# W O R L D W I D E
# wwPDB
## P R O T E I N   D A T A   B A N K

# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2017 – 11:35 PM EDT

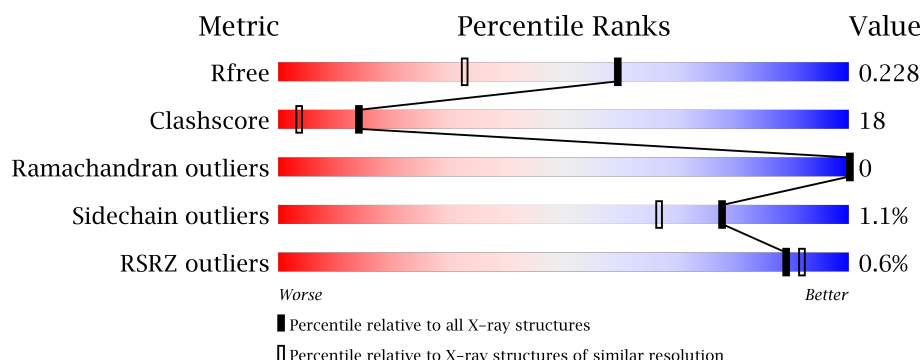|  |  |  |
|---|---|---|
| PDB ID | : | 4P7T |
| Title | : | Structural insights into higher-order assembly and function of the bacterial microcompartment protein PduA |
| Authors | : | Pickersgill, R.W.; Frank, S.; Pang, A.; Warren, M.J. |
| Deposited on | : | unknown |
| Resolution | : | 1.72 Å(reported) |

# 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 1.72 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 | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.228 |
| Clashscore | | 18 |
| Ramachandran outliers | | 0 |
| Sidechain outliers | | 1.1% |
| RSRZ outliers | | 0.6% |

*Worse*　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|:---:|:---:|
| $R_{free}$ | 100719 | 4385 (1.74-1.70) |
| Clashscore | 112137 | 4841 (1.74-1.70) |
| Ramachandran outliers | 110173 | 4771 (1.74-1.70) |
| Sidechain outliers | 110143 | 4771 (1.74-1.70) |
| RSRZ outliers | 101464 | 4426 (1.74-1.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 115 | 2% / 50% / 22% / · / 26% |
| 1 | B | 115 | 64% / 10% / · / 25% |
| 1 | C | 115 | 53% / 11% / 36% |
| 1 | D | 115 | .% / 54% / 18% / · / 25% |
| 1 | E | 115 | 58% / 15% / · / 25% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 115 | |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3837 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 Polyhedral bodies.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 600 | 373 | 106 | 118 | 3 | | | |
| 1 | B | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 606 | 379 | 106 | 118 | 3 | | | |
| 1 | C | 74 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 512 | 319 | 91 | 99 | 3 | | | |
| 1 | D | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 606 | 379 | 106 | 118 | 3 | | | |
| 1 | E | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 606 | 379 | 106 | 118 | 3 | | | |
| 1 | F | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 590 | 369 | 104 | 114 | 3 | | | |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | -1 | GLY | - | expression tag | UNP B1VB62 |
| A | 0 | SER | - | expression tag | UNP B1VB62 |
| A | 26 | ASP | LYS | engineered mutation | UNP B1VB62 |
| A | 93 | ARG | - | expression tag | UNP B1VB62 |
| A | 94 | LEU | - | expression tag | UNP B1VB62 |
| A | 95 | VAL | - | expression tag | UNP B1VB62 |
| A | 96 | LYS | - | expression tag | UNP B1VB62 |
| A | 97 | ASP | - | expression tag | UNP B1VB62 |
| A | 98 | PRO | - | expression tag | UNP B1VB62 |
| A | 99 | ALA | - | expression tag | UNP B1VB62 |
| A | 100 | ALA | - | expression tag | UNP B1VB62 |
| A | 101 | ASN | - | expression tag | UNP B1VB62 |
| A | 102 | LYS | - | expression tag | UNP B1VB62 |
| A | 103 | ALA | - | expression tag | UNP B1VB62 |
| A | 104 | ARG | - | expression tag | UNP B1VB62 |
| A | 105 | LYS | - | expression tag | UNP B1VB62 |
| A | 106 | GLU | - | expression tag | UNP B1VB62 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 107 | ALA | - | expression tag | UNP B1VB62 |
| A | 108 | GLU | - | expression tag | UNP B1VB62 |
