

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 03:28 am BST

| PDB ID | : | $3 \mathrm{MML}$ | | | | | |
|-----------------------------|---|------------------|---------------|---------------|-----------|------------------|-----------------------------|
| Title | : | Allophanate | Hydrolase | Complex | from | Mycobacterium | $\operatorname{smegmatis},$ |
| | | Msmeg0435-M | 1 meg 0436 | | | | |
| Authors | : | Kaufmann, M | .; Chernishof | , I.; Shin, A | .; Germ | ano, D.; Sawaya, | M.R.; Waldo, |
| | | G.S.; Arbing, | M.A.; Perry, | J.; Eisenber | rg, D.; I | ntegrated Center | for Structure |
| | | and Function | Innovation (| ISFI); TB S | Structur | al Genomics Con | sortium (TB- |
| | | SGC) | | | | | |
| Deposited on | : | 2010-04-20 | | | | | |
| $\operatorname{Resolution}$ | : | 2.50 Å(reporte | ed) | | | | |

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

| MolProbity | : | 4.02b-467 |
|--|---|---|
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| $\operatorname{CCP4}$ | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |
| EDS Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP) | ::::::::::::::::::::::::::::::::::::::: | 2.11 20191225.v01 (using entries in the PDB archive December 25th 2015 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996) 2.11 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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 | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$ |
|-----------------------|--|---|
| R _{free} | 130704 | 4661 (2.50-2.50) |
| Clashscore | 141614 | $5346\ (2.50-2.50)$ |
| Ramachandran outliers | 138981 | 5231(2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

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 <=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 | | |
|-----|-------|--------|------------------|-----|------|
| | | 210 | 2% | | |
| 1 | А | 318 | 80% | 10% | • 9% |
| | | | 3% | | |
| 1 | C | 318 | 82% | 9% | 9% |
| | | | 4% | | |
| 1 | E | 318 | 83% | 8% | 8% |
| | | | 4% | | |
| 1 | G | 318 | 83% | 7% | 9% |
| | | | 6% | | |
| 2 | В | 228 | 80% | 11% | • 8% |
| | | | 15% | | |
| 2 | D | 228 | 81% | 10% | 8% |



| Mol | Chain | Length | Quality of chain | | | |
|-----|-------|--------|------------------------|-----|-----|----|
| 2 | F | 228 | <mark>6%</mark> 82% | 10% | • | 8% |
| 2 | Н | 228 | 82% | 9% | • { | 8% |



$3 \mathrm{MML}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15919 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.

| Mol | Chain | Residues | | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-----|-----|--------------|---------------|---------|---------|-------|
| 1 | Δ | 280 | Total | С | Ν | Ο | \mathbf{S} | \mathbf{Se} | 0 | 0 | 0 |
| | A | 209 | 2160 | 1351 | 395 | 409 | 1 | 4 | 0 | 0 | 0 |
| 1 | C | 290 | Total | С | Ν | Ο | S | Se | 0 | 0 | 0 |
| 1 | | | 2167 | 1356 | 396 | 410 | 1 | 4 | | | 0 |
| 1 | Б | 20.2 | Total | С | Ν | Ο | S | Se | 0 | 0 | 0 |
| | I L | 292 | 2187 | 1370 | 398 | 414 | 1 | 4 | | | 0 |
| 1 | 1 C | 000 | Total | С | Ν | Ο | S | Se | 0 | 0 | 0 |
| I G | 200 | 2149 | 1345 | 391 | 408 | 1 | 4 | 0 | U | U | |

• Molecule 1 is a protein called Allophanate hydrolase subunit 2.

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| А | 295 | LEU | - | expression tag | UNP A0QPL0 |
| А | 296 | GLU | - | expression tag | UNP A0QPL0 |
| А | 297 | SER | - | expression tag | UNP A0QPL0 |
| А | 298 | GLY | - | expression tag | UNP A0QPL0 |
| А | 299 | LYS | - | expression tag | UNP A0QPL0 |
| А | 300 | GLU | - | expression tag | UNP A0QPL0 |
| А | 301 | THR | - | expression tag | UNP A0QPL0 |
| А | 302 | ALA | - | expression tag | UNP A0QPL0 |
| А | 303 | ALA | - | expression tag | UNP A0QPL0 |
| А | 304 | ALA | - | expression tag | UNP A0QPL0 |
| А | 305 | LYS | - | expression tag | UNP A0QPL0 |
| А | 306 | PHE | - | expression tag | UNP A0QPL0 |
| А | 307 | GLU | - | expression tag | UNP A0QPL0 |
| A | 308 | ARG | - | expression tag | UNP A0QPL0 |
| А | 309 | GLN | - | expression tag | UNP A0QPL0 |
| А | 310 | HIS | - | expression tag | UNP A0QPL0 |
| A | 311 | MSE | - | expression tag | UNP A0QPL0 |
| A | 312 | ASP | - | expression tag | UNP A0QPL0 |
| A | 313 | SER | - | expression tag | UNP A0QPL0 |
| A | 314 | SER | - | expression tag | UNP A0QPL0 |
| A | 315 | THR | - | expression tag | UNP A0QPL0 |



