# Full wwPDB Geometry-Only Validation Report (i)

May 29, 2020 – 05:02 am BST

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|---|---|---|
| PDB ID | : | 4IDW |
| Title | : | Polycrystalline T6 Bovine Insulin: Anisotropic Lattice Evolution and Novel Structure Refinement Strategy |
| Authors | : | Margiolaki, I.; Giannopoulou, A.E.; Wright, J.P.; Knight, L.; Norrman, M.; Schluckebier, G.; Fitch, A.; Von Dreele, R.B. |
| Deposited on | : | 2012-12-13 |
| Resolution | : | 2.70 Å(reported) |



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

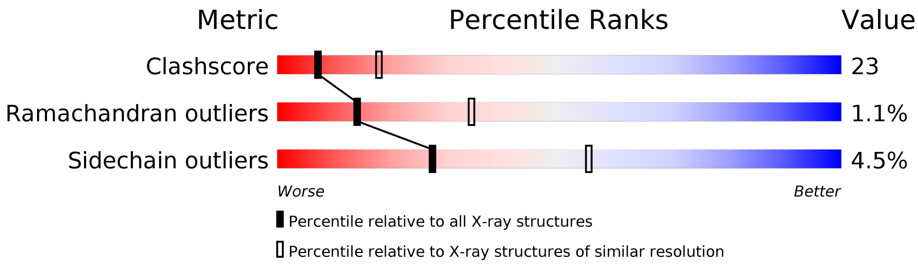
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*POWDER DIFFRACTION*

The reported resolution of this entry is 2.70 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)) |
|---|---|---|
| Clashscore | 141614 | 3122 (2.70-2.70) |
| Ramachandran outliers | 138981 | 3069 (2.70-2.70) |
| Sidechain outliers | 138945 | 3069 (2.70-2.70) |

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 on 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%

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 21 | 57% 43% |
| 1 | C | 21 | 67% 29% 5% |
| 2 | B | 30 | 47% 50% • |
| 2 | D | 30 | 60% 37% • |

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 846 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 Insulin A chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 21 | Total<br>160 | C<br>97 | N<br>25 | O<br>34 | S<br>4 | 0 | 0 | 0 |
| 1 | C | 21 | Total<br>160 | C<br>97 | N<br>25 | O<br>34 | S<br>4 | 0 | 0 | 0 |

- Molecule 2 is a protein called Insulin B chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 30 | Total<br>240 | C<br>157 | N<br>40 | O<br>41 | S<br>2 | 0 | 0 | 0 |
| 2 | D | 30 | Total<br>240 | C<br>157 | N<br>40 | O<br>41 | S<br>2 | 0 | 0 | 0 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | B | 1 | Total<br>1 | Zn<br>1 | 0 | 0 |
| 3 | D | 1 | Total<br>1 | Zn<br>1 | 0 | 0 |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | A | 8 | Total<br>8 | O<br>8 | 0 | 0 |
| 4 | B | 20 | Total<br>20 | O<br>20 | 0 | 0 |
| 4 | C | 5 | Total<br>5 | O<br>5 | 0 | 0 |
| 4 | D | 11 | Total<br>11 | O<br>11 | 0 | 0 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

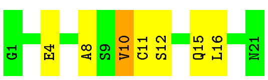
- Molecule 1: Insulin A chain

Chain A: 



- Molecule 1: Insulin A chain

Chain C: 

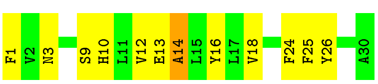

- Molecule 2: Insulin B chain

Chain B: 



- Molecule 2: Insulin B chain

Chain D: 

# 4 Model quality (i)

## 4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 | 0.64 | 0/161 | 0.88 | 0/216 |
| 1 | C | 0.66 | 0/161 | 0.84 | 0/216 |
| 2 | B | 0.70 | 0/247 | 0.95 | 0/332 |
| 2 | D | 0.67 | 0/247 | 0.86 | 0/332 |
| All | All | 0.67 | 0/816 | 0.89 | 0/1096 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | D | 0 | 1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | D | 14 | ALA | Mainchain |

## 4.2 Too-close contacts (i)

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 | 160 | 0 | 145 | 8 | 0 |
| 1 | C | 160 | 0 | 145 | 7 | 0 |
| 2 | B | 240 | 0 | 230 | 18 | 2 |
| 2 | D | 240 | 0 | 230 | 18 | 1 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 8 | 0 | 0 | 1 | 0 |
| 4 | B | 20 | 0 | 0 | 1 | 0 |
| 4 | C | 5 | 0 | 0 | 2 | 0 |
| 4 | D | 11 | 0 | 0 | 1 | 0 |
| All | All | 846 | 0 | 750 | 35 | 3 |

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 23.

