K1340 P1345 Q1349
H1372 L1373 F1376 L1385 D1411

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 94.61Å 151.94Å 114.01Å<br>90.00° 94.63° 90.00° | Depositor |
| Resolution (Å) | 47.92 – 2.29<br>47.92 – 2.29 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.0 (47.92-2.29)<br>98.0 (47.92-2.29) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.56 (at 2.29Å) | Xtriage |
| Refinement program | REFMAC 5.8.0267 | Depositor |
| R, $R_{free}$ | 0.205 , 0.246<br>0.205 , 0.246 | Depositor<br>DCC |
| $R_{free}$ test set | 6947 reflections (4.92%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 28.4 | Xtriage |
| Anisotropy | 0.380 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 27.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.34$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 20790 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 32.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, CA, MVL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.46 | 0/10900 | 0.80 | 0/14803 |
| 1 | B | 0.45 | 0/9721 | 0.79 | 0/13195 |
| All | All | 0.46 | 0/20621 | 0.80 | 0/27998 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 10648 | 0 | 10216 | 84 | 0 |
| 1 | B | 9492 | 0 | 9068 | 67 | 0 |
| 2 | A | 5 | 0 | 0 | 0 | 0 |
| 2 | B | 4 | 0 | 0 | 0 | 0 |
| 3 | A | 28 | 0 | 22 | 2 | 0 |
| 3 | B | 14 | 0 | 10 | 3 | 0 |
| 4 | A | 19 | 0 | 26 | 1 | 0 |
| 4 | B | 19 | 0 | 26 | 1 | 0 |
| 5 | A | 318 | 0 | 0 | 6 | 0 |
| 5 | B | 243 | 0 | 0 | 7 | 0 |
| All | All | 20790 | 0 | 19368 | 153 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 153 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:995:ILE:HG12 | 1:A:998:MET:CE | 1.71 | 1.19 |
| 1:A:995:ILE:HG12 | 1:A:998:MET:HE2 | 1.27 | 1.15 |
| 1:A:995:ILE:H | 1:A:998:MET:HE3 | 1.11 | 1.14 |
| 1:B:534:THR:HG22 | 1:B:537:ALA:H | 1.20 | 1.05 |
| 1:A:995:ILE:H | 1:A:998:MET:CE | 1.71 | 1.04 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 1369/1411 (97%) | 1312 (96%) | 55 (4%) | 2 (0%) | 51 | 64 |
| 1 | B | 1220/1411 (86%) | 1175 (96%) | 44 (4%) | 1 (0%) | 51 | 64 |
| All | All | 2589/2822 (92%) | 2487 (96%) | 99 (4%) | 3 (0%) | 51 | 64 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 743 | ASN |
| 1 | B | 743 | ASN |
| 1 | A | 794 | MET |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 1138/1178 (97%) | 1096 (96%) | 42 (4%) | 34 | 48 |
| 1 | B | 1010/1178 (86%) | 978 (97%) | 32 (3%) | 39 | 54 |
| All | All | 2148/2356 (91%) | 2074 (97%) | 74 (3%) | 37 | 51 |

5 of 74 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 627 | VAL |
| 1 | B | 1292 | LYS |
| 1 | B | 634 | THR |
| 1 | B | 909 | MET |
| 1 | A | 603 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1360 | HIS |
| 1 | B | 1351 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | MVL | B | 1505 | 2 | 13,15,15 | 0.94 | 1 (7%) | 11,22,22 | 2.36 | 3 (27%) |
| 4 | B3P | B | 1506 | - | 18,18,18 | 0.43 | 0 | 21,23,23 | 0.98 | 2 (9%) |
| 3 | MVL | A | 1505 | 2 | 13,15,15 | 0.85 | 1 (7%) | 11,22,22 | 2.41 | 4 (36%) |
| 4 | B3P | A | 1506 | - | 18,18,18 | 0.47 | 0 | 21,23,23 | 0.92 | 1 (4%) |
| 3 | MVL | A | 1508 | - | 13,15,15 | 0.43 | 0 | 11,22,22 | 1.47 | 2 (18%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | MVL | B | 1505 | 2 | - | 0/2/22/22 | 0/1/2/2 |
| 4 | B3P | B | 1506 | - | - | 18/28/28/28 | - |
| 3 | MVL | A | 1505 | 2 | - | 1/2/22/22 | 0/1/2/2 |
| 4 | B3P | A | 1506 | - | - | 17/28/28/28 | - |
| 3 | MVL | A | 1508 | - | - | 2/2/22/22 | 0/1/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | B | 1505 | MVL | C1-C2 | -2.79 | 1.47 | 1.51 |
| 3 | A | 1505 | MVL | C1-C2 | -2.03 | 1.48 | 1.51 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | B | 1505 | MVL | C4-C3-C2 | 5.28 | 118.26 | 110.24 |
| 3 | A | 1505 | MVL | C4-C3-C2 | 4.79 | 117.51 | 110.24 |
| 3 | A | 1505 | MVL | C6-C5-C4 | -4.25 | 104.78 | 112.45 |
| 3 | B | 1505 | MVL | C8-N10-C1 | -3.96 | 105.30 | 109.05 |
| 3 | A | 1505 | MVL | C8-N10-C1 | -3.78 | 105.48 | 109.05 |

