



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2024 – 03:02 pm GMT

PDB ID : 6QCM
EMDB ID : EMD-4508
Title : Cryo em structure of the Listeria stressosome
Authors : Williams, A.H.; Redzej, A.; Waksman, G.; Cossart, P.
Deposited on : 2018-12-28
Resolution : 4.21 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

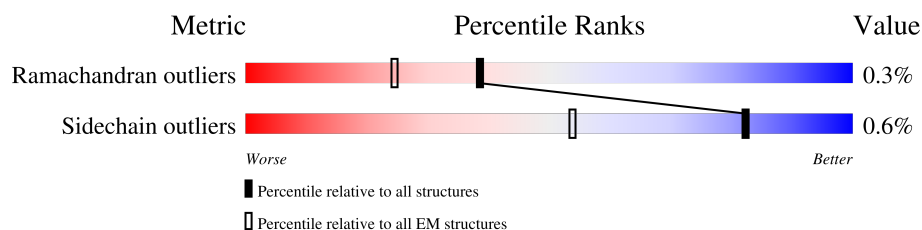
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.21 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AB | 128 | 88% • 10% |
| 1 | BC | 128 | 89% • 10% |
| 1 | DC | 128 | 88% • 10% |
| 1 | EB | 128 | 90% 10% |
| 1 | FA | 128 | 87% • 10% |
| 1 | FB | 128 | 88% • 10% |
| 1 | FC | 128 | 88% • 10% |
| 1 | GC | 128 | 90% 10% |
| 1 | HC | 128 | 88% •• 10% |
| 1 | IC | 128 | 87% • 10% |


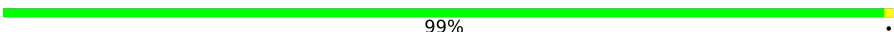
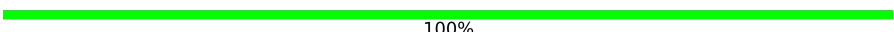
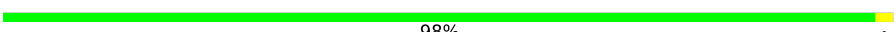
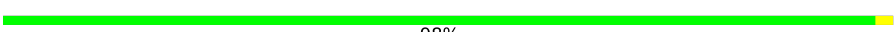







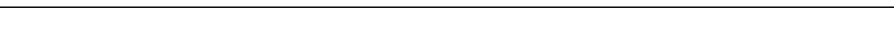

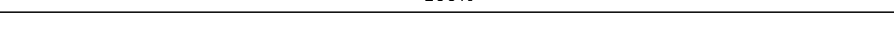
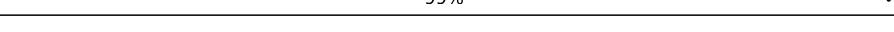
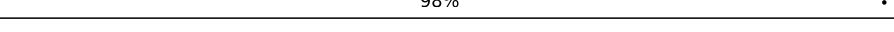
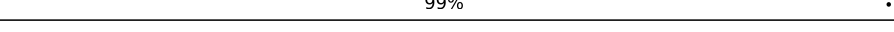
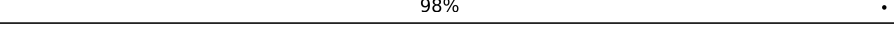
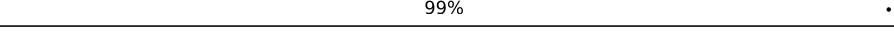
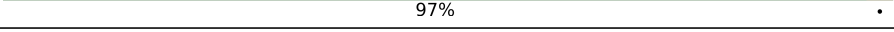
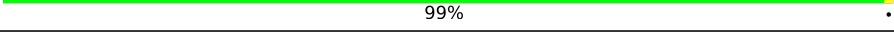
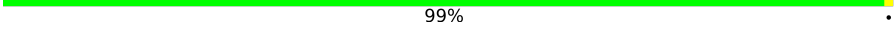