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 316 | SER | - | expression tag | UNP A0QPL0 |
| A | 317 | ALA | - | expression tag | UNP A0QPL0 |
| А | 318 | ALA | - | expression tag | UNP A0QPL0 |
| С | 295 | LEU | - | expression tag | UNP A0QPL0 |
| С | 296 | GLU | - | expression tag | UNP A0QPL0 |
| С | 297 | SER | - | expression tag | UNP A0QPL0 |
| С | 298 | GLY | - | expression tag | UNP A0QPL0 |
| С | 299 | LYS | - | expression tag | UNP A0QPL0 |
| С | 300 | GLU | - | expression tag | UNP A0QPL0 |
| С | 301 | THR | - | expression tag | UNP A0QPL0 |
| С | 302 | ALA | - | expression tag | UNP A0QPL0 |
| С | 303 | ALA | - | expression tag | UNP A0QPL0 |
| С | 304 | ALA | - | expression tag | UNP A0QPL0 |
| С | 305 | LYS | - | expression tag | UNP A0QPL0 |
| С | 306 | PHE | - | expression tag | UNP A0QPL0 |
| С | 307 | GLU | - | expression tag | UNP A0QPL0 |
| С | 308 | ARG | - | expression tag | UNP A0QPL0 |
| С | 309 | GLN | - | expression tag | UNP A0QPL0 |
| С | 310 | HIS | - | expression tag | UNP A0QPL0 |
| С | 311 | MSE | - | expression tag | UNP A0QPL0 |
| С | 312 | ASP | - | expression tag | UNP A0QPL0 |
| С | 313 | SER | - | expression tag | UNP A0QPL0 |
| С | 314 | SER | - | expression tag | UNP A0QPL0 |
| С | 315 | THR | - | expression tag | UNP A0QPL0 |
| С | 316 | SER | - | expression tag | UNP A0QPL0 |
| С | 317 | ALA | - | expression tag | UNP A0QPL0 |
| С | 318 | ALA | - | expression tag | UNP A0QPL0 |
| E | 295 | LEU | - | expression tag | UNP A0QPL0 |
| E | 296 | GLU | - | expression tag | UNP A0QPL0 |
| E | 297 | SER | - | expression tag | UNP A0QPL0 |
| E | 298 | GLY | - | expression tag | UNP A0QPL0 |
| E | 299 | LYS | - | expression tag | UNP A0QPL0 |
| E | 300 | GLU | - | expression tag | UNP A0QPL0 |
| E | 301 | THR | - | expression tag | UNP A0QPL0 |
| E | 302 | ALA | - | expression tag | UNP A0QPL0 |
| E | 303 | ALA | - | expression tag | UNP A0QPL0 |
| E | 304 | ALA | - | expression tag | UNP A0QPL0 |
| E | 305 | LYS | - | expression tag | UNP A0QPL0 |
| E | 306 | PHE | - | expression tag | UNP A0QPL0 |
| E | 307 | GLU | - | expression tag | UNP A0QPL0 |
| E | 308 | ARG | - | expression tag | UNP A0QPL0 |
| E | 309 | GLN | - | expression tag | UNP A0QPL0 |



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Е | 310 | HIS | _ | expression tag | UNP A0QPL0 |
| Е | 311 | MSE | _ | expression tag | UNP A0QPL0 |
| Е | 312 | ASP | - | expression tag | UNP A0QPL0 |
| Е | 313 | SER | - | expression tag | UNP A0QPL0 |
| Е | 314 | SER | - | expression tag | UNP A0QPL0 |
| Е | 315 | THR | - | expression tag | UNP A0QPL0 |
| Е | 316 | SER | - | expression tag | UNP A0QPL0 |
| Е | 317 | ALA | - | expression tag | UNP A0QPL0 |
| Е | 318 | ALA | - | expression tag | UNP A0QPL0 |
| G | 295 | LEU | - | expression tag | UNP A0QPL0 |
| G | 296 | GLU | - | expression tag | UNP A0QPL0 |
| G | 297 | SER | _ | expression tag | UNP A0QPL0 |
| G | 298 | GLY | - | expression tag | UNP A0QPL0 |
| G | 299 | LYS | - | expression tag | UNP A0QPL0 |
| G | 300 | GLU | - | expression tag | UNP A0QPL0 |
| G | 301 | THR | - | expression tag | UNP A0QPL0 |
| G | 302 | ALA | - | expression tag | UNP A0QPL0 |
| G | 303 | ALA | - | expression tag | UNP A0QPL0 |
| G | 304 | ALA | - | expression tag | UNP A0QPL0 |
| G | 305 | LYS | - | expression tag | UNP A0QPL0 |
| G | 306 | PHE | - | expression tag | UNP A0QPL0 |
| G | 307 | GLU | - | expression tag | UNP A0QPL0 |
| G | 308 | ARG | - | expression tag | UNP A0QPL0 |
| G | 309 | GLN | _ | expression tag | UNP A0QPL0 |
| G | 310 | HIS | - | expression tag | UNP A0QPL0 |
| G | 311 | MSE | - | expression tag | UNP A0QPL0 |
| G | 312 | ASP | - | expression tag | UNP A0QPL0 |
| G | 313 | SER | _ | expression tag | UNP A0QPL0 |
| G | 314 | SER | - | expression tag | UNP A0QPL0 |
| G | 315 | THR | - | expression tag | UNP A0QPL0 |
| G | 316 | SER | - | expression tag | UNP A0QPL0 |
| G | 317 | ALA | - | expression tag | UNP A0QPL0 |
| G | 318 | ALA | - | expression tag | UNP A0QPL0 |

• Molecule 2 is a protein called Allophanate hydrolase subunit 1.

| Mol | Chain | Residues | | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-----|-----|---|----|---------|---------|-------|
| 2 | В | 210 | Total | С | Ν | Ο | S | Se | 0 | 0 | 0 |
| | D | 210 | 1596 | 1013 | 286 | 293 | 1 | 3 | | | |
| 2 | П | 209 | Total | С | Ν | Ο | S | Se | 0 | 0 | 0 |
| | | | 1591 | 1011 | 285 | 291 | 1 | 3 | | | |
| 2 | Б | 910 | Total | С | Ν | Ο | S | Se | 0 | 0 | 0 |
| | 210 | 1596 | 1013 | 286 | 293 | 1 | 3 | 0 | U | U | |



Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------------|---------|-------|---|
| 2 | Н | 209 | Total 1587 | C 1009 | N 284 | O 290 | ${ m S}$ | ${ m Se} \ 3$ | 0 | 0 | 0 |

