



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2020 – 02:41 PM BST

PDB ID : 4JCQ
Title : ClpP1 from *Listeria monocytogenes*
Authors : Zeiler, E.; List, A.; Alte, F.; Gersch, M.; Wachtel, R.; Groll, M.; Sieber, S.
Deposited on : 2013-02-22
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) | : | 1.13 |
| EDS | : | 2.13 |
| 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) | : | 2.13 |

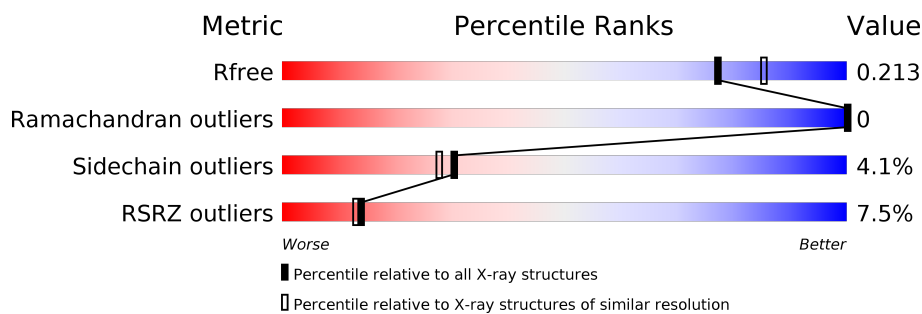
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.






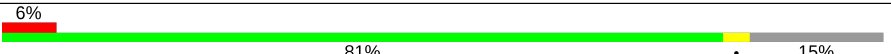
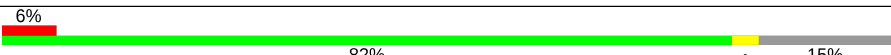
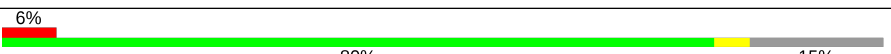
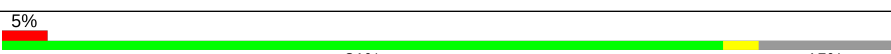
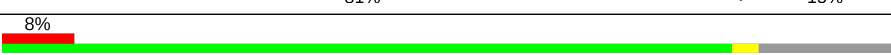

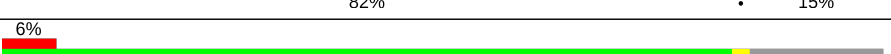
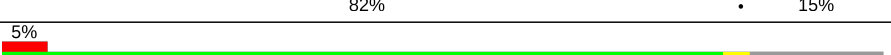

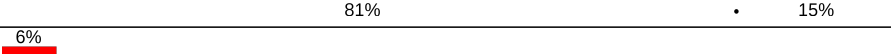
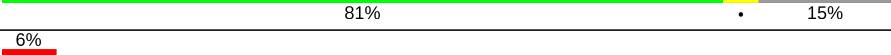






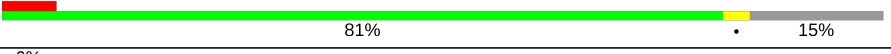
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 8085 (2.00-2.00) |
| Ramachandran outliers | 138981 | 9054 (2.00-2.00) |
| Sidechain outliers | 138945 | 9053 (2.00-2.00) |
| RSRZ outliers | 127900 | 7900 (2.00-2.00) |

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 $\leq 5\%$. 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.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 201 | <div> <div>5%</div> <div>82%</div> <div>15%</div> </div> |
| 1 | B | 201 | <div> <div>5%</div> <div>82%</div> <div>15%</div> </div> |
| 1 | C | 201 | <div> <div>8%</div> <div>82%</div> <div>15%</div> </div> |
| 1 | D | 201 | <div> <div>7%</div> <div>82%</div> <div>15%</div> </div> |
| 1 | E | 201 | <div> <div>7%</div> <div>81%</div> <div>15%</div> </div> |
| 1 | F | 201 | <div> <div>6%</div> <div>81%</div> <div>15%</div> </div> |
| 1 | G | 201 | <div> <div>7%</div> <div>81%</div> <div>15%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | H | 201 |  |
| 1 | I | 201 |  |
| 1 | J | 201 |  |
| 1 | K | 201 |  |
| 1 | L | 201 |  |
| 1 | M | 201 |  |
| 1 | N | 201 |  |
| 1 | O | 201 |  |
| 1 | P | 201 |  |
| 1 | Q | 201 |  |
| 1 | R | 201 |  |
| 1 | S | 201 |  |
| 1 | T | 201 |  |
| 1 | U | 201 |  |
| 1 | V | 201 |  |
| 1 | W | 201 |  |
| 1 | X | 201 |  |
| 1 | Y | 201 |  |
| 1 | Z | 201 |  |
| 1 | a | 201 |  |
| 1 | b | 201 |  |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40559 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 ATP-dependent Clp protease proteolytic subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | B | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | C | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | D | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | E | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | F | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | G | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | H | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | I | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | J | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | K | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | L | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | M | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | N | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | O | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | P | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | Q | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | R | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | S | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | T | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | U | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | V | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | W | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | X | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | Y | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | Z | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | a | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |
| 1 | b | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1345 | 850 | 232 | 260 | 3 | | | |

There are 308 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| A | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| B | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| C | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| D | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| E | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| F | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| F | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| G | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| H | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| I | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| J | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| J | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| K | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| L | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| M | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| N | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| O | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| P | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Q | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Q | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| R | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| S | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| T | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| U | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| U | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| V | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| W | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| X | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Y | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Y | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| Z | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| a | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 191 | MET | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 192 | ALA | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 193 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 194 | TRP | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 195 | SER | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 196 | HIS | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 197 | PRO | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 198 | GLN | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 199 | PHE | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 200 | GLU | - | EXPRESSION TAG | UNP Q8Y7Y1 |
| b | 201 | LYS | - | EXPRESSION TAG | UNP Q8Y7Y1 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2 | A | 88 | Total O 88 88 | 0 | 0 |
| 2 | B | 93 | Total O 93 93 | 0 | 0 |
| 2 | C | 80 | Total O 80 80 | 0 | 0 |
| 2 | D | 72 | Total O 72 72 | 0 | 0 |
| 2 | E | 102 | Total O 102 102 | 0 | 0 |
| 2 | F | 135 | Total O 135 135 | 0 | 0 |
| 2 | G | 107 | Total O 107 107 | 0 | 0 |
| 2 | H | 89 | Total O 89 89 | 0 | 0 |
| 2 | I | 81 | Total O 81 81 | 0 | 0 |
| 2 | J | 87 | Total O 87 87 | 0 | 0 |
| 2 | K | 111 | Total O 111 111 | 0 | 0 |
| 2 | L | 108 | Total O 108 108 | 0 | 0 |
| 2 | M | 134 | Total O 134 134 | 0 | 0 |
| 2 | N | 147 | Total O 147 147 | 0 | 0 |
| 2 | O | 83 | Total O 83 83 | 0 | 0 |
| 2 | P | 76 | Total O 76 76 | 0 | 0 |
| 2 | Q | 100 | Total O 100 100 | 0 | 0 |
| 2 | R | 99 | Total O 99 99 | 0 | 0 |
| 2 | S | 124 | Total O 124 124 | 0 | 0 |
| 2 | T | 157 | Total O 157 157 | 0 | 0 |
| 2 | U | 93 | Total O 93 93 | 0 | 0 |
| 2 | V | 106 | Total O 106 106 | 0 | 0 |