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | K | 128 |  88% • 10% |
| 1 | KB | 128 |  88% • 10% |
| 1 | L | 128 |  88% • 10% |
| 1 | LB | 128 |  88% • 10% |
| 1 | M | 128 |  88% • 10% |
| 1 | OB | 128 |  87% • 10% |
| 1 | P | 128 |  88% • 10% |
| 1 | PB | 128 |  89% • 10% |
| 1 | Q | 128 |  88% • 10% |
| 1 | SB | 128 |  89% • 10% |
| 1 | T | 128 |  88% • 10% |
| 1 | TB | 128 |  88% • 10% |
| 1 | U | 128 |  89% • 10% |
| 1 | UB | 128 |  88% • 10% |
| 1 | V | 128 |  88% • 10% |
| 1 | VB | 128 |  88% • 10% |
| 1 | W | 128 |  88% •• 10% |
| 1 | X | 128 |  87% • 10% |
| 1 | Y | 128 |  88% • 10% |
| 1 | Z | 128 |  89% • 10% |
| 2 | CB | 129 |  88% •• 10% |
| 2 | DB | 129 |  88% • 10% |
| 2 | E | 129 |  88% • 10% |
| 2 | F | 129 |  88% • 10% |
| 2 | GB | 129 |  87% • 10% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | IB | 129 |  89% 10% |
| 3 | A | 118 |  99% |
| 3 | B | 118 |  100% |
| 3 | C | 118 |  98% |
| 3 | D | 118 |  98% |
| 3 | I | 118 |  100% |
| 3 | J | 118 |  99% |
| 3 | N | 118 |  100% |
| 3 | O | 118 |  100% |
| 3 | R | 118 |  100% |
| 3 | S | 118 |  100% |
| 3 | a | 118 |  98% |
| 3 | b | 118 |  100% |
| 3 | c | 118 |  100% |
| 3 | d | 118 |  99% |
| 3 | e | 118 |  98% |
| 3 | f | 118 |  99% |
| 3 | g | 118 |  98% |
| 3 | h | 118 |  99% |
| 3 | i | 118 |  97% |
| 3 | j | 118 |  99% |
| 4 | AD | 123 |  99% |
| 5 | CD | 136 |  88% 10% |
| 5 | FD | 136 |  88% 10% |
| 5 | HD | 136 |  89% 10% |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52697 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 RsbR protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | AB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | BC | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 555 | 150 | 160 | 6 | | |
| 1 | DC | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | EB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | FA | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 555 | 150 | 160 | 6 | | |
| 1 | FB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | FC | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | GC | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | HC | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 555 | 150 | 160 | 6 | | |
| 1 | IC | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | K | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | KB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | L | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | LB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | M | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 555 | 150 | 160 | 6 | | |
| 1 | OB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | P | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | PB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | Q | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 554 | 149 | 162 | 6 | | |
| 1 | SB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | T | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 867 | 551 | 148 | 162 | 6 | | |
| 1 | TB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | U | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | UB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 869 | 554 | 147 | 162 | 6 | | |
| 1 | V | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 554 | 149 | 162 | 6 | | |
| 1 | VB | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | W | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | X | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 865 | 552 | 147 | 160 | 6 | | |
| 1 | Y | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |
| 1 | Z | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 557 | 150 | 162 | 6 | | |

- Molecule 2 is a protein called RsbR protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | CB | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 563 | 152 | 163 | 6 | | |
| 2 | DB | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 563 | 152 | 163 | 6 | | |
| 2 | E | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 563 | 152 | 163 | 6 | | |
| 2 | F | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 563 | 152 | 163 | 6 | | |
| 2 | GB | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 563 | 152 | 163 | 6 | | |
| 2 | IB | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 563 | 152 | 163 | 6 | | |

- Molecule 3 is a protein called RsbS protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 3 | A | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | B | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | C | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | D | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | I | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | J | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | N | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | O | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | R | 118 | Total 871 | C 556 | N 135 | O 175 | S 5 | 0 | 0 |
| 3 | S | 118 | Total 871 | C 556 | N 135 | O 175 | S 5 | 0 | 0 |
| 3 | a | 118 | Total 871 | C 556 | N 135 | O 175 | S 5 | 0 | 0 |
| 3 | b | 118 | Total 871 | C 556 | N 135 | O 175 | S 5 | 0 | 0 |
| 3 | c | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | d | 118 | Total 872 | C 557 | N 136 | O 175 | S 4 | 0 | 0 |
| 3 | e | 118 | Total 868 | C 555 | N 135 | O 173 | S 5 | 0 | 0 |
| 3 | f | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | g | 118 | Total 875 | C 559 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | h | 118 | Total 871 | C 556 | N 135 | O 175 | S 5 | 0 | 0 |
| 3 | i | 118 | Total 872 | C 556 | N 136 | O 175 | S 5 | 0 | 0 |
| 3 | j | 118 | Total 871 | C 556 | N 135 | O 175 | S 5 | 0 | 0 |

- Molecule 4 is a protein called RsbR protein,RsbR protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | AD | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 935 | 594 | 160 | 175 | 6 | | |

- Molecule 5 is a protein called RsbR protein.