There are 76 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference | | |
|-------|---------|----------|--------|----------------|------------|--|--|
| В | -17 | MSE | - | expression tag | UNP A0QPL1 | | |
| В | -16 | GLY | _ | expression tag | UNP A0QPL1 | | |
| В | -15 | SER | - | expression tag | UNP A0QPL1 | | |
| В | -14 | SER | _ | expression tag | UNP A0QPL1 | | |
| В | -13 | HIS | _ | expression tag | UNP A0QPL1 | | |
| В | -12 | HIS | _ | expression tag | UNP A0QPL1 | | |
| В | -11 | HIS | _ | expression tag | UNP A0QPL1 | | |
| В | -10 | HIS | - | expression tag | UNP A0QPL1 | | |
| В | -9 | HIS | - | expression tag | UNP A0QPL1 | | |
| В | -8 | HIS | _ | expression tag | UNP A0QPL1 | | |
| В | -7 | GLU | - | expression tag | UNP A0QPL1 | | |
| В | -6 | ASN | _ | expression tag | UNP A0QPL1 | | |
| В | -5 | LEU | - | expression tag | UNP A0QPL1 | | |
| В | -4 | TYR | _ | expression tag | UNP A0QPL1 | | |
| В | -3 | PHE | - | expression tag | UNP A0QPL1 | | |
| В | -2 | GLN | _ | expression tag | UNP A0QPL1 | | |
| В | -1 | GLY | _ | expression tag | UNP A0QPL1 | | |
| В | 0 | GLY | _ | expression tag | UNP A0QPL1 | | |
| В | 1 | SER | - | expression tag | UNP A0QPL1 | | |
| D | -17 | MSE | _ | expression tag | UNP A0QPL1 | | |
| D | -16 | GLY | _ | expression tag | UNP A0QPL1 | | |
| D | -15 | SER | - | expression tag | UNP A0QPL1 | | |
| D | -14 | SER | - | expression tag | UNP A0QPL1 | | |
| D | -13 | HIS | - | expression tag | UNP A0QPL1 | | |
| D | -12 | HIS | - | expression tag | UNP A0QPL1 | | |
| D | -11 | HIS | - | expression tag | UNP A0QPL1 | | |
| D | -10 | HIS | - | expression tag | UNP A0QPL1 | | |
| D | -9 | HIS | - | expression tag | UNP A0QPL1 | | |
| D | -8 | HIS | _ | expression tag | UNP A0QPL1 | | |
| D | -7 | GLU | - | expression tag | UNP A0QPL1 | | |
| D | -6 | ASN | _ | expression tag | UNP A0QPL1 | | |
| D | -5 | LEU | - | expression tag | UNP A0QPL1 | | |
| D | -4 | TYR | - | expression tag | UNP A0QPL1 | | |
| D | -3 | PHE | - | expression tag | UNP A0QPL1 | | |
| D | -2 | GLN | - | expression tag | UNP A0QPL1 | | |
| D | -1 | GLY | - | expression tag | UNP A0QPL1 | | |



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|------------|--------|----------------|------------|
| D | 0 | GLY | - | expression tag | UNP A0QPL1 |
| D | 1 | SER | - | expression tag | UNP A0QPL1 |
| F | -17 | MSE | - | expression tag | UNP A0QPL1 |
| F | -16 | GLY | - | expression tag | UNP A0QPL1 |
| F | -15 | SER | - | expression tag | UNP A0QPL1 |
| F | -14 | SER | - | expression tag | UNP A0QPL1 |
| F | -13 | HIS | - | expression tag | UNP A0QPL1 |
| F | -12 | HIS | - | expression tag | UNP A0QPL1 |
| F | -11 | HIS | - | expression tag | UNP A0QPL1 |
| F | -10 | HIS | - | expression tag | UNP A0QPL1 |
| F | -9 | HIS | - | expression tag | UNP A0QPL1 |
| F | -8 | HIS | - | expression tag | UNP A0QPL1 |
| F | -7 | GLU | - | expression tag | UNP A0QPL1 |
| F | -6 | ASN | - | expression tag | UNP A0QPL1 |
| F | -5 | LEU | - | expression tag | UNP A0QPL1 |
| F | -4 | TYR | - | expression tag | UNP A0QPL1 |
| F | -3 | PHE | - | expression tag | UNP A0QPL1 |
| F | -2 | GLN | - | expression tag | UNP A0QPL1 |
| F | -1 | GLY | - | expression tag | UNP A0QPL1 |
| F | 0 | GLY | - | expression tag | UNP A0QPL1 |
| F | 1 | SER | - | expression tag | UNP A0QPL1 |
| H | -17 | MSE | - | expression tag | UNP A0QPL1 |
| H | -16 | GLY | - | expression tag | UNP A0QPL1 |
| H | -15 | SER | - | expression tag | UNP A0QPL1 |
| H | -14 | SER | - | expression tag | UNP A0QPL1 |
| H | -13 | HIS | - | expression tag | UNP A0QPL1 |
| H | -12 | HIS | - | expression tag | UNP A0QPL1 |
| H | -11 | HIS | - | expression tag | UNP A0QPL1 |
| H | -10 | HIS | - | expression tag | UNP A0QPL1 |
| H | -9 | HIS | - | expression tag | UNP A0QPL1 |
| H | -8 | HIS | - | expression tag | UNP A0QPL1 |
| H | -7 | GLU | - | expression tag | UNP A0QPL1 |
| H | -6 | ASN | - | expression tag | UNP A0QPL1 |
| H | | | - | expression tag | UNP A0QPL1 |
| | -4 | | - | expression tag | UNP A0QPLI |
| | -3 | PHE CLN | - | expression tag | UNP AUQPLI |
| | -2 | GLN | - | expression tag | UNP AUQPLI |
| | -1 | GLY | - | expression tag | UNP AUQPLI |
| | U 1 | | - | expression tag | UNP AUQPLI |
| L H | | SER | - | expression tag | UNP A0QPLI |