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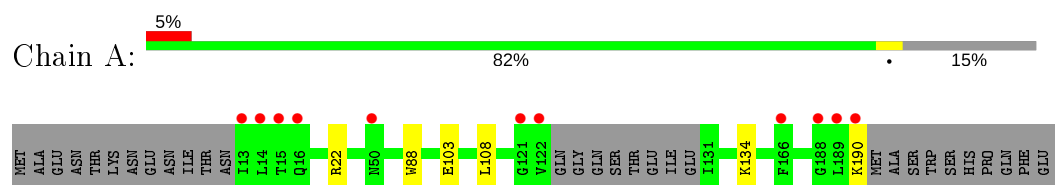
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 2 | W | 93 | Total 93 | O 93 | 0 | 0 |
| 2 | X | 84 | Total 84 | O 84 | 0 | 0 |
| 2 | Y | 90 | Total 90 | O 90 | 0 | 0 |
| 2 | Z | 93 | Total 93 | O 93 | 0 | 0 |
| 2 | a | 124 | Total 124 | O 124 | 0 | 0 |
| 2 | b | 143 | Total 143 | O 143 | 0 | 0 |

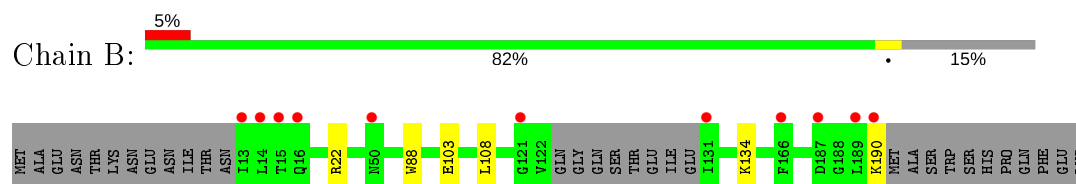
3 Residue-property plots [i](#)

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.

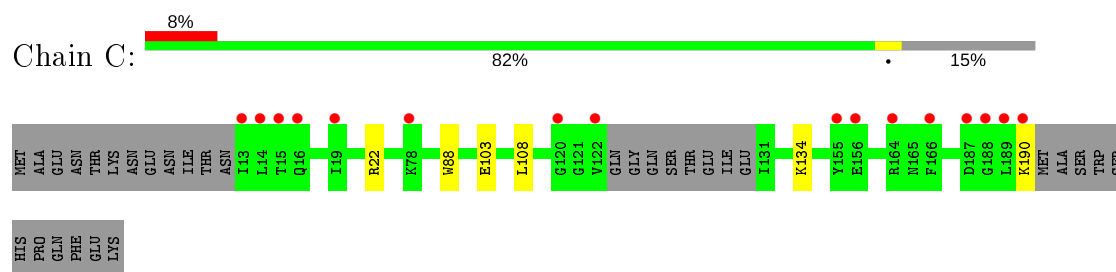
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



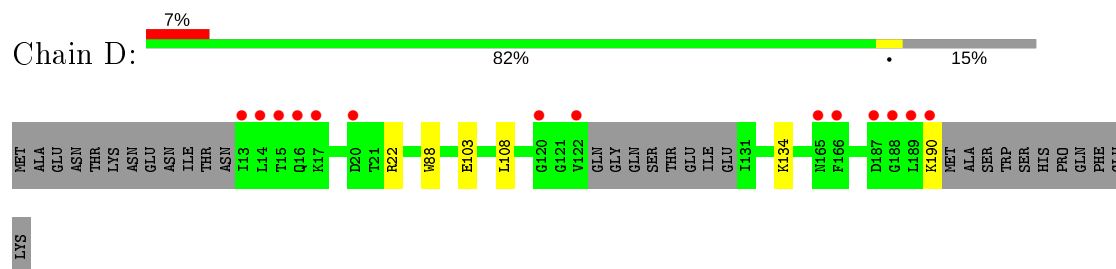
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



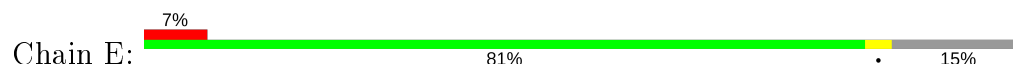
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

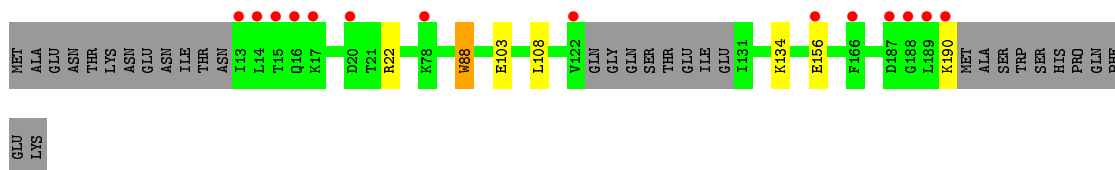


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

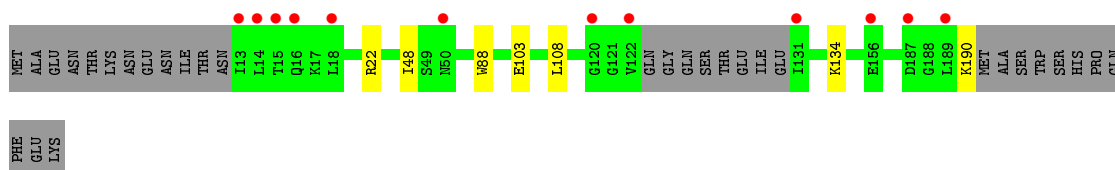
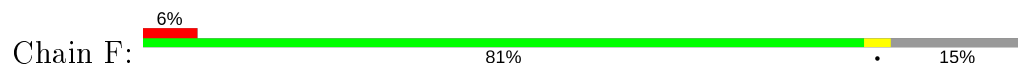


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

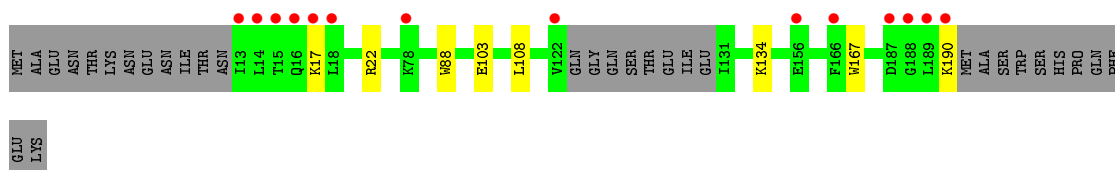
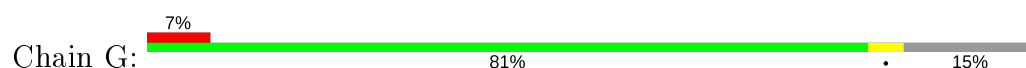




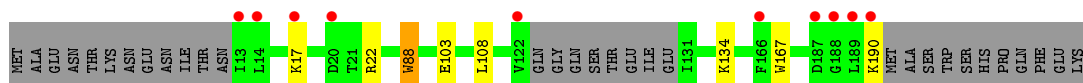
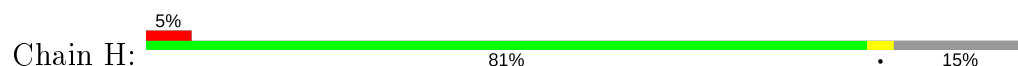
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