| A | 109 | LEU | - | expression tag | UNP B1VB62 |
| A | 110 | ALA | - | expression tag | UNP B1VB62 |
| A | 111 | ALA | - | expression tag | UNP B1VB62 |
| A | 112 | ALA | - | expression tag | UNP B1VB62 |
| A | 113 | THR | - | expression tag | UNP B1VB62 |
| B | -1 | GLY | - | expression tag | UNP B1VB62 |
| B | 0 | SER | - | expression tag | UNP B1VB62 |
| B | 26 | ASP | LYS | engineered mutation | UNP B1VB62 |
| B | 93 | ARG | - | expression tag | UNP B1VB62 |
| B | 94 | LEU | - | expression tag | UNP B1VB62 |
| B | 95 | VAL | - | expression tag | UNP B1VB62 |
| B | 96 | LYS | - | expression tag | UNP B1VB62 |
| B | 97 | ASP | - | expression tag | UNP B1VB62 |
| B | 98 | PRO | - | expression tag | UNP B1VB62 |
| B | 99 | ALA | - | expression tag | UNP B1VB62 |
| B | 100 | ALA | - | expression tag | UNP B1VB62 |
| B | 101 | ASN | - | expression tag | UNP B1VB62 |
| B | 102 | LYS | - | expression tag | UNP B1VB62 |
| B | 103 | ALA | - | expression tag | UNP B1VB62 |
| B | 104 | ARG | - | expression tag | UNP B1VB62 |
| B | 105 | LYS | - | expression tag | UNP B1VB62 |
| B | 106 | GLU | - | expression tag | UNP B1VB62 |
| B | 107 | ALA | - | expression tag | UNP B1VB62 |
| B | 108 | GLU | - | expression tag | UNP B1VB62 |
| B | 109 | LEU | - | expression tag | UNP B1VB62 |
| B | 110 | ALA | - | expression tag | UNP B1VB62 |
| B | 111 | ALA | - | expression tag | UNP B1VB62 |
| B | 112 | ALA | - | expression tag | UNP B1VB62 |
| B | 113 | THR | - | expression tag | UNP B1VB62 |
| C | -1 | GLY | - | expression tag | UNP B1VB62 |
| C | 0 | SER | - | expression tag | UNP B1VB62 |
| C | 26 | ASP | LYS | engineered mutation | UNP B1VB62 |
| C | 93 | ARG | - | expression tag | UNP B1VB62 |
| C | 94 | LEU | - | expression tag | UNP B1VB62 |
| C | 95 | VAL | - | expression tag | UNP B1VB62 |
| C | 96 | LYS | - | expression tag | UNP B1VB62 |
| C | 97 | ASP | - | expression tag | UNP B1VB62 |
| C | 98 | PRO | - | expression tag | UNP B1VB62 |
| C | 99 | ALA | - | expression tag | UNP B1VB62 |
| C | 100 | ALA | - | expression tag | UNP B1VB62 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| C | 101 | ASN | - | expression tag | UNP B1VB62 |
| C | 102 | LYS | - | expression tag | UNP B1VB62 |
| C | 103 | ALA | - | expression tag | UNP B1VB62 |
| C | 104 | ARG | - | expression tag | UNP B1VB62 |
| C | 105 | LYS | - | expression tag | UNP B1VB62 |
| C | 106 | GLU | - | expression tag | UNP B1VB62 |
| C | 107 | ALA | - | expression tag | UNP B1VB62 |
| C | 108 | GLU | - | expression tag | UNP B1VB62 |
| C | 109 | LEU | - | expression tag | UNP B1VB62 |
| C | 110 | ALA | - | expression tag | UNP B1VB62 |
| C | 111 | ALA | - | expression tag | UNP B1VB62 |
| C | 112 | ALA | - | expression tag | UNP B1VB62 |
| C | 113 | THR | - | expression tag | UNP B1VB62 |
| D | -1 | GLY | - | expression tag | UNP B1VB62 |
| D | 0 | SER | - | expression tag | UNP B1VB62 |
| D | 26 | ASP | LYS | engineered mutation | UNP B1VB62 |
| D | 93 | ARG | - | expression tag | UNP B1VB62 |
| D | 94 | LEU | - | expression tag | UNP B1VB62 |
| D | 95 | VAL | - | expression tag | UNP B1VB62 |
