



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2021 – 03:03 PM BST

PDB ID : 7O85
EMDB ID : EMD-12761
Title : Anthrax toxin prepore in complex with the neutralizing Fab cAb29
Authors : Hoelzgen, F.; Zalk, R.; Alcalay, R.; Cohen-Schwartz, S.; Garau, G.; Shahar, A.; Mazor, O.; Frank, G.A.
Deposited on : 2021-04-14
Resolution : 3.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
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) : 2.23.1

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| Mol | Chain | Length | Quality of chain | |
|-----|-------|--------|------------------|-----|
| 2 | H | 104 | 84% | 16% |
| 2 | K | 104 | 84% | 16% |
| 2 | N | 104 | 81% | 19% |
| 2 | Q | 104 | 84% | 16% |
| 2 | T | 104 | 83% | 17% |
| 3 | C | 113 | 91% | 9% |
| 3 | F | 113 | 91% | 9% |
| 3 | I | 113 | 91% | 9% |
| 3 | L | 113 | 91% | 9% |
| 3 | O | 113 | 91% | 9% |
| 3 | R | 113 | 91% | 9% |
| 3 | U | 113 | 91% | 9% |

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28525 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protective antigen PA-63.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |
| 1 | D | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |
| 1 | G | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |
| 1 | J | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |
| 1 | M | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |
| 1 | P | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |
| 1 | S | 332 | Total 2620 | C 1642 | N 456 | O 520 | S 2 | 0 | 0 |

- Molecule 2 is a protein called Fab.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |
| 2 | E | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |
| 2 | H | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |
| 2 | K | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |
| 2 | N | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |
| 2 | Q | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |
| 2 | T | 104 | Total 706 | C 444 | N 124 | O 136 | S 2 | 0 | 0 |

- Molecule 3 is a protein called Fab.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | C | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |
| 3 | F | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |
| 3 | I | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |
| 3 | L | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |
| 3 | O | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |
| 3 | R | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |
| 3 | U | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 470 | 133 | 142 | 2 | | |

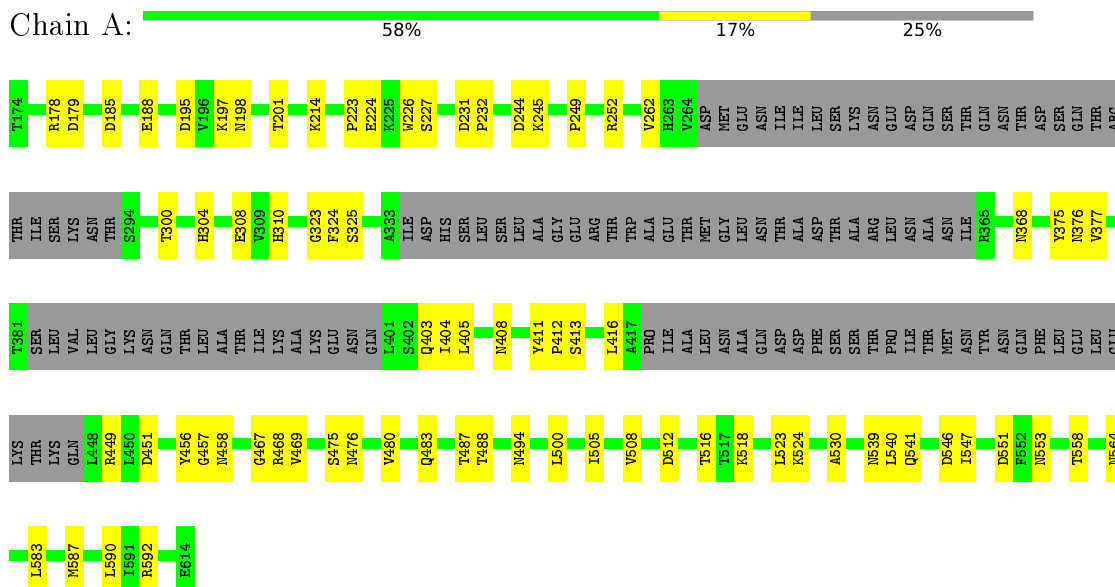
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 4 | A | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |
| 4 | D | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |
| 4 | G | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |
| 4 | J | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |
| 4 | M | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |
| 4 | P | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |
| 4 | S | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |