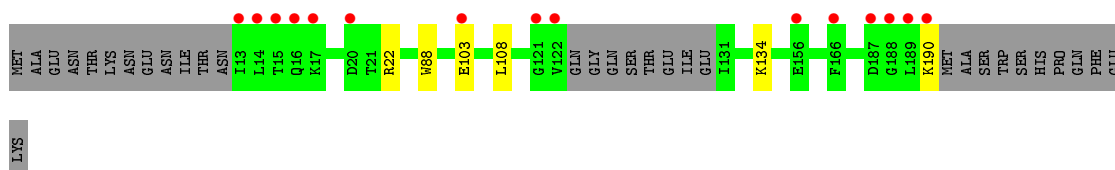
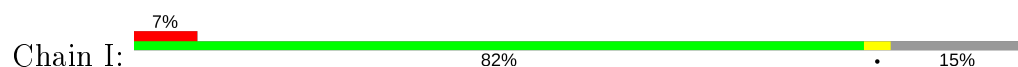
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



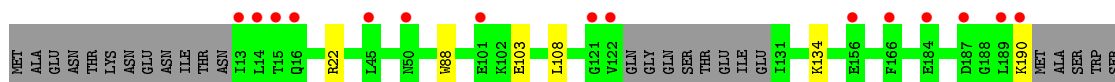
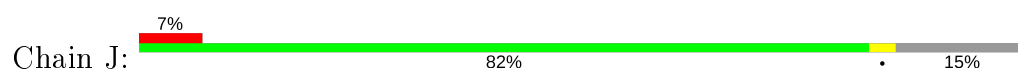
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



HIS
PRO
GLN
PHE
GLU
LYS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 6% 81% 15%

MET ALA GLU ASN THR LYS ASN GLU ASN ILE THR ASN I13 L14 L15 Q16 K17 R22 P52 W88 E103 L108 V122 GLN GLY GLN SER THR GLU ILE GLU I131 K134 F166 D187 G188 L189 K190 MET ALA SER TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 6% 82% 15%

MET ALA GLU ASN THR LYS ASN GLU ASN ILE THR ASN I13 L14 L15 Q16 D20 T21 R22 W88 E103 L108 V122 GLN GLY GLN SER THR GLU ILE GLU I131 K134 E156 F166 D187 G188 L189 K190 MET ALA SER TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 6% 80% 15%

MET ALA GLU ASN THR LYS ASN GLU ASN ILE THR ASN I13 L14 L15 Q16 K17 L18 I19 R22 W88 E103 L108 V122 GLN GLY GLN SER THR GLU ILE GLU I131 K134 E156 F166 W167 D187 G188 L189 K190 MET ALA SER TRP SER HIS PRO GLN PHE GLU

LYS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N: 5% 81% 15%

MET ALA GLU ASN THR LYS ASN GLU ASN ILE THR ASN I13 L14 L17 L19 R22 I48 S49 N50 W88 E103 L108 V122 GLN GLY GLN SER THR GLU ILE GLU I131 K134 F166 D187 G188 L189 K190 MET ALA SER TRP SER HIS PRO GLN PHE GLU

LYS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

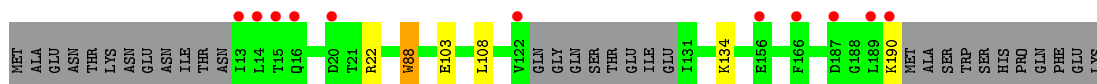
Chain O: 8% 82% 15%

MET ALA GLU ASN THR LYS ASN GLU ASN ILE THR ASN I13 L14 L15 Q16 K17 R20 T21 R22 L45 N50 W88 E103 L108 G121 V122 GLN GLY GLN SER THR GLU ILE GLU I131 K134 E156 F166 G188 L189 K190 MET ALA SER TRP SER HIS PRO

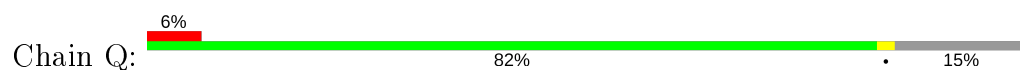
GLN
PHE
GLU
LYS

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

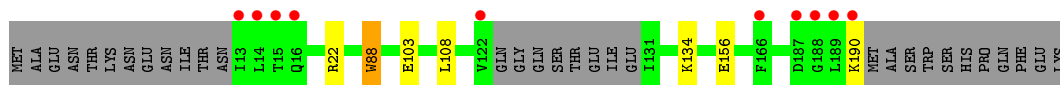
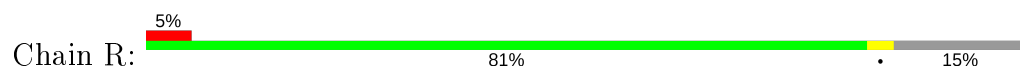
Chain P: 5% 82% 15%



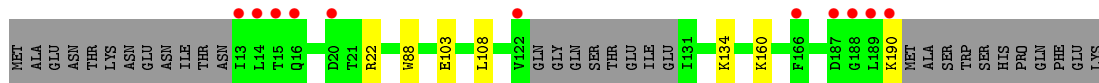
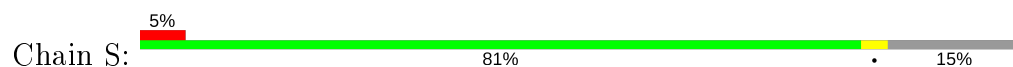
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



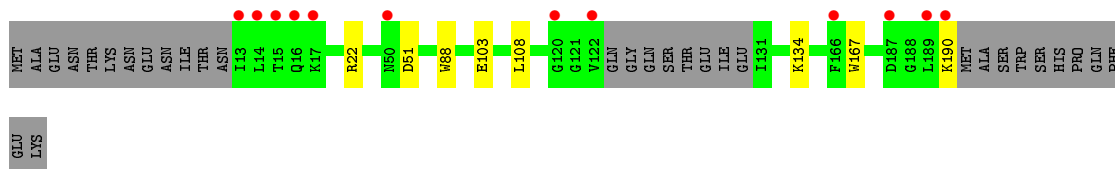
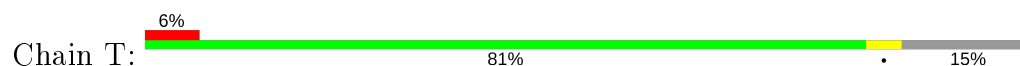
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



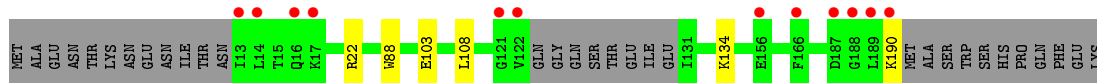
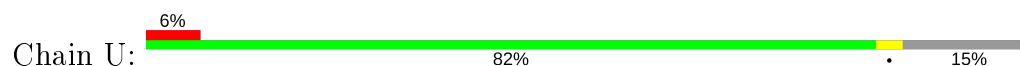
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



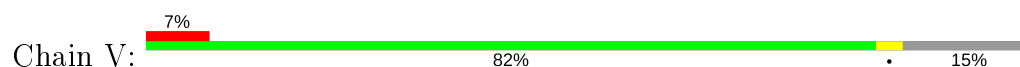
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit




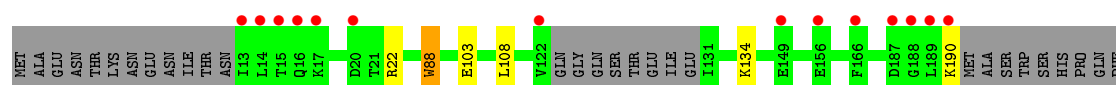
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