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 1506 | B3P | N1-C4-C6-O5 |
| 4 | A | 1506 | B3P | C5-C4-C6-O5 |
| 4 | A | 1506 | B3P | C7-C4-C6-O5 |
| 4 | A | 1506 | B3P | N1-C4-C7-O6 |
| 4 | A | 1506 | B3P | C5-C4-C7-O6 |

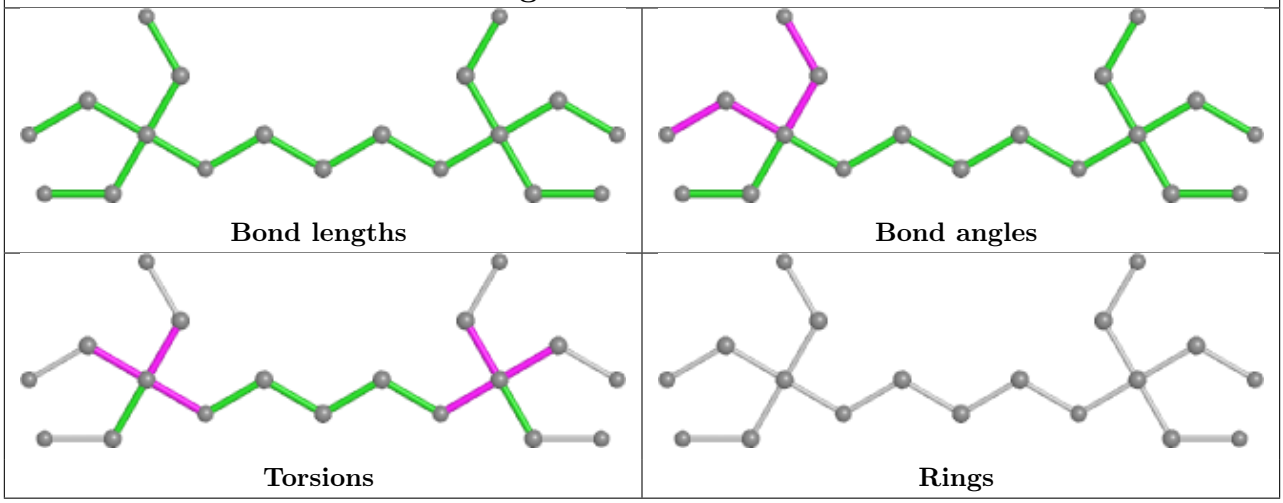
There are no ring outliers.

4 monomers are involved in 7 short contacts:

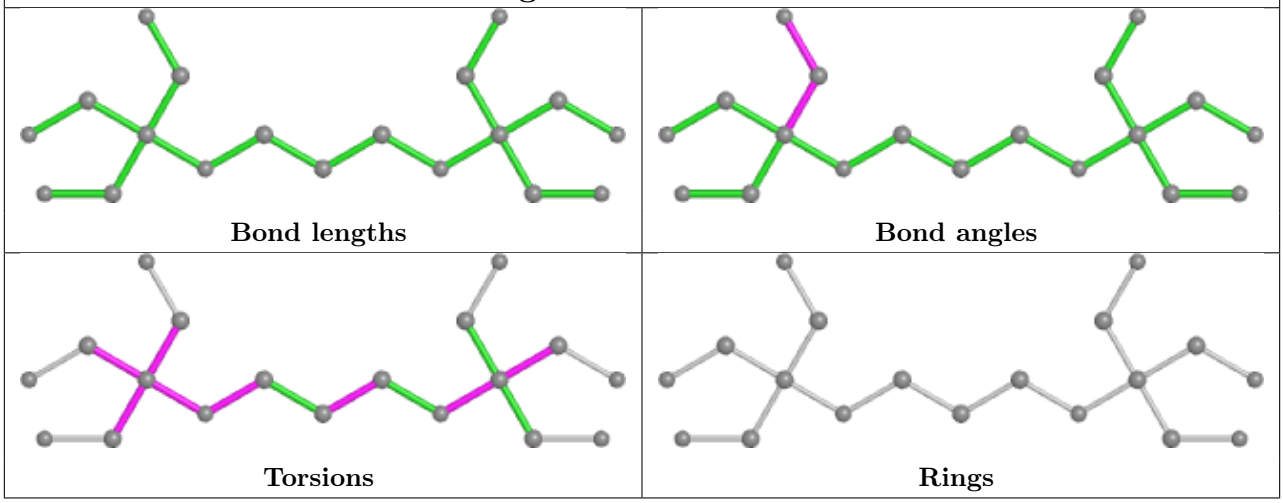
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | B | 1505 | MVL | 3 | 0 |
| 4 | B | 1506 | B3P | 1 | 0 |
| 3 | A | 1505 | MVL | 2 | 0 |
| 4 | A | 1506 | B3P | 1 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight $> 250$ and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand B3P B 1506**




