



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 10:14 am GMT

PDB ID : 1A1Q
Title : HEPATITIS C VIRUS NS3 PROTEINASE
Authors : Love, R.A.; Parge, H.E.; Wickersham, J.A.; Hostomsky, Z.; Habuka, N.;
Moomaw, E.W.; Adachi, T.; Hostomska, Z.
Deposited on : 1997-12-12
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

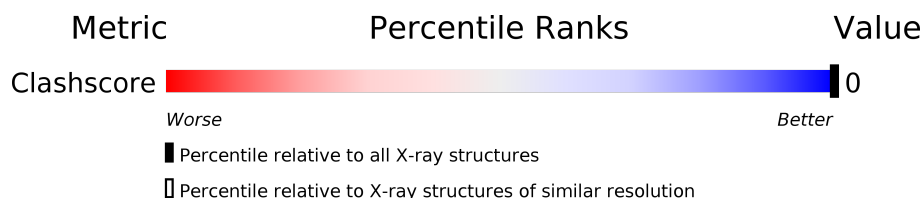
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

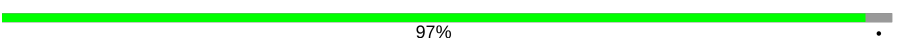


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 122078 | 3953 (2.40-2.40) |

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. 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 $\leq 5\%$. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 189 |  97% . |
| 1 | B | 189 |  90% 10% |
| 1 | C | 189 |  94% 6% |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 534 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 NS3 PROTEINASE.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 1 | A | 183 | Total C 183 183 | 0 | 0 | 183 |
| 1 | B | 170 | Total C 170 170 | 0 | 0 | 170 |
| 1 | C | 178 | Total C 178 178 | 0 | 0 | 178 |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 66 | GLY | ALA | CONFLICT | UNP P26663 |
| A | 86 | GLN | PRO | CONFLICT | UNP P26663 |
| A | 87 | ALA | LYS | CONFLICT | UNP P26663 |
| A | 147 | SER | PHE | CONFLICT | UNP P26663 |
| B | 66 | GLY | ALA | CONFLICT | UNP P26663 |
| B | 86 | GLN | PRO | CONFLICT | UNP P26663 |
| B | 87 | ALA | LYS | CONFLICT | UNP P26663 |
| B | 147 | SER | PHE | CONFLICT | UNP P26663 |
| C | 66 | GLY | ALA | CONFLICT | UNP P26663 |
| C | 86 | GLN | PRO | CONFLICT | UNP P26663 |
| C | 87 | ALA | LYS | CONFLICT | UNP P26663 |
| C | 147 | SER | PHE | CONFLICT | UNP P26663 |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2 | B | 1 | Total Zn 1 1 | 0 | 0 |
| 2 | A | 1 | Total Zn 1 1 | 0 | 0 |
| 2 | C | 1 | Total Zn 1 1 | 0 | 0 |

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 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.


Note EDS was not executed.

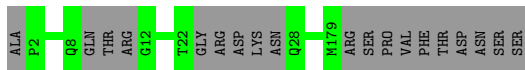
• Molecule 1: NS3 PROTEINASE

Chain A:  97% .



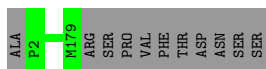
• Molecule 1: NS3 PROTEINASE

Chain B:  90% 10%



• Molecule 1: NS3 PROTEINASE

Chain C:  94% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | H 3 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 133.00Å 133.00Å 223.00Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 8.00 – 2.40 | Depositor |
| % Data completeness (in resolution range) | 98.0 (8.00-2.40) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.08 | Depositor |
| Refinement program | X-PLOR 3.1 | Depositor |
| R, R_{free} | 0.225 , 0.320 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 534 | wwPDB-VP |
| Average B, all atoms (Å ²) | 18.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 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).

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.

5.2 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 | 183 | 0 | 0 | 0 | 0 |
| 1 | B | 170 | 0 | 0 | 0 | 0 |
| 1 | C | 178 | 0 | 0 | 0 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| All | All | 534 | 0 | 0 | 0 | 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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.