PRO
GLN
PHE
GLU
LYS


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

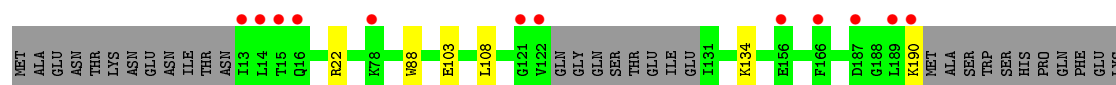
Chain W:  7% 82% 15%




GLU
LYS

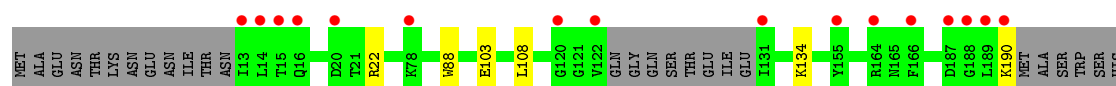
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:  6% 82% 15%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

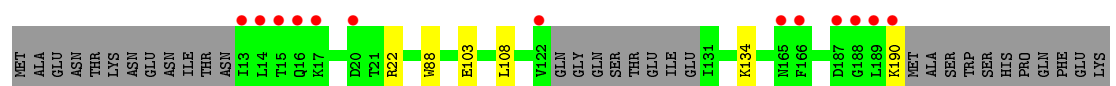
Chain Y:  8% 82% 15%




PRO
GLN
PHE
GLU
LYS

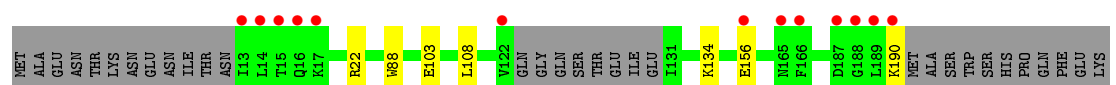
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:  6% 82% 15%




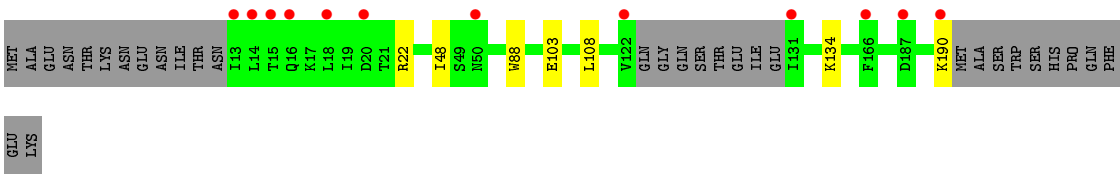
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:  6% 81% 15%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:  6% 81% 15%