**Ligand B3P A 1506**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 1371/1411 (97%) | -0.37 | 4 (0%) | 94 | 96 | 16, 28, 50, 80 | 0 |
| 1 | B | 1224/1411 (86%) | -0.17 | 14 (1%) | 80 | 85 | 16, 32, 65, 112 | 0 |
| All | All | 2595/2822 (91%) | -0.27 | 18 (0%) | 87 | 91 | 16, 30, 58, 112 | 0 |

The worst 5 of 18 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 227 | ALA | 5.5 |
| 1 | A | 566 | ALA | 3.2 |
| 1 | B | 652 | LEU | 3.2 |
| 1 | A | 567 | LYS | 3.1 |
| 1 | B | 1372 | HIS | 2.9 |

## 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates

There are no monosaccharides in this entry.

## 6.4 Ligands

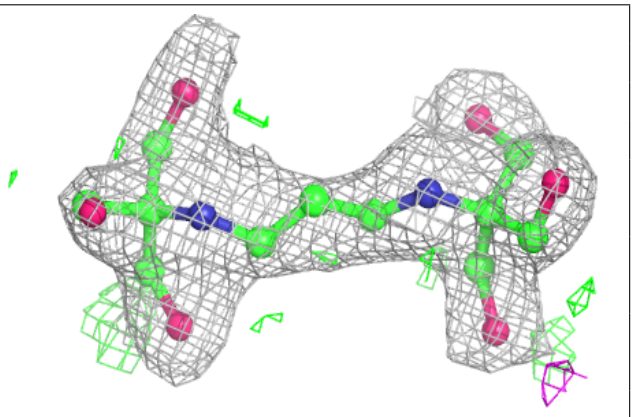
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

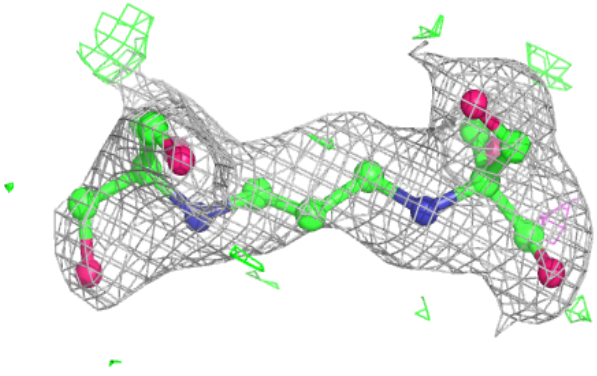
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | B3P | A | 1506 | 19/19 | 0.89 | 0.15 | 37,50,60,61 | 0 |
| 4 | B3P | B | 1506 | 19/19 | 0.89 | 0.15 | 36,49,77,78 | 0 |
| 2 | CA | B | 1503 | 1/1 | 0.94 | 0.06 | 54,54,54,54 | 0 |
| 2 | CA | A | 1503 | 1/1 | 0.95 | 0.04 | 39,39,39,39 | 0 |
| 3 | MVL | A | 1508 | 14/14 | 0.96 | 0.12 | 28,38,42,46 | 0 |
| 2 | CA | A | 1504 | 1/1 | 0.96 | 0.11 | 21,21,21,21 | 0 |
| 3 | MVL | A | 1505 | 14/14 | 0.96 | 0.18 | 25,26,28,30 | 0 |
| 3 | MVL | B | 1505 | 14/14 | 0.98 | 0.14 | 20,22,26,27 | 0 |
| 2 | CA | B | 1502 | 1/1 | 0.98 | 0.06 | 24,24,24,24 | 0 |
| 2 | CA | B | 1504 | 1/1 | 0.98 | 0.06 | 36,36,36,36 | 0 |
| 2 | CA | A | 1507 | 1/1 | 0.99 | 0.05 | 25,25,25,25 | 0 |
| 2 | CA | A | 1501 | 1/1 | 0.99 | 0.11 | 25,25,25,25 | 0 |
| 2 | CA | A | 1502 | 1/1 | 0.99 | 0.08 | 29,29,29,29 | 0 |
| 2 | CA | B | 1501 | 1/1 | 1.00 | 0.09 | 22,22,22,22 | 0 |