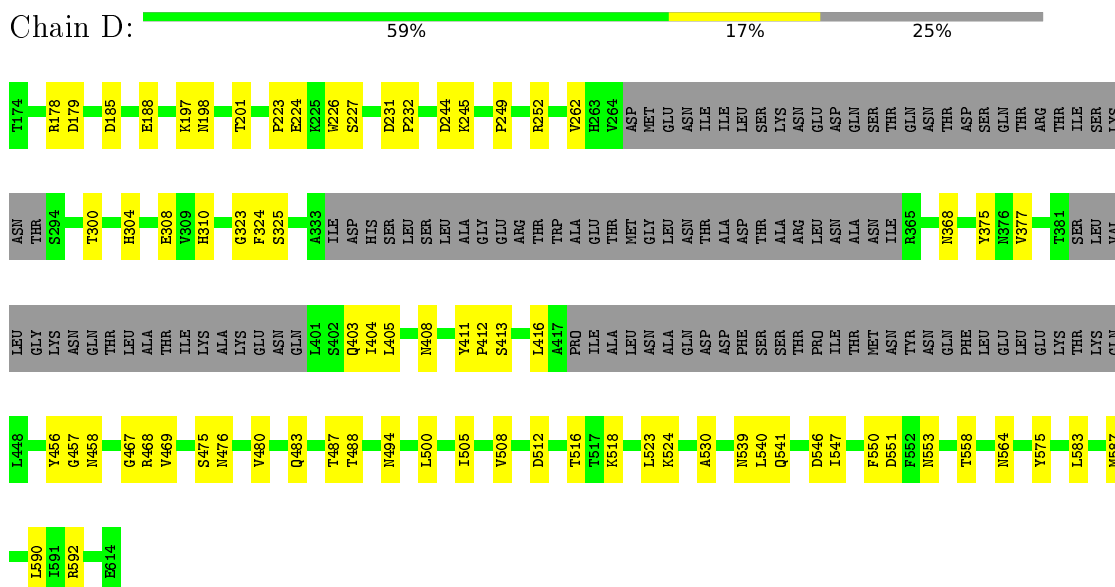
3 Residue-property plots [i](#)

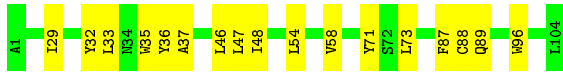
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

- Molecule 1: Protective antigen PA-63

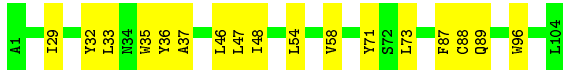
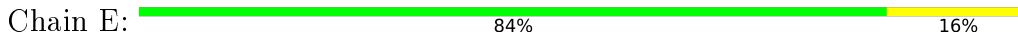


- Molecule 1: Protective antigen PA-63

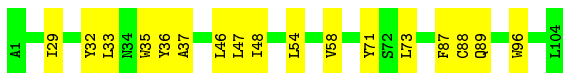
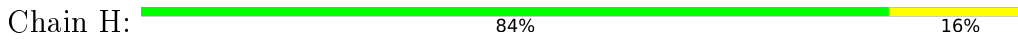




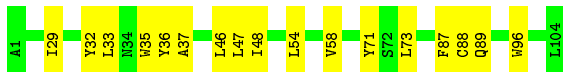
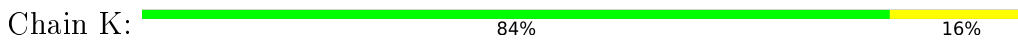
• Molecule 2: Fab



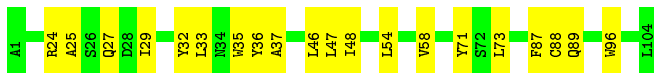
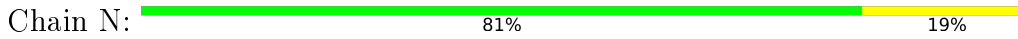
• Molecule 2: Fab



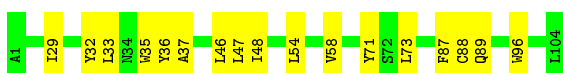
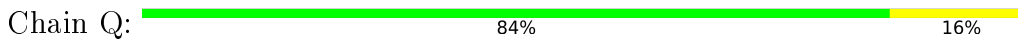
• Molecule 2: Fab



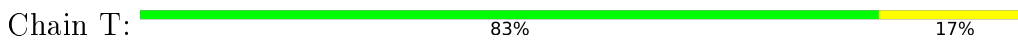
• Molecule 2: Fab



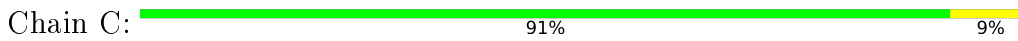
• Molecule 2: Fab



• Molecule 2: Fab

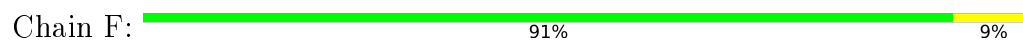


• Molecule 3: Fab

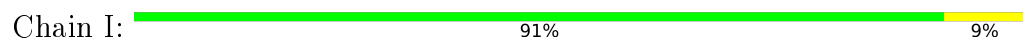




- Molecule 3: Fab



- Molecule 3: Fab



- Molecule 3: Fab



- Molecule 3: Fab



- Molecule 3: Fab



- Molecule 3: Fab



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 211098 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 80 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |

5 Model quality

5.1 Standard geometry

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

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 | 0.24 | 0/2671 | 0.48 | 0/3627 |
| 1 | D | 0.24 | 0/2671 | 0.48 | 0/3627 |
| 1 | G | 0.24 | 0/2671 | 0.47 | 0/3627 |
| 1 | J | 0.24 | 0/2671 | 0.48 | 0/3627 |
| 1 | M | 0.24 | 0/2671 | 0.47 | 0/3627 |
| 1 | P | 0.24 | 0/2671 | 0.48 | 0/3627 |
| 1 | S | 0.24 | 0/2671 | 0.47 | 0/3627 |
| 2 | B | 0.27 | 0/720 | 0.54 | 0/985 |
| 2 | E | 0.27 | 0/720 | 0.53 | 0/985 |
| 2 | H | 0.27 | 0/720 | 0.53 | 0/985 |
| 2 | K | 0.27 | 0/720 | 0.54 | 0/985 |
| 2 | N | 0.27 | 0/720 | 0.54 | 0/985 |
| 2 | Q | 0.27 | 0/720 | 0.54 | 0/985 |
| 2 | T | 0.27 | 0/720 | 0.54 | 0/985 |
| 3 | C | 0.26 | 0/763 | 0.47 | 0/1046 |
| 3 | F | 0.26 | 0/763 | 0.47 | 0/1046 |
| 3 | I | 0.26 | 0/763 | 0.47 | 0/1046 |
| 3 | L | 0.26 | 0/763 | 0.47 | 0/1046 |
| 3 | O | 0.26 | 0/763 | 0.47 | 0/1046 |
| 3 | R | 0.26 | 0/763 | 0.47 | 0/1046 |
| 3 | U | 0.26 | 0/763 | 0.47 | 0/1046 |
| All | All | 0.25 | 0/29078 | 0.49 | 0/39606 |

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 | 2620 | 0 | 2552 | 56 | 0 |
| 1 | D | 2620 | 0 | 2552 | 52 | 0 |
| 1 | G | 2620 | 0 | 2552 | 51 | 0 |
| 1 | J | 2620 | 0 | 2552 | 50 | 0 |
| 1 | M | 2620 | 0 | 2552 | 50 | 0 |
| 1 | P | 2620 | 0 | 2552 | 51 | 0 |
| 1 | S | 2620 | 0 | 2552 | 51 | 0 |
| 2 | B | 706 | 0 | 686 | 12 | 0 |
| 2 | E | 706 | 0 | 686 | 12 | 0 |
| 2 | H | 706 | 0 | 686 | 12 | 0 |
| 2 | K | 706 | 0 | 686 | 12 | 0 |
| 2 | N | 706 | 0 | 686 | 14 | 0 |
| 2 | Q | 706 | 0 | 686 | 12 | 0 |
| 2 | T | 706 | 0 | 686 | 13 | 0 |
| 3 | C | 747 | 0 | 716 | 5 | 0 |
| 3 | F | 747 | 0 | 716 | 5 | 0 |
| 3 | I | 747 | 0 | 716 | 5 | 0 |
| 3 | L | 747 | 0 | 716 | 5 | 0 |
| 3 | O | 747 | 0 | 716 | 5 | 0 |
| 3 | R | 747 | 0 | 716 | 5 | 0 |
| 3 | U | 747 | 0 | 716 | 5 | 0 |
| 4 | A | 2 | 0 | 0 | 0 | 0 |
| 4 | D | 2 | 0 | 0 | 0 | 0 |
| 4 | G | 2 | 0 | 0 | 0 | 0 |
| 4 | J | 2 | 0 | 0 | 0 | 0 |
| 4 | M | 2 | 0 | 0 | 0 | 0 |
| 4 | P | 2 | 0 | 0 | 0 | 0 |
| 4 | S | 2 | 0 | 0 | 0 | 0 |
| All | All | 28525 | 0 | 27678 | 421 | 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 7.

The worst 5 of 421 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:201:THR:HG22 | 1:D:224:GLU:HG3 | 1.74 | 0.70 |
| 1:D:201:THR:HG22 | 1:G:224:GLU:HG3 | 1.73 | 0.70 |
| 1:G:487:THR:OG1 | 1:G:518:LYS:NZ | 2.24 | 0.70 |
| 1:A:224:GLU:HG3 | 1:S:201:THR:HG22 | 1.74 | 0.70 |
| 1:G:201:THR:HG22 | 1:J:224:GLU:HG3 | 1.73 | 0.69 |

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 PDB entries followed by that with respect to all EM entries.

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 | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 1 | D | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 1 | G | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 1 | J | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 1 | M | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 1 | P | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 1 | S | 322/441 (73%) | 310 (96%) | 12 (4%) | 0 | 100 | 100 |
| 2 | B | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | E | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | H | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | K | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | N | 102/104 (98%) | 99 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | Q | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | T | 102/104 (98%) | 99 (97%) | 3 (3%) | 0 | 100 | 100 |
| 3 | C | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | F | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | I | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | L | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | O | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | R | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | U | 111/113 (98%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| All | All | 3745/4606 (81%) | 3621 (97%) | 124 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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 | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 1 | D | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 1 | G | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 1 | J | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 1 | M | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 1 | P | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 1 | S | 293/390 (75%) | 293 (100%) | 0 | 100 | 100 |
| 2 | B | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 2 | E | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 2 | H | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 2 | K | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 2 | N | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 2 | Q | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 2 | T | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 3 | C | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 3 | F | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 3 | I | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 3 | L | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 3 | O | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 3 | R | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 3 | U | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| All | All | 2772/3451 (80%) | 2772 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 14 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.