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[•] Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | В | 1 | Total Cl 1 1 | 0 | 0 |

• Molecule 4 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 4 | А | 214 | Total O 214 214 | 0 | 0 |
| 4 | В | 106 | Total O 106 106 | 0 | 0 |
| 4 | С | 166 | Total O 166 166 | 0 | 0 |
| 4 | D | 32 | $\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$ | 0 | 0 |
| 4 | Ε | 157 | Total O 157 157 | 0 | 0 |
| 4 | F | 79 | Total O 79 79 | 0 | 0 |
| 4 | G | 110 | Total O 110 110 | 0 | 0 |
| 4 | Н | 21 | Total O 21 21 | 0 | 0 |



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



83%

• Molecule 1: Allophanate hydrolase subunit 2



7%

9 CLU CLEBU CLEBU

• Molecule 2: Allophanate hydrolase subunit 1



• Molecule 2: Allophanate hydrolase subunit 1

| <u> </u> | | • ••• | | |
|--|--|---|---|----------------------|
| NSE SER SER SER SER SER HIS ASN HIS ASN CLU CLU CLU CLU CLV CLU | R32 150 151 165 165 166 166 166 | P81 082 183 184 184 188 189 198 1108 11105 | G106 M107 T108 P109 A110 Q111 T119 | R122 V123 G127 |
| Chain D: | 81% | | 10% 8% | - |
| 15% | | | | |

F132 F132 R141 R141 R145 P1455 P145 R141 P1455 R145 R141 R145 R146 R172 R145 R146 R146 R172 R146 R172 R146 R182 R183 R183 R184 R182 R184 R182 R184 R182 R184 R184<

• Molecule 2: Allophanate hydrolase subunit 1



V123 R141 T152 Q178 V190 P200 **C210**

• Molecule 2: Allophanate hydrolase subunit 1





4 Data and refinement statistics (i)

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants | 77.48Å 84.24Å 402.07Å | Depositor |
| a, b, c, α , β , γ | 90.00° 90.00° 90.00° | Depositor |
| $\mathbf{B}_{\mathrm{ascolution}}(\mathbf{\hat{A}})$ | 19.92 - 2.50 | Depositor |
| Resolution (A) | 19.92 - 2.50 | EDS |
| % Data completeness | (Not available) $(19.92-2.50)$ | Depositor |
| (in resolution range) | 97.9(19.92-2.50) | EDS |
| R_{merge} | 0.10 | Depositor |
| R _{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | $4.61 (at 2.50 \text{\AA})$ | Xtriage |
| Refinement program | TNT, BUSTER 2.8.0 | Depositor |
| B B. | 0.169 , 0.202 | Depositor |
| 10, 10 free | 0.169 , 0.204 | DCC |
| R_{free} test set | 4507 reflections $(5.01%)$ | wwPDB-VP |
| Wilson B-factor (Å ²) | 36.2 | Xtriage |
| Anisotropy | 0.053 | Xtriage |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$ | 0.32 , 54.8 | EDS |
| L-test for twinning ² | $ < L >=0.49, < L^2>=0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 15919 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

| Mal | Chain | Bond | lengths | Bond | angles |
|-----|-------|------|----------|------|----------|
| | Cham | RMSZ | # Z > 5 | RMSZ | # Z > 5 |
| 1 | А | 0.59 | 0/2208 | 0.75 | 0/3017 |
| 1 | С | 0.54 | 0/2216 | 0.71 | 0/3029 |
| 1 | Е | 0.51 | 0/2237 | 0.71 | 0/3057 |
| 1 | G | 0.48 | 0/2197 | 0.72 | 0/3003 |
| 2 | В | 0.53 | 0/1633 | 0.72 | 0/2228 |
| 2 | D | 0.44 | 0/1628 | 0.68 | 0/2223 |
| 2 | F | 0.48 | 0/1633 | 0.70 | 0/2228 |
| 2 | Н | 0.43 | 0/1624 | 0.67 | 0/2218 |
| All | All | 0.51 | 0/15376 | 0.71 | 0/21003 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | А | 2160 | 0 | 2132 | 14 | 0 |
| 1 | С | 2167 | 0 | 2139 | 13 | 0 |
| 1 | Е | 2187 | 0 | 2154 | 9 | 0 |
| 1 | G | 2149 | 0 | 2119 | 9 | 0 |
| 2 | В | 1596 | 0 | 1587 | 9 | 0 |