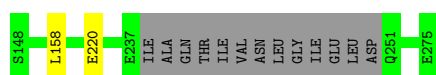
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | CD | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 935 | 595 | 161 | 173 | 6 | | |
| 5 | FD | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 927 | 589 | 159 | 173 | 6 | | |
| 5 | HD | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 931 | 591 | 159 | 175 | 6 | | |

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.

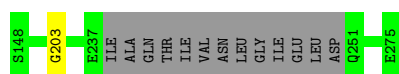
- Molecule 1: RsbR protein

Chain AB:  88% 10%



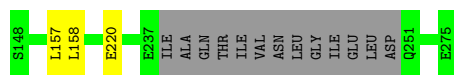
- Molecule 1: RsbR protein

Chain BC:  89% 10%



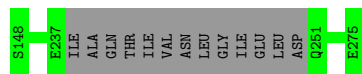
- Molecule 1: RsbR protein

Chain DC:  88% 10%




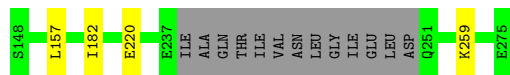
- Molecule 1: RsbR protein

Chain EB:  90% 10%




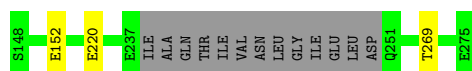
- Molecule 1: RsbR protein

Chain FA:  87% 10%



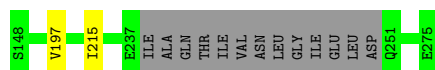
- Molecule 1: RsbR protein

Chain FB:  88% 10%



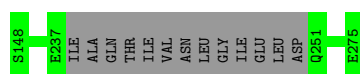
- Molecule 1: RsbR protein

Chain FC: 88% 10%



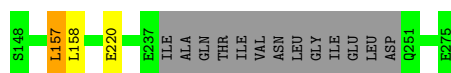
- Molecule 1: RsbR protein

Chain GC: 90% 10%



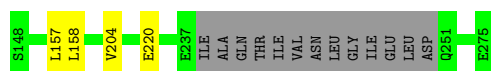
- Molecule 1: RsbR protein

Chain HC: 88% 10%



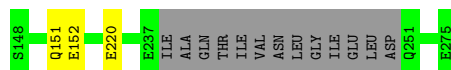
- Molecule 1: RsbR protein

Chain IC: 87% 10%



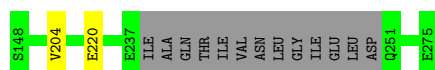
- Molecule 1: RsbR protein

Chain K: 88% 10%



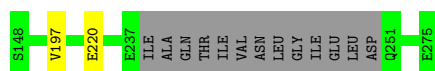
- Molecule 1: RsbR protein

Chain KB: 88% 10%



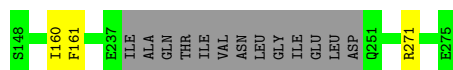
- Molecule 1: RsbR protein

Chain L: 88% 10%



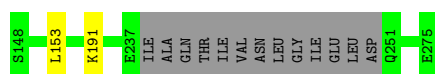
- Molecule 1: RsbR protein

Chain LB: 88% 10%



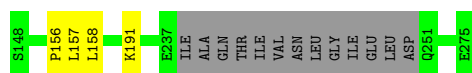
- Molecule 1: RsbR protein

Chain M: 88% 10%



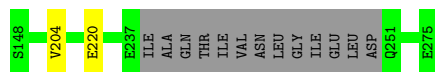
- Molecule 1: RsbR protein

Chain OB: 87% 10%



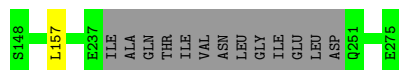
- Molecule 1: RsbR protein

Chain P: 88% 10%



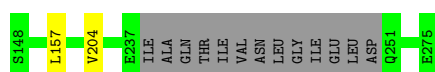
- Molecule 1: RsbR protein

Chain PB: 89% 10%



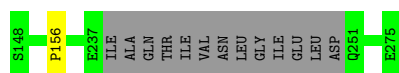
- Molecule 1: RsbR protein

Chain Q: 88% 10%




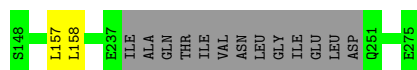
- Molecule 1: RsbR protein

Chain SB: 89% 10%




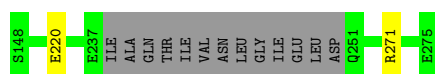
- Molecule 1: RsbR protein

Chain T:  88% 10%




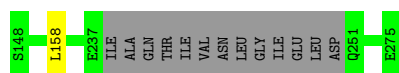
- Molecule 1: RsbR protein

Chain TB:  88% 10%