GLU
LYS

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 140.95Å 109.06Å 196.26Å 90.00° 93.16° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 2.00 15.00 – 2.00 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (15.00-2.00) 99.7 (15.00-2.00) | Depositor EDS |
| R_{merge} | 0.06 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.19 (at 2.00Å) | Xtriage |
| Refinement program | REFMAC 5.6.0117 | Depositor |
| R, R_{free} | 0.192 , 0.213 0.192 , 0.213 | Depositor DCC |
| R_{free} test set | 19880 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 26.7 | Xtriage |
| Anisotropy | 0.048 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.39 , 54.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 40559 | wwPDB-VP |
| Average B, all atoms (Å ²) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to $7.0334e-06$. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | B | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | C | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | D | 0.40 | 0/1363 | 0.48 | 0/1841 |
| 1 | E | 0.41 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | F | 0.41 | 0/1363 | 0.49 | 0/1841 |
| 1 | G | 0.40 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | H | 0.41 | 2/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | I | 0.40 | 0/1363 | 0.48 | 0/1841 |
| 1 | J | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | K | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | L | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | M | 0.41 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | N | 0.41 | 0/1363 | 0.49 | 0/1841 |
| 1 | O | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | P | 0.40 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | Q | 0.41 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | R | 0.40 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | S | 0.41 | 0/1363 | 0.49 | 0/1841 |
| 1 | T | 0.41 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | U | 0.40 | 0/1363 | 0.49 | 0/1841 |
| 1 | V | 0.41 | 0/1363 | 0.49 | 0/1841 |
| 1 | W | 0.41 | 1/1363 (0.1%) | 0.49 | 0/1841 |
| 1 | X | 0.40 | 0/1363 | 0.48 | 0/1841 |
| 1 | Y | 0.41 | 0/1363 | 0.48 | 0/1841 |
| 1 | Z | 0.40 | 0/1363 | 0.48 | 0/1841 |
| 1 | a | 0.41 | 0/1363 | 0.49 | 0/1841 |
| 1 | b | 0.41 | 0/1363 | 0.49 | 0/1841 |
| All | All | 0.40 | 10/38164 (0.0%) | 0.49 | 0/51548 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | R | 88 | TRP | CD2-CE2 | 5.07 | 1.47 | 1.41 |
| 1 | Q | 88 | TRP | CD2-CE2 | 5.05 | 1.47 | 1.41 |
| 1 | M | 167 | TRP | CD2-CE2 | 5.04 | 1.47 | 1.41 |
| 1 | H | 167 | TRP | CD2-CE2 | 5.03 | 1.47 | 1.41 |
| 1 | P | 88 | TRP | CD2-CE2 | 5.03 | 1.47 | 1.41 |
| 1 | H | 88 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | W | 88 | TRP | CD2-CE2 | 5.01 | 1.47 | 1.41 |
| 1 | G | 167 | TRP | CD2-CE2 | 5.00 | 1.47 | 1.41 |
| 1 | T | 167 | TRP | CD2-CE2 | 5.00 | 1.47 | 1.41 |
| 1 | E | 88 | TRP | CD2-CE2 | 5.00 | 1.47 | 1.41 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | B | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | C | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | D | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | E | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | F | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | G | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | H | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | I | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | J | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | K | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | L | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | M | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | N | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | O | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | P | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | Q | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | R | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | S | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | T | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | U | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | V | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | W | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | X | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | Y | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | Z | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | a | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | b | 166/201 (83%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| All | All | 4648/5628 (83%) | 4536 (98%) | 112 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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 | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | B | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | C | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | D | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | E | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | F | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | G | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | H | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | I | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | J | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | K | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | L | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | M | 147/175 (84%) | 140 (95%) | 7 (5%) | 25 | 22 |
| 1 | N | 147/175 (84%) | 140 (95%) | 7 (5%) | 25 | 22 |
| 1 | O | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | P | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | Q | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | R | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | S | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | T | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | U | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | V | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | W | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | X | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | Y | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | Z | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | a | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| 1 | b | 147/175 (84%) | 141 (96%) | 6 (4%) | 30 | 28 |
| All | All | 4116/4900 (84%) | 3946 (96%) | 170 (4%) | 30 | 28 |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 22 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 88 | TRP |