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | D | 1591 | 0 | 1584 | 9 | 0 |
| 2 | F | 1596 | 0 | 1587 | 8 | 0 |
| 2 | Н | 1587 | 0 | 1578 | 10 | 0 |
| 3 | В | 1 | 0 | 0 | 1 | 0 |
| 4 | А | 214 | 0 | 0 | 2 | 0 |
| 4 | В | 106 | 0 | 0 | 0 | 0 |
| 4 | С | 166 | 0 | 0 | 1 | 0 |
| 4 | D | 32 | 0 | 0 | 0 | 0 |
| 4 | Е | 157 | 0 | 0 | 1 | 0 |
| 4 | F | 79 | 0 | 0 | 0 | 0 |
| 4 | G | 110 | 0 | 0 | 0 | 0 |
| 4 | Н | 21 | 0 | 0 | 0 | 0 |
| All | All | 15919 | 0 | 14880 | 72 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom 1 | Atom 9 | Interatomic | Clash |
|------------------|-----------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:216:MSE:HE3 | 1:A:217:PRO:HD2 | 1.55 | 0.89 |
| 1:C:216:MSE:HE3 | 1:C:217:PRO:HD2 | 1.65 | 0.79 |
| 2:H:107:MSE:HE2 | 2:H:111:GLN:HB3 | 1.62 | 0.79 |
| 1:G:216:MSE:HE3 | 1:G:217:PRO:HD2 | 1.66 | 0.77 |
| 2:B:107:MSE:HE2 | 2:B:111:GLN:HB3 | 1.69 | 0.73 |
| 2:D:107:MSE:HE2 | 2:D:111:GLN:HB3 | 1.72 | 0.72 |
| 2:F:26:ALA:HB2 | 2:F:74:GLU:HB3 | 1.75 | 0.68 |
| 1:G:233:THR:HG22 | 2:H:52:LYS:HD3 | 1.74 | 0.67 |
| 1:C:95:ILE:HD12 | 1:C:160:PHE:HZ | 1.59 | 0.66 |
| 2:D:123:VAL:HG22 | 2:D:200:PRO:HA | 1.77 | 0.65 |
| 1:C:233:THR:HG22 | 2:D:52:LYS:HD3 | 1.78 | 0.64 |
| 1:C:95:ILE:CD1 | 1:C:160:PHE:HZ | 2.09 | 0.64 |
| 2:F:29:GLU:HB3 | 2:F:72:ARG:HD3 | 1.79 | 0.63 |
| 2:B:123:VAL:HG22 | 2:B:200:PRO:HA | 1.80 | 0.63 |
| 2:F:123:VAL:HG22 | 2:F:200:PRO:HA | 1.82 | 0.62 |
| 1:A:47:VAL:O | 1:A:120:ARG:HD3 | 2.00 | 0.62 |
| 2:H:123:VAL:HG22 | 2:H:200:PRO:HA | 1.81 | 0.61 |
| 1:A:52:GLU:HG3 | 4:A:425:HOH:O | 2.02 | 0.59 |
| 1:C:95:ILE:HD12 | 1:C:160:PHE:CZ | 2.38 | 0.58 |
| 2:B:168:VAL:HB | 2:B:187:MSE:HE2 | 1.86 | 0.58 |
| 1:C:234:ARG:NH2 | 4:C:328:HOH:O | 2.35 | 0.57 |



| | i i i i i i i i i i i i i i i i i i i | Interatomic | Clash | |
|------------------|---------------------------------------|-------------------------|-------------|--|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 2:D:199:THR:H | 2:D:202:MSE:SE | 2.38 | 0.57 | |
| 1:E:201:LEU:HD11 | 1:G:203:THR:HG22 | 1.87 | 0.56 | |
| 2:F:36:LEU:HD23 | 2:F:65:ARG:NH1 | 2.21 | 0.55 | |
| 1:G:163:LEU:H | 1:G:163:LEU:HD13 | 1.71 | 0.55 | |
| 1:E:95:ILE:HD11 | 1:E:160:PHE:HZ | 1.74 | 0.53 | |
| 1:E:77:THR:HG22 | 1:E:93:ASN:HD22 | 1.76 | 0.51 | |
| 1:A:233:THR:HG22 | 2:B:52:LYS:HD3 | 1.92 | 0.51 | |
| 1:A:77:THR:HG22 | 1:A:93:ASN:HD22 | 1.76 | 0.51 | |
| 1:E:233:THR:HG22 | 2:F:52:LYS:HD3 | 1.93 | 0.50 | |
| 2:F:107:MSE:HE2 | 2:F:111:GLN:HB3 | 1.94 | 0.50 | |
| 2:D:60:ALA:HA | 2:H:106:GLY:O | 2.12 | 0.50 | |
| 1:A:194:ILE:HD13 | 4:A:543:HOH:O | 2.10 | 0.49 | |
| 1:A:201:LEU:HG | 1:C:214:VAL:HG21 | 1.95 | 0.49 | |
| 2:D:122:ARG:HD2 | 2:D:203:TRP:CZ2 | 2.47 | 0.49 | |
| 1:A:137:MSE:HE2 | 1:A:253:PRO:HD3 | 1.94 | 0.49 | |
| 1:C:27:MSE:HE1 | 2:D:195:PRO:HD2 | 1.96 | 0.48 | |
| 1:G:77:THR:HG22 | 1:G:93:ASN:HD22 | 1.78 | 0.48 | |
| 2:D:63:ARG:HD3 | 2:H:106:GLY:O | 2.13 | 0.48 | |
| 1:G:41:THR:HG22 | 1:G:45:ARG:HH21 | 1.79 | 0.48 | |
| 1:G:43:ALA:HB1 | 1:G:118:ALA:HB2 | 1.96 | 0.47 | |
| 2:H:199:THR:O | 2:H:202:MSE:HB2 | 2.15 | 0.47 | |
| 2:H:22:ALA:HB1 | 2:H:76:ILE:HG23 | 1.97 | 0.47 | |
| 1:C:95:ILE:CD1 | 1:C:160:PHE:CZ | 2.96 | 0.46 | |
| 2:B:56:PRO:HD2 | 3:B:211:CL:CL | 2.53 | 0.46 | |
| 1:A:191:ASP:HB3 | 1:A:194:ILE:HD12 | 1.97 | 0.45 | |
| 1:C:77:THR:HG22 | 1:C:93:ASN:HD22 | 1.80 | 0.45 | |
| 1:A:285:TRP:CZ2 | 1:A:289:ARG:HD3 | 2.52 | 0.44 | |
| 1:E:45:ARG:NH2 | 4:E:560:HOH:O | 2.51 | 0.44 | |
| 2:F:36:LEU:HD23 | 2:F:65:ARG:HH11 | 1.82 | 0.44 | |
| 1:C:41:THR:HG22 | 1:C:45:ARG:HH21 | 1.83 | 0.43 | |
| 1:G:83:PRO:HB2 | 1:G:90:PHE:CZ | 2.54 | 0.42 | |
| 2:B:80:PRO:HA | 2:B:81:PRO:HD3 | 1.94 | 0.42 | |
| 1:E:83:PRO:HB2 | 1:E:90:PHE:CZ | 2.55 | 0.42 | |
| 2:B:71:VAL:HG22 | 2:B:73:PRO:HD2 | 2.01 | 0.41 | |
| 2:B:85:VAL:HG21 | 2:B:205:GLN:HB2 | 2.02 | 0.41 | |
| 1:A:83:PRO:HB2 | 1:A:90:PHE:CZ | 2.55 | 0.41 | |
| 2:F:27:TRP:CE2 | 2:F:71:VAL:HB | 2.55 | 0.41 | |
| 2:H:85:VAL:HG21 | 2:H:205:GLN:HB2 | 2.02 | 0.41 | |
| 2:B:127:GLY:O | 2:B:132:PHE:HB3 | 2.21 | 0.41 | |
| 1:C:83:PRO:HB2 | 1:C:90:PHE:CZ | 2.55 | 0.41 | |
| 1:A:73:ALA:HB1 | 1:A:95:ILE:HD11 | 2.03 | 0.41 | |