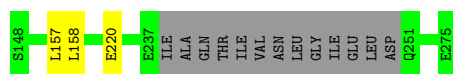
- Molecule 1: RsbR protein

Chain U:  89% 10%




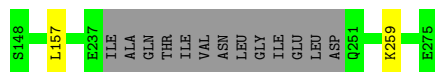
- Molecule 1: RsbR protein

Chain UB:  88% 10%



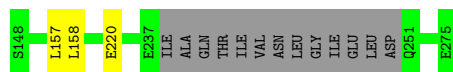
- Molecule 1: RsbR protein

Chain V:  88% 10%




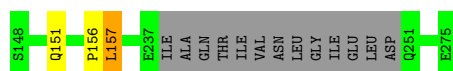
- Molecule 1: RsbR protein

Chain VB:  88% 10%



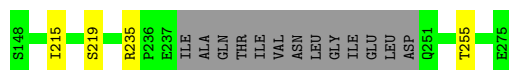
- Molecule 1: RsbR protein

Chain W:  88% 10%



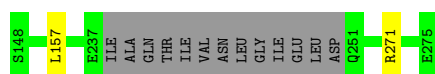
- Molecule 1: RsbR protein

Chain X: 87% 10%



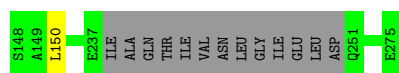
- Molecule 1: RsbR protein

Chain Y: 88% 10%



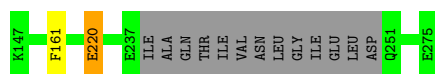
- Molecule 1: RsbR protein

Chain Z: 89% 10%



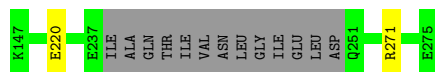
- Molecule 2: RsbR protein

Chain CB: 88% 10%



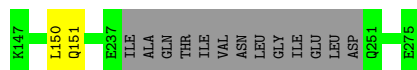
- Molecule 2: RsbR protein

Chain DB: 88% 10%



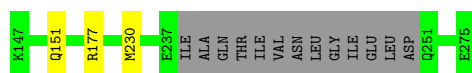
- Molecule 2: RsbR protein

Chain E: 88% 10%



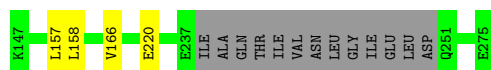
- Molecule 2: RsbR protein

Chain F: 88% 10%



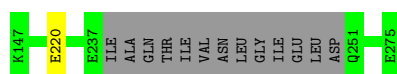
- Molecule 2: RsbR protein

Chain GB: 87% 10%



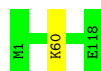
- Molecule 2: RsbR protein

Chain IB: 89% 10%



- Molecule 3: RsbS protein

Chain A: 99%



- Molecule 3: RsbS protein

Chain B: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain C: 98%



- Molecule 3: RsbS protein

Chain D: 98%



- Molecule 3: RsbS protein

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain J:  99% .



- Molecule 3: RsbS protein

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain R:  100%

There are no outlier residues recorded for this chain.

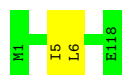
- Molecule 3: RsbS protein

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain a:  98% .



- Molecule 3: RsbS protein

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain d:  99% .



- Molecule 3: RsbS protein

Chain e:  98%



- Molecule 3: RsbS protein

Chain f:  99%



- Molecule 3: RsbS protein

Chain g:  98%



- Molecule 3: RsbS protein

Chain h:  99%



- Molecule 3: RsbS protein

Chain i:  97%



- Molecule 3: RsbS protein

Chain j:  99%

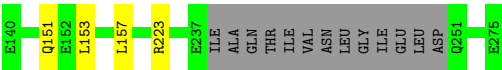
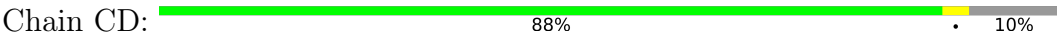


- Molecule 4: RsbR protein,RsbR protein

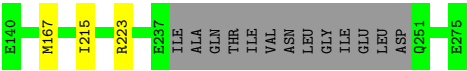
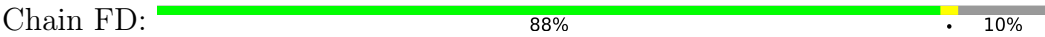
Chain AD:  99%