| 1 | A | 103 | GLU |
| 1 | A | 108 | LEU |
| 1 | A | 134 | LYS |
| 1 | A | 190 | LYS |
| 1 | B | 22 | ARG |
| 1 | B | 88 | TRP |
| 1 | B | 103 | GLU |
| 1 | B | 108 | LEU |
| 1 | B | 134 | LYS |
| 1 | B | 190 | LYS |
| 1 | C | 22 | ARG |
| 1 | C | 88 | TRP |
| 1 | C | 103 | GLU |
| 1 | C | 108 | LEU |
| 1 | C | 134 | LYS |
| 1 | C | 190 | LYS |
| 1 | D | 22 | ARG |
| 1 | D | 88 | TRP |
| 1 | D | 103 | GLU |
| 1 | D | 108 | LEU |
| 1 | D | 134 | LYS |
| 1 | D | 190 | LYS |
| 1 | E | 22 | ARG |
| 1 | E | 88 | TRP |
| 1 | E | 103 | GLU |
| 1 | E | 108 | LEU |
| 1 | E | 134 | LYS |
| 1 | E | 190 | LYS |
| 1 | F | 22 | ARG |
| 1 | F | 88 | TRP |
| 1 | F | 103 | GLU |
| 1 | F | 108 | LEU |
| 1 | F | 134 | LYS |
| 1 | F | 190 | LYS |
| 1 | G | 22 | ARG |
| 1 | G | 88 | TRP |
| 1 | G | 103 | GLU |
| 1 | G | 108 | LEU |
| 1 | G | 134 | LYS |
| 1 | G | 190 | LYS |
| 1 | H | 22 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 88 | TRP |
| 1 | H | 103 | GLU |
| 1 | H | 108 | LEU |
| 1 | H | 134 | LYS |
| 1 | H | 190 | LYS |
| 1 | I | 22 | ARG |
| 1 | I | 88 | TRP |
| 1 | I | 103 | GLU |
| 1 | I | 108 | LEU |
| 1 | I | 134 | LYS |
| 1 | I | 190 | LYS |
| 1 | J | 22 | ARG |
| 1 | J | 88 | TRP |
| 1 | J | 103 | GLU |
| 1 | J | 108 | LEU |
| 1 | J | 134 | LYS |
| 1 | J | 190 | LYS |
| 1 | K | 22 | ARG |
| 1 | K | 88 | TRP |
| 1 | K | 103 | GLU |
| 1 | K | 108 | LEU |
| 1 | K | 134 | LYS |
| 1 | K | 190 | LYS |
| 1 | L | 22 | ARG |
| 1 | L | 88 | TRP |
| 1 | L | 103 | GLU |
| 1 | L | 108 | LEU |
| 1 | L | 134 | LYS |
| 1 | L | 190 | LYS |
| 1 | M | 19 | ILE |
| 1 | M | 22 | ARG |
| 1 | M | 88 | TRP |
| 1 | M | 103 | GLU |
| 1 | M | 108 | LEU |
| 1 | M | 134 | LYS |
| 1 | M | 190 | LYS |
| 1 | N | 19 | ILE |
| 1 | N | 22 | ARG |
| 1 | N | 88 | TRP |
| 1 | N | 103 | GLU |
| 1 | N | 108 | LEU |
| 1 | N | 134 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 190 | LYS |
| 1 | O | 22 | ARG |
| 1 | O | 88 | TRP |
| 1 | O | 103 | GLU |
| 1 | O | 108 | LEU |
| 1 | O | 134 | LYS |
| 1 | O | 190 | LYS |
| 1 | P | 22 | ARG |
| 1 | P | 88 | TRP |
| 1 | P | 103 | GLU |
| 1 | P | 108 | LEU |
| 1 | P | 134 | LYS |
| 1 | P | 190 | LYS |
| 1 | Q | 22 | ARG |
| 1 | Q | 88 | TRP |
| 1 | Q | 103 | GLU |
| 1 | Q | 108 | LEU |
| 1 | Q | 134 | LYS |
| 1 | Q | 190 | LYS |
| 1 | R | 22 | ARG |
| 1 | R | 88 | TRP |
| 1 | R | 103 | GLU |
| 1 | R | 108 | LEU |
| 1 | R | 134 | LYS |
| 1 | R | 190 | LYS |
| 1 | S | 22 | ARG |
| 1 | S | 88 | TRP |
| 1 | S | 103 | GLU |
| 1 | S | 108 | LEU |
| 1 | S | 134 | LYS |
| 1 | S | 190 | LYS |
| 1 | T | 22 | ARG |
| 1 | T | 88 | TRP |
| 1 | T | 103 | GLU |
| 1 | T | 108 | LEU |
| 1 | T | 134 | LYS |
| 1 | T | 190 | LYS |
| 1 | U | 22 | ARG |
| 1 | U | 88 | TRP |
| 1 | U | 103 | GLU |
| 1 | U | 108 | LEU |
| 1 | U | 134 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | U | 190 | LYS |
| 1 | V | 22 | ARG |
| 1 | V | 88 | TRP |
| 1 | V | 103 | GLU |
| 1 | V | 108 | LEU |
| 1 | V | 134 | LYS |
| 1 | V | 190 | LYS |
| 1 | W | 22 | ARG |
| 1 | W | 88 | TRP |
| 1 | W | 103 | GLU |
| 1 | W | 108 | LEU |
| 1 | W | 134 | LYS |
| 1 | W | 190 | LYS |
| 1 | X | 22 | ARG |
| 1 | X | 88 | TRP |
| 1 | X | 103 | GLU |
| 1 | X | 108 | LEU |
| 1 | X | 134 | LYS |
| 1 | X | 190 | LYS |
| 1 | Y | 22 | ARG |
| 1 | Y | 88 | TRP |
| 1 | Y | 103 | GLU |
| 1 | Y | 108 | LEU |
| 1 | Y | 134 | LYS |
| 1 | Y | 190 | LYS |
| 1 | Z | 22 | ARG |
| 1 | Z | 88 | TRP |
| 1 | Z | 103 | GLU |
| 1 | Z | 108 | LEU |
| 1 | Z | 134 | LYS |
| 1 | Z | 190 | LYS |
| 1 | a | 22 | ARG |
| 1 | a | 88 | TRP |
| 1 | a | 103 | GLU |
| 1 | a | 108 | LEU |
| 1 | a | 134 | LYS |
| 1 | a | 190 | LYS |
| 1 | b | 22 | ARG |
| 1 | b | 88 | TRP |
| 1 | b | 103 | GLU |
| 1 | b | 108 | LEU |
| 1 | b | 134 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | b | 190 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 50 | ASN |
| 1 | B | 180 | ASN |
| 1 | E | 180 | ASN |
| 1 | F | 50 | ASN |
| 1 | F | 185 | ASN |
| 1 | G | 180 | ASN |
| 1 | L | 63 | HIS |
| 1 | M | 50 | ASN |
| 1 | N | 50 | ASN |
| 1 | O | 180 | ASN |
| 1 | P | 16 | GLN |
| 1 | R | 180 | ASN |
| 1 | S | 180 | ASN |
| 1 | T | 50 | ASN |
| 1 | T | 180 | ASN |
| 1 | U | 63 | HIS |
| 1 | U | 180 | ASN |
| 1 | V | 16 | GLN |
| 1 | W | 16 | GLN |
| 1 | Z | 63 | HIS |
| 1 | b | 16 | GLN |
| 1 | b | 50 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th 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 | 170/201 (84%) | 0.14 | 11 (6%) 18 18 | 19, 30, 67, 111 | 0 |
| 1 | B | 170/201 (84%) | 0.19 | 11 (6%) 18 18 | 23, 35, 71, 116 | 0 |
| 1 | C | 170/201 (84%) | 0.31 | 16 (9%) 8 8 | 24, 36, 74, 121 | 0 |
| 1 | D | 170/201 (84%) | 0.43 | 14 (8%) 11 11 | 23, 36, 74, 118 | 0 |
| 1 | E | 170/201 (84%) | 0.19 | 14 (8%) 11 11 | 16, 27, 66, 111 | 0 |
| 1 | F | 170/201 (84%) | 0.11 | 12 (7%) 16 15 | 15, 25, 60, 102 | 0 |
| 1 | G | 170/201 (84%) | 0.12 | 14 (8%) 11 11 | 16, 27, 65, 107 | 0 |
| 1 | H | 170/201 (84%) | 0.17 | 10 (5%) 22 21 | 17, 29, 63, 106 | 0 |
| 1 | I | 170/201 (84%) | 0.37 | 15 (8%) 10 9 | 22, 34, 69, 112 | 0 |
| 1 | J | 170/201 (84%) | 0.27 | 15 (8%) 10 9 | 25, 36, 67, 114 | 0 |
| 1 | K | 170/201 (84%) | 0.27 | 12 (7%) 16 15 | 22, 32, 72, 114 | 0 |
| 1 | L | 170/201 (84%) | 0.16 | 12 (7%) 16 15 | 18, 30, 66, 112 | 0 |
| 1 | M | 170/201 (84%) | 0.13 | 12 (7%) 16 15 | 13, 23, 62, 108 | 0 |
| 1 | N | 170/201 (84%) | 0.08 | 11 (6%) 18 18 | 13, 23, 55, 101 | 0 |
| 1 | O | 170/201 (84%) | 0.25 | 16 (9%) 8 8 | 21, 33, 67, 114 | 0 |
| 1 | P | 170/201 (84%) | 0.24 | 11 (6%) 18 18 | 23, 35, 70, 114 | 0 |
| 1 | Q | 170/201 (84%) | 0.19 | 13 (7%) 13 13 | 20, 31, 69, 112 | 0 |
| 1 | R | 170/201 (84%) | 0.10 | 10 (5%) 22 21 | 18, 28, 66, 110 | 0 |
| 1 | S | 170/201 (84%) | 0.12 | 11 (6%) 18 18 | 13, 23, 65, 109 | 0 |
| 1 | T | 170/201 (84%) | 0.03 | 12 (7%) 16 15 | 13, 23, 50, 100 | 0 |
| 1 | U | 170/201 (84%) | 0.16 | 12 (7%) 16 15 | 17, 28, 63, 108 | 0 |
| 1 | V | 170/201 (84%) | 0.13 | 15 (8%) 10 9 | 16, 27, 65, 109 | 0 |
| 1 | W | 170/201 (84%) | 0.20 | 14 (8%) 11 11 | 17, 28, 65, 110 | 0 |
| 1 | X | 170/201 (84%) | 0.17 | 12 (7%) 16 15 | 21, 33, 68, 114 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-------|-----------------------|-------|
| 1 | Y | 170/201 (84%) | 0.33 | 16 (9%) | 8 8 | 21, 32, 69, 116 | 0 |
| 1 | Z | 170/201 (84%) | 0.21 | 13 (7%) | 13 13 | 21, 32, 70, 114 | 0 |
| 1 | a | 170/201 (84%) | 0.12 | 13 (7%) | 13 13 | 15, 25, 65, 107 | 0 |
| 1 | b | 170/201 (84%) | 0.10 | 12 (7%) | 16 15 | 14, 23, 59, 102 | 0 |
| All | All | 4760/5628 (84%) | 0.19 | 359 (7%) | 14 13 | 13, 30, 73, 121 | 0 |