| Atom-1 | Atom-2 | ${f Interatomic} \ {f distance} \ ({ m \AA})$ | Clash overlap (Å) |
|------------------|------------------|---|----------------------|
| 2:H:199:THR:H | 2:H:202:MSE:SE | 2.54 | 0.40 |
| 1:A:176:VAL:HG21 | 1:A:275:VAL:HG22 | 2.04 | 0.40 |
| 1:A:33:GLY:HA2 | 1:A:133:SER:OG | 2.21 | 0.40 |
| 1:C:61:GLY:HA3 | 1:C:107:GLY:O | 2.21 | 0.40 |
| 1:G:202:VAL:HG21 | 1:G:275:VAL:CG1 | 2.51 | 0.40 |
| 1:E:33:GLY:HA2 | 1:E:133:SER:OG | 2.20 | 0.40 |
| 1:E:41:THR:HG22 | 1:E:45:ARG:HH21 | 1.85 | 0.40 |
| 2:D:127:GLY:O | 2:D:132:PHE:HB3 | 2.22 | 0.40 |
| 1:E:18:ASP:HA | 1:E:40:HIS:CE1 | 2.56 | 0.40 |
| 2:H:80:PRO:HA | 2:H:81:PRO:HD3 | 1.96 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | Perce | entiles |
|-----|-------|-----------------|------------|---------|----------|-------|---------|
| 1 | А | 287/318~(90%) | 280~(98%) | 7(2%) | 0 | 100 | 100 |
| 1 | С | 288/318~(91%) | 281~(98%) | 7(2%) | 0 | 100 | 100 |
| 1 | E | 290/318~(91%) | 284 (98%) | 6 (2%) | 0 | 100 | 100 |
| 1 | G | 286/318~(90%) | 278~(97%) | 8 (3%) | 0 | 100 | 100 |
| 2 | В | 208/228~(91%) | 200~(96%) | 7(3%) | 1 (0%) | 29 | 48 |
| 2 | D | 207/228~(91%) | 203~(98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | F | 208/228~(91%) | 200~(96%) | 7(3%) | 1 (0%) | 29 | 48 |
| 2 | Н | 207/228 (91%) | 202 (98%) | 5 (2%) | 0 | 100 | 100 |
| All | All | 1981/2184~(91%) | 1928 (97%) | 51 (3%) | 2(0%) | 51 | 73 |

All (2) Ramachandran outliers are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | В | 73 | PRO |
| 2 | F | 83 | ASP |

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | Perce | entiles |
|-----|-------|-----------------|------------|----------|-------|---------|
| 1 | А | 232/249~(93%) | 218~(94%) | 14~(6%) | 19 | 37 |
| 1 | С | 233/249~(94%) | 219~(94%) | 14~(6%) | 19 | 37 |
| 1 | Е | 235/249~(94%) | 221 (94%) | 14~(6%) | 19 | 37 |
| 1 | G | 231/249~(93%) | 221~(96%) | 10 (4%) | 29 | 53 |
| 2 | В | 164/175~(94%) | 151 (92%) | 13 (8%) | 12 | 24 |
| 2 | D | 164/175~(94%) | 153~(93%) | 11 (7%) | 16 | 31 |
| 2 | F | 164/175~(94%) | 152~(93%) | 12 (7%) | 14 | 27 |
| 2 | Η | 163/175~(93%) | 153 (94%) | 10(6%) | 18 | 36 |
| All | All | 1586/1696~(94%) | 1488 (94%) | 98 (6%) | 18 | 35 |