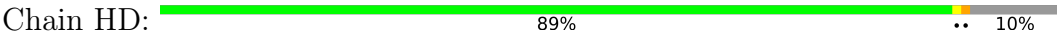
- Molecule 5: RsbR protein



- Molecule 5: RsbR protein



- Molecule 5: RsbR protein



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 78000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 2.25 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 | AB | 0.30 | 0/881 | 0.65 | 0/1193 |
| 1 | BC | 0.28 | 0/877 | 0.65 | 0/1188 |
| 1 | DC | 0.28 | 0/881 | 0.66 | 1/1193 (0.1%) |
| 1 | EB | 0.29 | 0/881 | 0.63 | 0/1193 |
| 1 | FA | 0.30 | 0/877 | 0.60 | 1/1188 (0.1%) |
| 1 | FB | 0.29 | 0/881 | 0.61 | 0/1193 |
| 1 | FC | 0.27 | 0/881 | 0.64 | 0/1193 |
| 1 | GC | 0.27 | 0/881 | 0.61 | 0/1193 |
| 1 | HC | 0.29 | 0/877 | 0.63 | 1/1188 (0.1%) |
| 1 | IC | 0.28 | 0/881 | 0.64 | 1/1193 (0.1%) |
| 1 | K | 0.28 | 0/881 | 0.64 | 0/1193 |
| 1 | KB | 0.30 | 0/881 | 0.61 | 0/1193 |
| 1 | L | 0.27 | 0/881 | 0.58 | 0/1193 |
| 1 | LB | 0.28 | 0/881 | 0.63 | 0/1193 |
| 1 | M | 0.27 | 0/877 | 0.66 | 1/1188 (0.1%) |
| 1 | OB | 0.30 | 0/881 | 0.66 | 2/1193 (0.2%) |
| 1 | P | 0.27 | 0/881 | 0.60 | 0/1193 |
| 1 | PB | 0.27 | 0/881 | 0.60 | 0/1193 |
| 1 | Q | 0.31 | 0/877 | 0.63 | 1/1189 (0.1%) |
| 1 | SB | 0.28 | 0/881 | 0.60 | 0/1193 |
| 1 | T | 0.30 | 0/873 | 0.64 | 1/1185 (0.1%) |
| 1 | TB | 0.29 | 0/881 | 0.65 | 0/1193 |
| 1 | U | 0.29 | 0/881 | 0.63 | 0/1193 |
| 1 | UB | 0.30 | 0/875 | 0.64 | 1/1186 (0.1%) |
| 1 | V | 0.29 | 0/877 | 0.58 | 0/1189 |
| 1 | VB | 0.28 | 0/881 | 0.66 | 1/1193 (0.1%) |
| 1 | W | 0.28 | 0/881 | 0.62 | 0/1193 |
| 1 | X | 0.29 | 0/871 | 0.68 | 1/1181 (0.1%) |
| 1 | Y | 0.29 | 0/881 | 0.62 | 0/1193 |
| 1 | Z | 0.29 | 0/881 | 0.63 | 1/1193 (0.1%) |
| 2 | CB | 0.29 | 0/890 | 0.63 | 0/1204 |
| 2 | DB | 0.27 | 0/890 | 0.62 | 0/1204 |
| 2 | E | 0.27 | 0/890 | 0.61 | 0/1204 |
| 2 | F | 0.27 | 0/890 | 0.61 | 0/1204 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | GB | 0.29 | 0/890 | 0.65 | 0/1204 |
| 2 | IB | 0.27 | 0/890 | 0.59 | 0/1204 |
| 3 | A | 0.27 | 0/881 | 0.55 | 0/1188 |
| 3 | B | 0.26 | 0/881 | 0.51 | 0/1188 |
| 3 | C | 0.26 | 0/881 | 0.49 | 0/1188 |
| 3 | D | 0.28 | 0/881 | 0.59 | 1/1188 (0.1%) |
| 3 | I | 0.27 | 0/881 | 0.56 | 0/1188 |
| 3 | J | 0.26 | 0/881 | 0.51 | 0/1188 |
| 3 | N | 0.27 | 0/881 | 0.56 | 0/1188 |
| 3 | O | 0.26 | 0/881 | 0.51 | 0/1188 |
| 3 | R | 0.26 | 0/877 | 0.52 | 0/1184 |
| 3 | S | 0.26 | 0/877 | 0.51 | 0/1184 |
| 3 | a | 0.26 | 0/877 | 0.53 | 0/1184 |
| 3 | b | 0.25 | 0/877 | 0.49 | 0/1184 |
| 3 | c | 0.26 | 0/881 | 0.51 | 0/1188 |
| 3 | d | 0.26 | 0/878 | 0.56 | 1/1185 (0.1%) |
| 3 | e | 0.26 | 0/874 | 0.51 | 0/1180 |
| 3 | f | 0.27 | 0/881 | 0.55 | 1/1188 (0.1%) |
| 3 | g | 0.27 | 0/881 | 0.51 | 0/1188 |
| 3 | h | 0.27 | 0/877 | 0.52 | 0/1184 |
| 3 | i | 0.27 | 0/878 | 0.56 | 0/1184 |
| 3 | j | 0.26 | 0/877 | 0.52 | 1/1184 (0.1%) |
| 4 | AD | 0.28 | 0/941 | 0.64 | 0/1274 |
| 5 | CD | 0.27 | 0/941 | 0.63 | 1/1273 (0.1%) |
| 5 | FD | 0.27 | 0/933 | 0.62 | 0/1265 |
| 5 | HD | 0.27 | 0/935 | 0.68 | 1/1264 (0.1%) |
| All | All | 0.28 | 0/53055 | 0.60 | 19/71756 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AB | 0 | 2 |
| 1 | DC | 0 | 1 |
| 1 | FA | 0 | 1 |
| 1 | FB | 0 | 2 |
| 1 | FC | 0 | 1 |
| 1 | HC | 0 | 2 |
| 1 | IC | 0 | 1 |
| 1 | K | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | KB | 0 | 2 |
| 1 | L | 0 | 1 |
| 1 | P | 0 | 2 |
| 1 | PB | 0 | 1 |
| 1 | Q | 0 | 1 |
| 1 | TB | 0 | 1 |
| 1 | U | 0 | 1 |
| 1 | UB | 0 | 1 |
| 1 | VB | 0 | 1 |
| 1 | W | 0 | 2 |
| 2 | CB | 0 | 1 |
| 2 | DB | 0 | 1 |
| 2 | E | 0 | 1 |
| 2 | F | 0 | 1 |
| 2 | GB | 0 | 3 |
| 2 | IB | 0 | 1 |
| 3 | a | 0 | 1 |
| 3 | e | 0 | 1 |
| 4 | AD | 0 | 1 |
| 5 | CD | 0 | 2 |
| 5 | HD | 0 | 1 |
| All | All | 0 | 39 |

