



wwPDB Geometry-Only Validation Summary Report ⓘ

May 16, 2020 – 10:31 am BST

PDB ID : 3HQV
Title : Low resolution, molecular envelope structure of type I collagen in situ determined by fiber diffraction. Single type I collagen molecule, rigid body refinement
Authors : Orgel, J.P.
Deposited on : 2009-06-08
Resolution : 5.16 Å(reported)

This is a wwPDB Geometry-Only 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3134 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 Collagen alpha-1(I) chain.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------------|---------|---------|-------|
| 1 | A | 1054 | Total C 1054 1054 | 0 | 0 | 1054 |
| 1 | C | 1054 | Total C 1054 1054 | 0 | 0 | 1054 |

- Molecule 2 is a protein called Collagen alpha-2(I) chain.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------------|---------|---------|-------|
| 2 | B | 1026 | Total C 1026 1026 | 0 | 0 | 1026 |

3 Residue-property plots [i](#)

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: Collagen alpha-1(I) chain

Chain A:  100%



- Molecule 1: Collagen alpha-1(I) chain

Chain C:  100%



- Molecule 2: Collagen alpha-2(I) chain

Chain B:  100%



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: HYP, LYZ

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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 | 1054 | 0 | 0 | 1 | 0 |
| 1 | C | 1054 | 0 | 0 | 1 | 0 |
| 2 | B | 1026 | 0 | 0 | 1 | 0 |
| All | All | 3134 | 0 | 0 | 3 | 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 1.

All (3) 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:17:GLY:CA | 1:A:18:PRO:CA | 2.87 | 0.52 |
| 2:B:233:LEU:CA | 2:B:234:HYP:CA | 2.89 | 0.51 |
| 1:C:240:ALA:CA | 1:C:241:HYP:CA | 2.97 | 0.43 |

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Of 312 non-standard protein/DNA/RNA residues modelled in this entry, 312 are modelled with single atom - 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.

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.