All (35) 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:C:10:VAL:HB | 2:D:3:ASN:HB3 | 1.42 | 0.96 |
| 2:B:9:SER:HB2 | 2:D:13:GLU:HG3 | 1.64 | 0.78 |
| 2:D:9:SER:O | 2:D:12:VAL:HG22 | 1.89 | 0.72 |
| 1:A:10:VAL:HG11 | 2:B:3:ASN:HB3 | 1.73 | 0.69 |
| 2:B:12:VAL:HG22 | 2:D:12:VAL:HB | 1.78 | 0.66 |
| 2:B:12:VAL:CG2 | 2:D:12:VAL:HB | 2.31 | 0.59 |
| 1:A:13:LEU:HD12 | 2:B:1:PHE:CD1 | 2.37 | 0.58 |
| 2:B:16:TYR:CD1 | 2:D:9:SER:HB3 | 2.38 | 0.58 |
| 1:C:4:GLU:HA | 1:C:8:ALA:HB3 | 1.86 | 0.57 |
| 2:B:12:VAL:HG13 | 2:D:13:GLU:OE1 | 2.08 | 0.54 |
| 1:C:16:LEU:HD12 | 2:D:18:VAL:HG21 | 1.90 | 0.53 |
| 1:A:2:ILE:HB | 1:A:19:TYR:CE2 | 2.44 | 0.52 |
| 2:B:13:GLU:OE1 | 2:D:9:SER:HB2 | 2.09 | 0.52 |
| 1:A:12:SER:O | 1:A:16:LEU:HD23 | 2.13 | 0.49 |
| 4:C:104:HOH:O | 2:D:1:PHE:HB3 | 2.13 | 0.48 |
| 2:B:6:LEU:HD23 | 4:B:604:HOH:O | 2.14 | 0.47 |
| 2:B:13:GLU:O | 2:B:17:LEU:HG | 2.15 | 0.47 |
| 1:A:15:GLN:HB3 | 4:A:106:HOH:O | 2.14 | 0.46 |
| 2:D:16:TYR:HA | 2:D:24:PHE:HE2 | 1.79 | 0.46 |
| 2:D:14:ALA:O | 2:D:18:VAL:HG23 | 2.15 | 0.46 |
| 2:B:13:GLU:HA | 2:B:13:GLU:OE1 | 2.16 | 0.46 |
| 2:D:26:TYR:HA | 4:D:203:HOH:O | 2.15 | 0.45 |
| 1:C:11:CYS:O | 2:D:3:ASN:HA | 2.17 | 0.45 |
| 2:B:24:PHE:C | 2:B:24:PHE:CD1 | 2.90 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:12:SER:HB2 | 4:C:104:HOH:O | 2.16 | 0.45 |
| 1:C:4:GLU:H | 1:C:4:GLU:CD | 2.20 | 0.45 |
| 2:B:25:PHE:CE1 | 2:D:25:PHE:HB2 | 2.53 | 0.44 |
| 1:A:20:CYS:HB2 | 2:B:22:ARG:NH1 | 2.33 | 0.44 |
| 2:D:12:VAL:HG23 | 2:D:13:GLU:OE1 | 2.18 | 0.44 |
| 1:A:10:VAL:CG1 | 2:B:3:ASN:HB3 | 2.45 | 0.43 |
| 2:B:9:SER:HB3 | 2:D:16:TYR:CD2 | 2.54 | 0.43 |
| 1:C:11:CYS:HB2 | 1:C:15:GLN:OE1 | 2.19 | 0.42 |
| 2:B:15:LEU:HB3 | 2:B:24:PHE:CD2 | 2.54 | 0.42 |
| 2:B:24:PHE:CE1 | 2:D:24:PHE:HE1 | 2.38 | 0.41 |
| 1:A:2:ILE:HG13 | 1:A:6:CYS:SG | 2.61 | 0.41 |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:10:HIS:CE1 | 2:B:10:HIS:CE1[2_555] | 1.57 | 0.63 |
| 2:D:10:HIS:CE1 | 2:D:10:HIS:CE1[2_555] | 2.03 | 0.17 |
| 2:B:10:HIS:CE1 | 2:B:10:HIS:NE2[2_555] | 2.18 | 0.02 |

## 4.3 Torsion angles (i)

### 4.3.1 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 | 19/21 (90%) | 18 (95%) | 1 (5%) | 0 | 100 | 100 |
| 1 | C | 19/21 (90%) | 19 (100%) | 0 | 0 | 100 | 100 |
| 2 | B | 28/30 (93%) | 26 (93%) | 1 (4%) | 1 (4%) | 3 | 7 |
| 2 | D | 28/30 (93%) | 28 (100%) | 0 | 0 | 100 | 100 |
| All | All | 94/102 (92%) | 91 (97%) | 2 (2%) | 1 (1%) | 14 | 34 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 19 | CYS |

### 4.3.2 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 | 19/19 (100%) | 19 (100%) | 0 | 100 | 100 |
| 1 | C | 19/19 (100%) | 18 (95%) | 1 (5%) | 22 | 48 |
| 2 | B | 25/25 (100%) | 22 (88%) | 3 (12%) | 5 | 11 |
| 2 | D | 25/25 (100%) | 25 (100%) | 0 | 100 | 100 |
| All | All | 88/88 (100%) | 84 (96%) | 4 (4%) | 27 | 55 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 2 | VAL |
| 2 | B | 5 | HIS |
| 2 | B | 24 | PHE |
| 1 | C | 10 | VAL |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 4 | GLN |
| 2 | D | 3 | ASN |

### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 4.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.