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3 | d | 100 | LEU | CA-CB-CG | 7.72 | 133.06 | 115.30 |
| 5 | CD | 153 | LEU | CA-CB-CG | 7.59 | 132.77 | 115.30 |
| 5 | HD | 158 | LEU | CA-CB-CG | 7.58 | 132.72 | 115.30 |
| 1 | UB | 158 | LEU | CA-CB-CG | 7.10 | 131.64 | 115.30 |
| 1 | OB | 157 | LEU | CA-CB-CG | 6.34 | 129.88 | 115.30 |

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | AB | 158 | LEU | Peptide |
| 1 | AB | 220 | GLU | Peptide |
| 2 | CB | 220 | GLU | Peptide |
| 2 | DB | 220 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | DC | 220 | GLU | Peptide |

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 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 | AB | 111/128 (87%) | 95 (86%) | 16 (14%) | 0 | 100 | 100 |
| 1 | BC | 111/128 (87%) | 91 (82%) | 19 (17%) | 1 (1%) | 14 | 50 |
| 1 | DC | 111/128 (87%) | 93 (84%) | 17 (15%) | 1 (1%) | 14 | 50 |
| 1 | EB | 111/128 (87%) | 90 (81%) | 21 (19%) | 0 | 100 | 100 |
| 1 | FA | 111/128 (87%) | 83 (75%) | 27 (24%) | 1 (1%) | 14 | 50 |
| 1 | FB | 111/128 (87%) | 89 (80%) | 22 (20%) | 0 | 100 | 100 |
| 1 | FC | 111/128 (87%) | 87 (78%) | 23 (21%) | 1 (1%) | 14 | 50 |
| 1 | GC | 111/128 (87%) | 98 (88%) | 13 (12%) | 0 | 100 | 100 |
| 1 | HC | 111/128 (87%) | 90 (81%) | 20 (18%) | 1 (1%) | 14 | 50 |
| 1 | IC | 111/128 (87%) | 88 (79%) | 22 (20%) | 1 (1%) | 14 | 50 |
| 1 | K | 111/128 (87%) | 88 (79%) | 23 (21%) | 0 | 100 | 100 |
| 1 | KB | 111/128 (87%) | 93 (84%) | 18 (16%) | 0 | 100 | 100 |
| 1 | L | 111/128 (87%) | 90 (81%) | 21 (19%) | 0 | 100 | 100 |
| 1 | LB | 111/128 (87%) | 91 (82%) | 18 (16%) | 2 (2%) | 7 | 34 |
| 1 | M | 111/128 (87%) | 88 (79%) | 23 (21%) | 0 | 100 | 100 |
| 1 | OB | 111/128 (87%) | 94 (85%) | 16 (14%) | 1 (1%) | 14 | 50 |
| 1 | P | 111/128 (87%) | 96 (86%) | 15 (14%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | PB | 111/128 (87%) | 93 (84%) | 18 (16%) | 0 | 100 | 100 |
| 1 | Q | 111/128 (87%) | 89 (80%) | 22 (20%) | 0 | 100 | 100 |
| 1 | SB | 111/128 (87%) | 94 (85%) | 16 (14%) | 1 (1%) | 14 | 50 |
| 1 | T | 111/128 (87%) | 93 (84%) | 17 (15%) | 1 (1%) | 14 | 50 |
| 1 | TB | 111/128 (87%) | 92 (83%) | 19 (17%) | 0 | 100 | 100 |
| 1 | U | 111/128 (87%) | 94 (85%) | 17 (15%) | 0 | 100 | 100 |
| 1 | UB | 111/128 (87%) | 92 (83%) | 18 (16%) | 1 (1%) | 14 | 50 |
| 1 | V | 111/128 (87%) | 91 (82%) | 19 (17%) | 1 (1%) | 14 | 50 |