All (359) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 14 | LEU | 14.8 |
| 1 | I | 14 | LEU | 13.7 |
| 1 | K | 13 | ILE | 13.2 |
| 1 | J | 14 | LEU | 12.3 |
| 1 | Q | 188 | GLY | 11.6 |
| 1 | W | 14 | LEU | 11.5 |
| 1 | W | 13 | ILE | 11.5 |
| 1 | C | 14 | LEU | 11.5 |
| 1 | R | 190 | LYS | 11.3 |
| 1 | D | 188 | GLY | 11.3 |
| 1 | P | 14 | LEU | 11.1 |
| 1 | E | 14 | LEU | 11.0 |
| 1 | X | 14 | LEU | 10.9 |
| 1 | Y | 13 | ILE | 10.5 |
| 1 | Z | 14 | LEU | 10.2 |
| 1 | I | 13 | ILE | 9.9 |
| 1 | P | 190 | LYS | 9.9 |
| 1 | Y | 14 | LEU | 9.8 |
| 1 | O | 13 | ILE | 9.4 |
| 1 | O | 14 | LEU | 9.3 |
| 1 | Q | 13 | ILE | 9.3 |
| 1 | U | 13 | ILE | 8.9 |
| 1 | U | 14 | LEU | 8.8 |
| 1 | R | 14 | LEU | 8.7 |
| 1 | X | 13 | ILE | 8.6 |
| 1 | M | 14 | LEU | 8.5 |
| 1 | P | 15 | THR | 8.5 |
| 1 | H | 13 | ILE | 8.4 |
| 1 | R | 13 | ILE | 8.3 |
| 1 | V | 13 | ILE | 8.3 |
| 1 | S | 188 | GLY | 8.1 |
| 1 | C | 188 | GLY | 8.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 13 | ILE | 8.0 |
| 1 | E | 13 | ILE | 7.8 |
| 1 | L | 14 | LEU | 7.8 |
| 1 | M | 122 | VAL | 7.7 |
| 1 | M | 188 | GLY | 7.7 |
| 1 | I | 15 | THR | 7.7 |
| 1 | a | 13 | ILE | 7.6 |
| 1 | Y | 188 | GLY | 7.6 |
| 1 | J | 15 | THR | 7.6 |
| 1 | L | 190 | LYS | 7.5 |
| 1 | A | 14 | LEU | 7.5 |
| 1 | a | 14 | LEU | 7.4 |
| 1 | Z | 188 | GLY | 7.4 |
| 1 | Q | 190 | LYS | 7.4 |
| 1 | I | 190 | LYS | 7.4 |
| 1 | N | 14 | LEU | 7.3 |
| 1 | D | 15 | THR | 7.2 |
| 1 | C | 190 | LYS | 7.2 |
| 1 | L | 189 | LEU | 7.1 |
| 1 | T | 14 | LEU | 7.0 |
| 1 | G | 13 | ILE | 7.0 |
| 1 | A | 13 | ILE | 7.0 |
| 1 | H | 122 | VAL | 7.0 |
| 1 | H | 14 | LEU | 6.8 |
| 1 | O | 16 | GLN | 6.8 |
| 1 | P | 13 | ILE | 6.8 |
| 1 | Z | 122 | VAL | 6.7 |
| 1 | D | 189 | LEU | 6.7 |
| 1 | J | 190 | LYS | 6.6 |
| 1 | K | 187 | ASP | 6.6 |
| 1 | S | 14 | LEU | 6.5 |
| 1 | Y | 190 | LYS | 6.5 |
| 1 | V | 122 | VAL | 6.5 |
| 1 | W | 15 | THR | 6.5 |
| 1 | Z | 189 | LEU | 6.5 |
| 1 | S | 15 | THR | 6.5 |
| 1 | B | 190 | LYS | 6.4 |
| 1 | B | 14 | LEU | 6.3 |
| 1 | C | 13 | ILE | 6.3 |
| 1 | U | 122 | VAL | 6.3 |
| 1 | Q | 14 | LEU | 6.1 |
| 1 | G | 14 | LEU | 6.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 16 | GLN | 6.0 |
| 1 | Y | 187 | ASP | 6.0 |
| 1 | I | 122 | VAL | 6.0 |
| 1 | D | 122 | VAL | 6.0 |
| 1 | V | 189 | LEU | 5.9 |
| 1 | N | 13 | ILE | 5.9 |
| 1 | E | 188 | GLY | 5.8 |
| 1 | G | 122 | VAL | 5.8 |
| 1 | V | 190 | LYS | 5.7 |
| 1 | D | 190 | LYS | 5.6 |
| 1 | I | 16 | GLN | 5.6 |
| 1 | A | 189 | LEU | 5.6 |
| 1 | V | 14 | LEU | 5.5 |
| 1 | O | 15 | THR | 5.5 |
| 1 | A | 190 | LYS | 5.4 |
| 1 | S | 16 | GLN | 5.4 |
| 1 | S | 190 | LYS | 5.4 |
| 1 | a | 188 | GLY | 5.4 |
| 1 | Z | 190 | LYS | 5.3 |
| 1 | b | 15 | THR | 5.3 |
| 1 | b | 13 | ILE | 5.3 |
| 1 | F | 13 | ILE | 5.2 |
| 1 | P | 16 | GLN | 5.2 |
| 1 | T | 187 | ASP | 5.2 |
| 1 | M | 190 | LYS | 5.2 |
| 1 | Q | 16 | GLN | 5.2 |
| 1 | K | 190 | LYS | 5.1 |
| 1 | M | 189 | LEU | 5.1 |
| 1 | J | 13 | ILE | 5.1 |
| 1 | L | 16 | GLN | 5.1 |
| 1 | Y | 16 | GLN | 5.0 |
| 1 | Z | 15 | THR | 5.0 |
| 1 | T | 13 | ILE | 5.0 |
| 1 | D | 187 | ASP | 5.0 |
| 1 | L | 188 | GLY | 5.0 |
| 1 | K | 14 | LEU | 4.9 |
| 1 | K | 122 | VAL | 4.9 |
| 1 | I | 188 | GLY | 4.9 |
| 1 | K | 15 | THR | 4.8 |
| 1 | Z | 13 | ILE | 4.8 |
| 1 | R | 188 | GLY | 4.7 |
| 1 | S | 189 | LEU | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | W | 190 | LYS | 4.7 |
| 1 | C | 189 | LEU | 4.7 |
| 1 | E | 15 | THR | 4.7 |
| 1 | S | 122 | VAL | 4.7 |
| 1 | O | 188 | GLY | 4.7 |
| 1 | W | 188 | GLY | 4.7 |
| 1 | E | 189 | LEU | 4.7 |
| 1 | Y | 15 | THR | 4.7 |
| 1 | B | 15 | THR | 4.6 |
| 1 | O | 17 | LYS | 4.6 |
| 1 | W | 122 | VAL | 4.6 |
| 1 | K | 166 | PHE | 4.6 |
| 1 | Z | 16 | GLN | 4.6 |
| 1 | B | 13 | ILE | 4.5 |
| 1 | A | 15 | THR | 4.5 |
| 1 | H | 190 | LYS | 4.5 |
| 1 | R | 122 | VAL | 4.5 |
| 1 | F | 187 | ASP | 4.5 |
| 1 | L | 15 | THR | 4.4 |
| 1 | L | 13 | ILE | 4.4 |
| 1 | a | 187 | ASP | 4.4 |
| 1 | C | 15 | THR | 4.4 |
| 1 | a | 15 | THR | 4.4 |
| 1 | D | 16 | GLN | 4.4 |
| 1 | K | 16 | GLN | 4.4 |
| 1 | C | 166 | PHE | 4.4 |
| 1 | Q | 189 | LEU | 4.4 |
| 1 | G | 190 | LYS | 4.3 |
| 1 | V | 188 | GLY | 4.3 |
| 1 | Q | 122 | VAL | 4.3 |
| 1 | J | 16 | GLN | 4.2 |
| 1 | b | 14 | LEU | 4.2 |
| 1 | P | 187 | ASP | 4.2 |
| 1 | W | 16 | GLN | 4.2 |
| 1 | Q | 187 | ASP | 4.2 |
| 1 | C | 187 | ASP | 4.1 |
| 1 | Y | 166 | PHE | 4.1 |
| 1 | a | 189 | LEU | 4.1 |
| 1 | E | 190 | LYS | 4.0 |
| 1 | Y | 189 | LEU | 4.0 |
| 1 | K | 188 | GLY | 4.0 |
| 1 | X | 122 | VAL | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | M | 16 | GLN | 4.0 |
| 1 | E | 187 | ASP | 3.9 |
| 1 | R | 16 | GLN | 3.9 |
| 1 | V | 16 | GLN | 3.9 |
| 1 | a | 16 | GLN | 3.9 |
| 1 | G | 189 | LEU | 3.9 |
| 1 | A | 122 | VAL | 3.9 |
| 1 | R | 189 | LEU | 3.9 |
| 1 | E | 166 | PHE | 3.9 |
| 1 | S | 166 | PHE | 3.9 |
| 1 | W | 166 | PHE | 3.9 |
| 1 | Q | 15 | THR | 3.9 |
| 1 | U | 190 | LYS | 3.9 |
| 1 | a | 156 | GLU | 3.8 |
| 1 | U | 187 | ASP | 3.8 |
| 1 | M | 166 | PHE | 3.8 |
| 1 | T | 122 | VAL | 3.7 |
| 1 | C | 122 | VAL | 3.7 |
| 1 | L | 122 | VAL | 3.7 |
| 1 | M | 15 | THR | 3.7 |
| 1 | X | 16 | GLN | 3.7 |