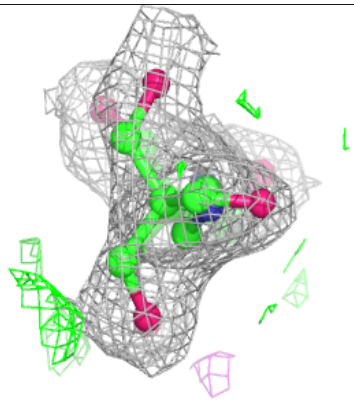
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around B3P A 1506:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

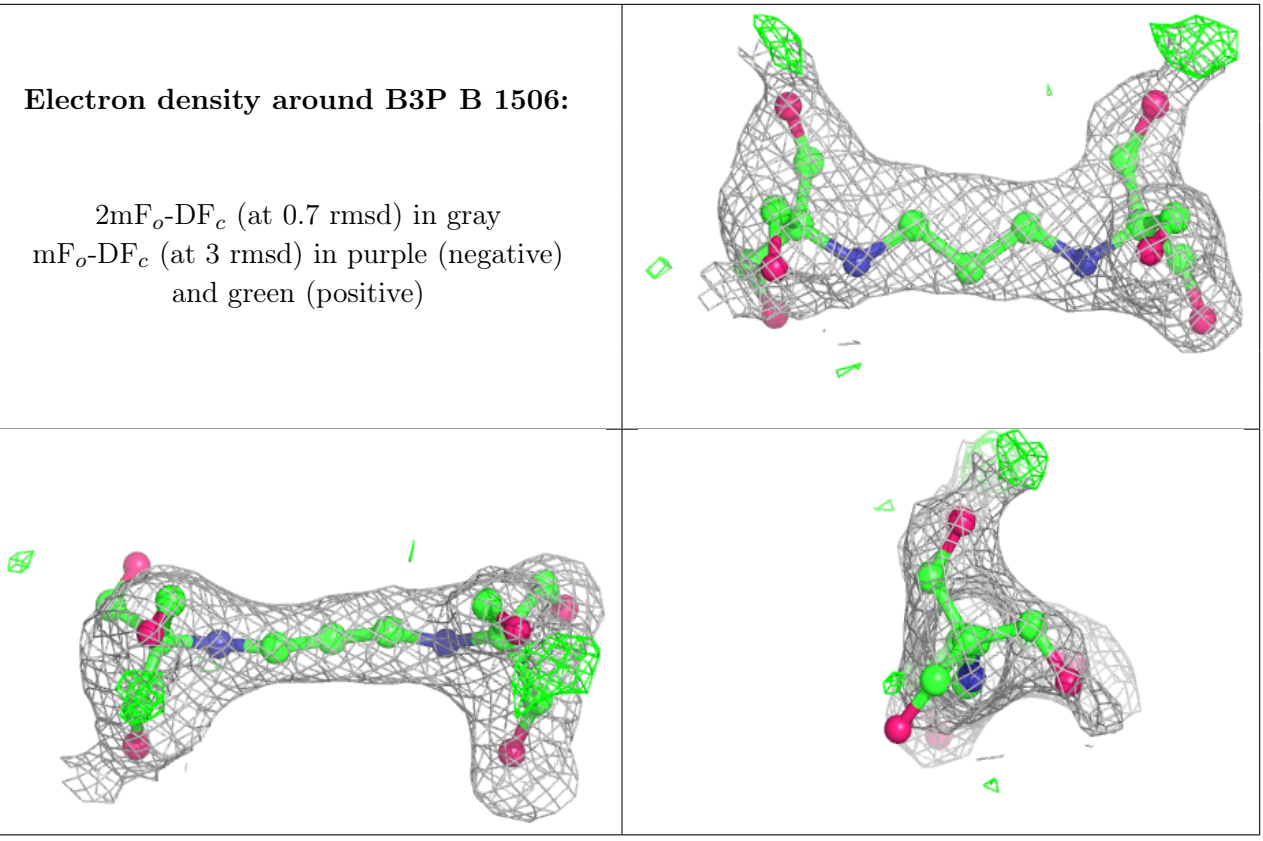






**Electron density around B3P B 1506:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.5 Other polymers (i)

There are no such residues in this entry.