| 1 | VB | 111/128 (87%) | 89 (80%) | 21 (19%) | 1 (1%) | 14 | 50 |
| 1 | W | 111/128 (87%) | 92 (83%) | 18 (16%) | 1 (1%) | 14 | 50 |
| 1 | X | 111/128 (87%) | 93 (84%) | 18 (16%) | 0 | 100 | 100 |
| 1 | Y | 111/128 (87%) | 93 (84%) | 18 (16%) | 0 | 100 | 100 |
| 1 | Z | 111/128 (87%) | 92 (83%) | 19 (17%) | 0 | 100 | 100 |
| 2 | CB | 112/129 (87%) | 96 (86%) | 16 (14%) | 0 | 100 | 100 |
| 2 | DB | 112/129 (87%) | 91 (81%) | 21 (19%) | 0 | 100 | 100 |
| 2 | E | 112/129 (87%) | 87 (78%) | 24 (21%) | 1 (1%) | 14 | 50 |
| 2 | F | 112/129 (87%) | 93 (83%) | 19 (17%) | 0 | 100 | 100 |
| 2 | GB | 112/129 (87%) | 97 (87%) | 14 (12%) | 1 (1%) | 14 | 50 |
| 2 | IB | 112/129 (87%) | 93 (83%) | 19 (17%) | 0 | 100 | 100 |
| 3 | A | 116/118 (98%) | 100 (86%) | 16 (14%) | 0 | 100 | 100 |
| 3 | B | 116/118 (98%) | 103 (89%) | 13 (11%) | 0 | 100 | 100 |
| 3 | C | 116/118 (98%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 3 | D | 116/118 (98%) | 101 (87%) | 15 (13%) | 0 | 100 | 100 |
| 3 | I | 116/118 (98%) | 107 (92%) | 9 (8%) | 0 | 100 | 100 |
| 3 | J | 116/118 (98%) | 105 (90%) | 11 (10%) | 0 | 100 | 100 |
| 3 | N | 116/118 (98%) | 106 (91%) | 10 (9%) | 0 | 100 | 100 |
| 3 | O | 116/118 (98%) | 105 (90%) | 11 (10%) | 0 | 100 | 100 |
| 3 | R | 116/118 (98%) | 105 (90%) | 11 (10%) | 0 | 100 | 100 |
| 3 | S | 116/118 (98%) | 100 (86%) | 16 (14%) | 0 | 100 | 100 |
| 3 | a | 116/118 (98%) | 109 (94%) | 7 (6%) | 0 | 100 | 100 |
| 3 | b | 116/118 (98%) | 108 (93%) | 8 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3 | c | 116/118 (98%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 3 | d | 116/118 (98%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 3 | e | 116/118 (98%) | 105 (90%) | 11 (10%) | 0 | 100 | 100 |
| 3 | f | 116/118 (98%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 3 | g | 116/118 (98%) | 107 (92%) | 9 (8%) | 0 | 100 | 100 |
| 3 | h | 116/118 (98%) | 106 (91%) | 10 (9%) | 0 | 100 | 100 |
| 3 | i | 116/118 (98%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 3 | j | 116/118 (98%) | 106 (91%) | 10 (9%) | 0 | 100 | 100 |
| 4 | AD | 119/123 (97%) | 99 (83%) | 20 (17%) | 0 | 100 | 100 |
| 5 | CD | 119/136 (88%) | 104 (87%) | 15 (13%) | 0 | 100 | 100 |
| 5 | FD | 119/136 (88%) | 98 (82%) | 21 (18%) | 0 | 100 | 100 |
| 5 | HD | 115/136 (85%) | 93 (81%) | 21 (18%) | 1 (1%) | 14 | 50 |
| All | All | 6794/7505 (90%) | 5785 (85%) | 991 (15%) | 18 (0%) | 38 | 72 |