| 1 | G | 188 | GLY | 3.7 |
| 1 | O | 189 | LEU | 3.6 |
| 1 | K | 131 | ILE | 3.6 |
| 1 | X | 15 | THR | 3.6 |
| 1 | D | 166 | PHE | 3.6 |
| 1 | F | 14 | LEU | 3.6 |
| 1 | J | 187 | ASP | 3.5 |
| 1 | U | 189 | LEU | 3.5 |
| 1 | W | 189 | LEU | 3.5 |
| 1 | O | 190 | LYS | 3.5 |
| 1 | M | 187 | ASP | 3.5 |
| 1 | G | 17 | LYS | 3.5 |
| 1 | C | 16 | GLN | 3.5 |
| 1 | I | 187 | ASP | 3.5 |
| 1 | P | 189 | LEU | 3.5 |
| 1 | F | 122 | VAL | 3.5 |
| 1 | N | 122 | VAL | 3.5 |
| 1 | H | 187 | ASP | 3.4 |
| 1 | A | 16 | GLN | 3.4 |
| 1 | T | 15 | THR | 3.4 |
| 1 | X | 190 | LYS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | U | 16 | GLN | 3.4 |
| 1 | V | 166 | PHE | 3.4 |
| 1 | A | 121 | GLY | 3.4 |
| 1 | b | 122 | VAL | 3.4 |
| 1 | E | 122 | VAL | 3.3 |
| 1 | G | 15 | THR | 3.3 |
| 1 | E | 16 | GLN | 3.2 |
| 1 | F | 50 | ASN | 3.2 |
| 1 | Z | 187 | ASP | 3.2 |
| 1 | H | 189 | LEU | 3.2 |
| 1 | J | 189 | LEU | 3.2 |
| 1 | K | 189 | LEU | 3.2 |
| 1 | P | 166 | PHE | 3.2 |
| 1 | a | 166 | PHE | 3.2 |
| 1 | Q | 166 | PHE | 3.2 |
| 1 | b | 187 | ASP | 3.2 |
| 1 | N | 187 | ASP | 3.1 |
| 1 | G | 166 | PHE | 3.1 |
| 1 | E | 156 | GLU | 3.1 |
| 1 | J | 166 | PHE | 3.1 |
| 1 | I | 121 | GLY | 3.1 |
| 1 | L | 20 | ASP | 3.1 |
| 1 | R | 187 | ASP | 3.1 |
| 1 | Y | 122 | VAL | 3.1 |
| 1 | C | 120 | GLY | 3.0 |
| 1 | I | 166 | PHE | 3.0 |
| 1 | B | 187 | ASP | 3.0 |
| 1 | O | 20 | ASP | 3.0 |
| 1 | V | 20 | ASP | 3.0 |
| 1 | S | 13 | ILE | 3.0 |
| 1 | F | 16 | GLN | 3.0 |
| 1 | b | 50 | ASN | 3.0 |
| 1 | B | 131 | ILE | 2.9 |
| 1 | T | 16 | GLN | 2.9 |
| 1 | N | 17 | LYS | 2.9 |
| 1 | C | 19 | ILE | 2.9 |
| 1 | N | 166 | PHE | 2.9 |
| 1 | X | 78 | LYS | 2.9 |
| 1 | a | 190 | LYS | 2.9 |
| 1 | V | 187 | ASP | 2.9 |
| 1 | T | 189 | LEU | 2.9 |
| 1 | H | 17 | LYS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | R | 15 | THR | 2.8 |
| 1 | X | 121 | GLY | 2.8 |
| 1 | X | 189 | LEU | 2.8 |
| 1 | V | 17 | LYS | 2.8 |
| 1 | Z | 166 | PHE | 2.8 |
| 1 | a | 122 | VAL | 2.8 |
| 1 | G | 187 | ASP | 2.7 |
| 1 | J | 121 | GLY | 2.7 |
| 1 | S | 187 | ASP | 2.7 |
| 1 | M | 17 | LYS | 2.7 |
| 1 | N | 50 | ASN | 2.7 |
| 1 | U | 156 | GLU | 2.7 |
| 1 | O | 166 | PHE | 2.7 |
| 1 | L | 187 | ASP | 2.7 |
| 1 | B | 166 | PHE | 2.7 |
| 1 | G | 18 | LEU | 2.7 |
| 1 | E | 78 | LYS | 2.6 |
| 1 | W | 17 | LYS | 2.6 |
| 1 | A | 188 | GLY | 2.6 |
| 1 | A | 166 | PHE | 2.6 |
| 1 | T | 190 | LYS | 2.6 |
| 1 | G | 16 | GLN | 2.6 |
| 1 | B | 121 | GLY | 2.6 |
| 1 | T | 166 | PHE | 2.6 |
| 1 | O | 122 | VAL | 2.6 |
| 1 | G | 156 | GLU | 2.6 |
| 1 | D | 20 | ASP | 2.6 |
| 1 | C | 78 | LYS | 2.6 |
| 1 | L | 166 | PHE | 2.6 |
| 1 | F | 189 | LEU | 2.6 |
| 1 | H | 188 | GLY | 2.5 |
| 1 | M | 13 | ILE | 2.5 |
| 1 | F | 156 | GLU | 2.5 |
| 1 | P | 122 | VAL | 2.5 |
| 1 | Y | 131 | ILE | 2.5 |
| 1 | R | 166 | PHE | 2.5 |
| 1 | D | 120 | GLY | 2.5 |
| 1 | N | 189 | LEU | 2.5 |
| 1 | W | 187 | ASP | 2.5 |
| 1 | X | 187 | ASP | 2.5 |
| 1 | E | 17 | LYS | 2.5 |
| 1 | Y | 78 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | O | 156 | GLU | 2.5 |
| 1 | C | 164 | ARG | 2.4 |
| 1 | D | 165 | ASN | 2.4 |
| 1 | Q | 17 | LYS | 2.4 |
| 1 | Z | 17 | LYS | 2.4 |
| 1 | C | 155 | TYR | 2.4 |
| 1 | F | 15 | THR | 2.4 |
| 1 | O | 121 | GLY | 2.4 |
| 1 | U | 121 | GLY | 2.4 |
| 1 | P | 20 | ASP | 2.4 |
| 1 | U | 17 | LYS | 2.4 |
| 1 | Y | 120 | GLY | 2.4 |
| 1 | J | 122 | VAL | 2.4 |
| 1 | b | 190 | LYS | 2.4 |
| 1 | Y | 164 | ARG | 2.4 |
| 1 | U | 166 | PHE | 2.4 |
| 1 | X | 156 | GLU | 2.4 |
| 1 | I | 20 | ASP | 2.4 |
| 1 | X | 166 | PHE | 2.3 |
| 1 | P | 156 | GLU | 2.3 |
| 1 | Q | 156 | GLU | 2.3 |
| 1 | I | 189 | LEU | 2.3 |
| 1 | E | 20 | ASP | 2.3 |
| 1 | V | 156 | GLU | 2.3 |
| 1 | O | 131 | ILE | 2.3 |
| 1 | F | 131 | ILE | 2.3 |
| 1 | V | 78 | LYS | 2.3 |
| 1 | M | 156 | GLU | 2.3 |
| 1 | V | 121 | GLY | 2.3 |
| 1 | W | 156 | GLU | 2.3 |
| 1 | b | 166 | PHE | 2.3 |
| 1 | G | 78 | LYS | 2.3 |
| 1 | b | 131 | ILE | 2.3 |
| 1 | Z | 165 | ASN | 2.2 |
| 1 | b | 16 | GLN | 2.2 |
| 1 | H | 20 | ASP | 2.2 |
| 1 | J | 156 | GLU | 2.2 |
| 1 | K | 17 | LYS | 2.2 |
| 1 | I | 156 | GLU | 2.2 |
| 1 | B | 50 | ASN | 2.2 |
| 1 | J | 101 | GLU | 2.2 |
| 1 | N | 131 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | S | 20 | ASP | 2.2 |
| 1 | b | 18 | LEU | 2.2 |
| 1 | T | 17 | LYS | 2.2 |
| 1 | H | 166 | PHE | 2.2 |
| 1 | A | 50 | ASN | 2.2 |
| 1 | O | 50 | ASN | 2.2 |
| 1 | I | 17 | LYS | 2.2 |
| 1 | V | 45 | LEU | 2.1 |
| 1 | T | 50 | ASN | 2.1 |
| 1 | J | 50 | ASN | 2.1 |
| 1 | W | 20 | ASP | 2.1 |
| 1 | b | 20 | ASP | 2.1 |
| 1 | Z | 20 | ASP | 2.1 |
| 1 | C | 156 | GLU | 2.1 |
| 1 | L | 156 | GLU | 2.1 |
| 1 | a | 17 | LYS | 2.1 |
| 1 | I | 103 | GLU | 2.1 |
| 1 | F | 120 | GLY | 2.1 |
| 1 | N | 48 | ILE | 2.1 |
| 1 | Q | 131 | ILE | 2.1 |
| 1 | B | 189 | LEU | 2.1 |
| 1 | J | 184 | GLU | 2.1 |
| 1 | N | 190 | LYS | 2.1 |
| 1 | U | 188 | GLY | 2.1 |
| 1 | F | 18 | LEU | 2.0 |
| 1 | O | 45 | LEU | 2.0 |
| 1 | Y | 155 | TYR | 2.0 |
| 1 | J | 45 | LEU | 2.0 |
| 1 | W | 149 | GLU | 2.0 |
| 1 | T | 120 | GLY | 2.0 |
| 1 | Y | 20 | ASP | 2.0 |
| 1 | D | 17 | LYS | 2.0 |
| 1 | a | 165 | ASN | 2.0 |

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.