All (98) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 30 | THR |
| 1 | А | 52 | GLU |
| 1 | А | 82 | ASP |
| 1 | А | 106 | LEU |
| 1 | А | 136 | VAL |
| 1 | А | 137 | MSE |
| 1 | А | 158 | ASP |
| 1 | А | 164 | ASP |
| 1 | А | 165 | GLN |
| 1 | А | 203 | THR |
| 1 | А | 212 | ARG |
| 1 | А | 218 | LEU |
| 1 | А | 267 | GLU |
| 1 | А | 290 | ARG |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | В | 2 | THR |
| 2 | В | 50 | LEU |
| 2 | В | 57 | ARG |
| 2 | В | 66 | LEU |
| 2 | В | 69 | LEU |
| 2 | В | 70 | ARG |
| 2 | В | 78 | HIS |
| 2 | В | 85 | VAL |
| 2 | В | 123 | VAL |
| 2 | В | 141 | ARG |
| 2 | В | 152 | THR |
| 2 | В | 178 | GLN |
| 2 | В | 190 | VAL |
| 1 | С | 30 | THR |
| 1 | С | 52 | GLU |
| 1 | С | 82 | ASP |
| 1 | С | 106 | LEU |
| 1 | С | 136 | VAL |
| 1 | С | 137 | MSE |
| 1 | С | 159 | GLU |
| 1 | С | 163 | LEU |
| 1 | С | 164 | ASP |
| 1 | С | 165 | GLN |
| 1 | С | 203 | THR |
| 1 | С | 212 | ARG |
| 1 | С | 218 | LEU |
| 1 | С | 289 | ARG |
| 2 | D | 32 | ARG |
| 2 | D | 50 | LEU |
| 2 | D | 57 | ARG |
| 2 | D | 66 | LEU |
| 2 | D | 85 | VAL |
| 2 | D | 123 | VAL |
| 2 | D | 141 | ARG |
| 2 | D | 146 | ARG |
| 2 | D | 152 | THR |
| 2 | D | 178 | GLN |
| 2 | D | 190 | VAL |
| 1 | Е | 30 | THR |
| 1 | Е | 38 | ARG |
| 1 | Е | 52 | GLU |
| 1 | Е | 82 | ASP |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Е | 106 | LEU |
| 1 | Е | 136 | VAL |
| 1 | Е | 137 | MSE |
| 1 | Е | 158 | ASP |
| 1 | Е | 159 | GLU |
| 1 | Е | 164 | ASP |
| 1 | Е | 165 | GLN |
| 1 | Е | 201 | LEU |
| 1 | Е | 212 | ARG |
| 1 | Е | 218 | LEU |
| 2 | F | 32 | ARG |
| 2 | F | 50 | LEU |
| 2 | F | 57 | ARG |
| 2 | F | 66 | LEU |
| 2 | F | 69 | LEU |
| 2 | F | 83 | ASP |
| 2 | F | 85 | VAL |
| 2 | F | 123 | VAL |
| 2 | F | 141 | ARG |
| 2 | F | 152 | THR |
| 2 | F | 178 | GLN |
| 2 | F | 190 | VAL |
| 1 | G | 30 | THR |
| 1 | G | 52 | GLU |
| 1 | G | 82 | ASP |
| 1 | G | 106 | LEU |
| 1 | G | 137 | MSE |
| 1 | G | 163 | LEU |
| 1 | G | 165 | GLN |
| 1 | G | 212 | ARG |
| 1 | G | 218 | LEU |
| 1 | G | 289 | ARG |
| 2 | Н | 32 | ARG |
| 2 | Н | 50 | LEU |
| 2 | Н | 66 | LEU |
| 2 | Н | 123 | VAL |
| 2 | Н | 141 | ARG |
| 2 | Н | 146 | ARG |
| 2 | Н | 152 | THR |
| 2 | Н | 178 | GLN |
| 2 | H | 190 | VAL |
| 2 | Н | 202 | MSE |

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Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 1 | А | 93 | ASN |
| 1 | С | 93 | ASN |
| 1 | Е | 93 | ASN |
| 1 | G | 93 | 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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 | $\mathbf{OWAB}(\mathbf{A}^2)$ | Q<0.9 |
|-----|-------|-----------------|-----------|----------------|-------------------------------|-------|
| 1 | А | 285/318~(89%) | -0.61 | 5 (1%) 68 71 | 15, 25, 54, 111 | 0 |
| 1 | С | 286/318~(89%) | -0.45 | 11 (3%) 40 43 | 17, 32, 73, 115 | 0 |
| 1 | E | 288/318~(90%) | -0.44 | 13 (4%) 33 36 | 24, 35, 70, 116 | 0 |
| 1 | G | 284/318~(89%) | -0.27 | 12 (4%) 36 39 | 24, 42, 83, 132 | 0 |
| 2 | В | 207/228~(90%) | -0.18 | 13 (6%) 20 21 | 18, 39, 107, 139 | 0 |
| 2 | D | 206/228~(90%) | 0.79 | 34~(16%) 1 1 | 32, 84, 155, 181 | 0 |
| 2 | F | 207/228~(90%) | -0.04 | 14 (6%) 17 17 | 29, 47, 100, 121 | 0 |
| 2 | Н | 206/228~(90%) | 0.62 | 30 (14%) 2 2 | 46, 73, 123, 146 | 0 |
| All | All | 1969/2184~(90%) | -0.13 | 132 (6%) 17 18 | 15, 41, 113, 181 | 0 |

All (132) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | F | 76 | ILE | 11.3 |
| 2 | F | 77 | THR | 10.5 |
| 2 | F | 75 | ALA | 7.1 |
| 2 | В | 76 | ILE | 6.0 |
| 2 | Н | 81 | PRO | 5.8 |
| 1 | Е | 164 | ASP | 5.8 |
| 2 | F | 73 | PRO | 5.7 |
| 2 | В | 74 | GLU | 5.6 |
| 2 | D | 85 | VAL | 5.5 |
| 2 | D | 152 | THR | 5.3 |
| 2 | Н | 82 | GLY | 5.2 |
| 1 | С | 291 | PRO | 5.2 |
| 2 | Н | 148 | ALA | 5.1 |
| 2 | D | 82 | GLY | 5.0 |
| 2 | В | 81 | PRO | 4.8 |
| 2 | В | 83 | ASP | 4.8 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | F | 78 | HIS | 4.8 |
| 1 | G | 166 | ALA | 4.7 |
| 1 | А | 161 | PRO | 4.7 |
| 1 | С | 164 | ASP | 4.7 |
| 2 | Н | 68 | LYS | 4.7 |
| 2 | Н | 85 | VAL | 4.6 |
| 2 | D | 180 | ILE | 4.6 |
| 2 | Н | 152 | THR | 4.6 |
| 2 | D | 103 | SER | 4.6 |
| 2 | В | 72 | ARG | 4.5 |
| 2 | Н | 149 | GLU | 4.5 |
| 1 | G | 163 | LEU | 4.4 |
| 2 | В | 73 | PRO | 4.3 |
| 2 | F | 1 | SER | 4.3 |
| 2 | D | 99 | HIS | 4.3 |
| 2 | D | 207 | ARG | 3.9 |
| 2 | D | 176 | GLY | 3.9 |
| 2 | D | 181 | GLY | 3.8 |
| 2 | В | 82 | GLY | 3.8 |
| 1 | Ε | 293 | GLU | 3.8 |
| 1 | G | 162 | GLU | 3.7 |
| 2 | Н | 73 | PRO | 3.7 |
| 2 | D | 84 | ARG | 3.7 |
| 2 | В | 75 | ALA | 3.7 |
| 2 | D | 149 | GLU | 3.7 |
| 1 | G | 159 | GLU | 3.6 |
| 2 | Н | 83 | ASP | 3.6 |
| 2 | Н | 84 | ARG | 3.6 |
| 1 | С | 167 | PRO | 3.6 |
| 1 | С | 290 | ARG | 3.6 |
| 1 | G | 224 | ASP | 3.6 |
| 2 | D | 141 | ARG | 3.6 |
| 2 | D | 83 | ASP | 3.5 |
| 1 | А | 160 | PHE | 3.5 |
| 2 | D | 209 | VAL | 3.5 |
| 2 | F | 82 | GLY | 3.5 |
| 1 | E | 292 | PHE | 3.5 |
| 1 | E | 167 | PRO | 3.4 |
| 1 | E | 169 | ALA | 3.4 |
| 2 | D | 179 | LEU | 3.4 |
| 1 | С | 166 | ALA | 3.4 |
| 2 | Н | 76 | ILE | 3.4 |