5 of 18 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | HD | 159 | PRO |
| 1 | BC | 203 | GLY |
| 1 | FC | 197 | VAL |
| 1 | UB | 157 | LEU |
| 1 | W | 157 | LEU |

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 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 | AB | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | BC | 99/111 (89%) | 99 (100%) | 0 | 100 | 100 |
| 1 | DC | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | EB | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | FA | 99/111 (89%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 1 | FB | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | FC | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | GC | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | HC | 99/111 (89%) | 99 (100%) | 0 | 100 | 100 |
| 1 | IC | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | K | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | KB | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | L | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | LB | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | M | 99/111 (89%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 1 | OB | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | P | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | PB | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | Q | 99/111 (89%) | 99 (100%) | 0 | 100 | 100 |
| 1 | SB | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | T | 98/111 (88%) | 98 (100%) | 0 | 100 | 100 |
| 1 | TB | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | U | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | UB | 99/111 (89%) | 99 (100%) | 0 | 100 | 100 |
| 1 | V | 99/111 (89%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 1 | VB | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 1 | W | 100/111 (90%) | 99 (99%) | 1 (1%) | 73 | 82 |
| 1 | X | 98/111 (88%) | 95 (97%) | 3 (3%) | 35 | 56 |
| 1 | Y | 100/111 (90%) | 98 (98%) | 2 (2%) | 50 | 69 |
| 1 | Z | 100/111 (90%) | 100 (100%) | 0 | 100 | 100 |
| 2 | CB | 101/112 (90%) | 99 (98%) | 2 (2%) | 50 | 69 |
| 2 | DB | 101/112 (90%) | 100 (99%) | 1 (1%) | 73 | 82 |
| 2 | E | 101/112 (90%) | 101 (100%) | 0 | 100 | 100 |
| 2 | F | 101/112 (90%) | 99 (98%) | 2 (2%) | 50 | 69 |
| 2 | GB | 101/112 (90%) | 101 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2 | IB | 101/112 (90%) | 101 (100%) | 0 | 100 | 100 |
| 3 | A | 99/100 (99%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 3 | B | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 3 | C | 99/100 (99%) | 97 (98%) | 2 (2%) | 50 | 69 |
| 3 | D | 99/100 (99%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 3 | I | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 3 | J | 99/100 (99%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 3 | N | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 3 | O | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 3 | R | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 3 | S | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 3 | a | 98/100 (98%) | 97 (99%) | 1 (1%) | 73 | 82 |
| 3 | b | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 3 | c | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 3 | d | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 3 | e | 97/100 (97%) | 96 (99%) | 1 (1%) | 73 | 82 |
| 3 | f | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 3 | g | 99/100 (99%) | 97 (98%) | 2 (2%) | 50 | 69 |
| 3 | h | 98/100 (98%) | 97 (99%) | 1 (1%) | 73 | 82 |
| 3 | i | 98/100 (98%) | 95 (97%) | 3 (3%) | 35 | 56 |
| 3 | j | 98/100 (98%) | 98 (100%) | 0 | 100 | 100 |
| 4 | AD | 107/108 (99%) | 107 (100%) | 0 | 100 | 100 |
| 5 | CD | 107/119 (90%) | 106 (99%) | 1 (1%) | 75 | 83 |
| 5 | FD | 105/119 (88%) | 102 (97%) | 3 (3%) | 37 | 58 |
| 5 | HD | 106/119 (89%) | 106 (100%) | 0 | 100 | 100 |
| All | All | 5990/6467 (93%) | 5952 (99%) | 38 (1%) | 82 | 88 |

5 of 38 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | g | 6 | LEU |
| 5 | FD | 167 | MET |
| 3 | g | 28 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | i | 23 | HIS |
| 5 | FD | 223 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | e | 29 | GLN |
| 5 | CD | 228 | GLN |
| 3 | f | 37 | HIS |
| 4 | AD | 146 | GLN |
| 5 | FD | 192 | ASN |

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 oligosaccharides 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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 5 | HD | 2 |
| 4 | AD | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | AD | 237:GLU | C | 238:GLN | N | 11.07 |
| 1 | HD | 220:GLU | C | 221:ALA | N | 5.35 |
| 1 | HD | 222:VAL | C | 223:ARG | N | 3.25 |

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4508. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.