| Conti | nued from | n previ | ous page | |
|-------|-----------|---------|----------|------|
| Mol | Chain | Res | Type | RSRZ |
| 1 | С | 163 | LEU | 3.4 |
| 1 | Е | 163 | LEU | 3.4 |
| 2 | Н | 77 | THR | 3.3 |
| 1 | G | 161 | PRO | 3.3 |
| 2 | D | 182 | HIS | 3.2 |
| 1 | Е | 166 | ALA | 3.2 |
| 2 | D | 172 | GLN | 3.2 |
| 1 | А | 164 | ASP | 3.2 |
| 2 | Η | 37 | LEU | 3.2 |
| 2 | В | 148 | ALA | 3.1 |
| 1 | Е | 160 | PHE | 3.1 |
| 2 | B | 149 | GLU | 3.1 |
| 2 | F | 83 | ASP | 3.1 |
| 2 | D | 109 | PRO | 3.0 |
| 2 | В | 78 | HIS | 3.0 |
| 1 | G | 158 | ASP | 3.0 |
| 2 | В | 84 | ARG | 2.9 |
| 2 | D | 104 | LEU | 2.9 |
| 2 | F | 74 | GLU | 2.9 |
| 2 | Н | 64 | GLN | 2.9 |
| 2 | D | 148 | ALA | 2.9 |
| 2 | D | 208 | ALA | 2.9 |
| 2 | D | 151 | ARG | 2.9 |
| 1 | С | 226 | GLN | 2.9 |
| 2 | D | 106 | GLY | 2.9 |
| 2 | D | 160 | ALA | 2.9 |
| 2 | H | 78 | HIS | 2.9 |
| 1 | С | 162 | GLU | 2.8 |
| 2 | H | 146 | ARG | 2.8 |
| 2 | H | 75 | ALA | 2.7 |
| 2 | F | 84 | ARG | 2.7 |
| 2 | H | 72 | ARG | 2.7 |
| 2 | F | 80 | PRO | 2.7 |
| 1 | A | 290 | ARG | 2.7 |
| 1 | E | 158 | ASP | 2.7 |
| 2 | D | 184 | ASP | 2.7 |
| 2 | D | 105 | THR | 2.7 |
| 1 | G | 165 | GLN | 2.7 |
| 2 | H | 137 | ASP | 2.6 |
| 2 | H | 33 | GLU | 2.5 |
| 1 | G | 157 | THR | 2.5 |
| 1 | A A | 166 | ALA | 2.5 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 119 | THR | 2.5 |
| 2 | D | 159 | VAL | 2.4 |
| 1 | G | 164 | ASP | 2.4 |
| 2 | Н | 176 | GLY | 2.4 |
| 2 | Н | 184 | ASP | 2.4 |
| 1 | С | 224 | ASP | 2.4 |
| 1 | G | 160 | PHE | 2.4 |
| 2 | F | 79 | GLN | 2.4 |
| 1 | Е | 161 | PRO | 2.4 |
| 2 | Н | 174 | PRO | 2.4 |
| 1 | G | 287 | TYR | 2.3 |
| 2 | Н | 35 | GLU | 2.3 |
| 1 | С | 159 | GLU | 2.3 |
| 1 | Е | 291 | PRO | 2.3 |
| 2 | D | 144 | VAL | 2.3 |
| 2 | F | 210 | GLY | 2.3 |
| 2 | Н | 186 | VAL | 2.3 |
| 2 | D | 81 | PRO | 2.2 |
| 2 | Н | 167 | GLY | 2.2 |
| 2 | D | 194 | LYS | 2.2 |
| 2 | Н | 201 | GLY | 2.2 |
| 1 | С | 158 | ASP | 2.1 |
| 1 | Е | 162 | GLU | 2.1 |
| 1 | Е | 290 | ARG | 2.1 |
| 2 | D | 185 | ALA | 2.1 |
| 2 | Н | 168 | VAL | 2.1 |
| 2 | F | 49 | VAL | 2.1 |
| 2 | D | 168 | VAL | 2.0 |
| 2 | D | 98 | LEU | 2.0 |
| 2 | В | 77 | THR | 2.0 |
| 2 | Н | 194 | LYS | 2.0 |
| 2 | Н | 104 | LEU | 2.0 |

Continued from previous page...

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | $\mathbf{B}	extsf{-}\mathbf{B}	extsf{-}\mathbf{factors}(\mathbf{A}^2)$ | Q<0.9 |
|-----|------|-------|-----|-------|------|------|--|-------|
| 3 | CL | В | 211 | 1/1 | 0.99 | 0.05 | $41,\!41,\!41,\!41$ | 0 |

6.5 Other polymers (i)

There are no such residues in this entry.