| D | 96 | LYS | - | expression tag | UNP B1VB62 |
| D | 97 | ASP | - | expression tag | UNP B1VB62 |
| D | 98 | PRO | - | expression tag | UNP B1VB62 |
| D | 99 | ALA | - | expression tag | UNP B1VB62 |
| D | 100 | ALA | - | expression tag | UNP B1VB62 |
| D | 101 | ASN | - | expression tag | UNP B1VB62 |
| D | 102 | LYS | - | expression tag | UNP B1VB62 |
| D | 103 | ALA | - | expression tag | UNP B1VB62 |
| D | 104 | ARG | - | expression tag | UNP B1VB62 |
| D | 105 | LYS | - | expression tag | UNP B1VB62 |
| D | 106 | GLU | - | expression tag | UNP B1VB62 |
| D | 107 | ALA | - | expression tag | UNP B1VB62 |
| D | 108 | GLU | - | expression tag | UNP B1VB62 |
| D | 109 | LEU | - | expression tag | UNP B1VB62 |
| D | 110 | ALA | - | expression tag | UNP B1VB62 |
| D | 111 | ALA | - | expression tag | UNP B1VB62 |
| D | 112 | ALA | - | expression tag | UNP B1VB62 |
| D | 113 | THR | - | expression tag | UNP B1VB62 |
| E | -1 | GLY | - | expression tag | UNP B1VB62 |
| E | 0 | SER | - | expression tag | UNP B1VB62 |
| E | 26 | ASP | LYS | engineered mutation | UNP B1VB62 |
| E | 93 | ARG | - | expression tag | UNP B1VB62 |
| E | 94 | LEU | - | expression tag | UNP B1VB62 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| E | 95 | VAL | - | expression tag | UNP B1VB62 |
| E | 96 | LYS | - | expression tag | UNP B1VB62 |
| E | 97 | ASP | - | expression tag | UNP B1VB62 |
| E | 98 | PRO | - | expression tag | UNP B1VB62 |
| E | 99 | ALA | - | expression tag | UNP B1VB62 |
| E | 100 | ALA | - | expression tag | UNP B1VB62 |
| E | 101 | ASN | - | expression tag | UNP B1VB62 |
| E | 102 | LYS | - | expression tag | UNP B1VB62 |
| E | 103 | ALA | - | expression tag | UNP B1VB62 |
| E | 104 | ARG | - | expression tag | UNP B1VB62 |
| E | 105 | LYS | - | expression tag | UNP B1VB62 |
| E | 106 | GLU | - | expression tag | UNP B1VB62 |
| E | 107 | ALA | - | expression tag | UNP B1VB62 |
| E | 108 | GLU | - | expression tag | UNP B1VB62 |
| E | 109 | LEU | - | expression tag | UNP B1VB62 |
| E | 110 | ALA | - | expression tag | UNP B1VB62 |
| E | 111 | ALA | - | expression tag | UNP B1VB62 |
| E | 112 | ALA | - | expression tag | UNP B1VB62 |
| E | 113 | THR | - | expression tag | UNP B1VB62 |
| F | -1 | GLY | - | expression tag | UNP B1VB62 |
| F | 0 | SER | - | expression tag | UNP B1VB62 |
| F | 26 | ASP | LYS | engineered mutation | UNP B1VB62 |
| F | 93 | ARG | - | expression tag | UNP B1VB62 |
| F | 94 | LEU | - | expression tag | UNP B1VB62 |
| F | 95 | VAL | - | expression tag | UNP B1VB62 |
| F | 96 | LYS | - | expression tag | UNP B1VB62 |
| F | 97 | ASP | - | expression tag | UNP B1VB62 |
| F | 98 | PRO | - | expression tag | UNP B1VB62 |
| F | 99 | ALA | - | expression tag | UNP B1VB62 |
| F | 100 | ALA | - | expression tag | UNP B1VB62 |
| F | 101 | ASN | - | expression tag | UNP B1VB62 |
| F | 102 | LYS | - | expression tag | UNP B1VB62 |
| F | 103 | ALA | - | expression tag | UNP B1VB62 |
| F | 104 | ARG | - | expression tag | UNP B1VB62 |
| F | 105 | LYS | - | expression tag | UNP B1VB62 |
| F | 106 | GLU | - | expression tag | UNP B1VB62 |
| F | 107 | ALA | - | expression tag | UNP B1VB62 |
| F | 108 | GLU | - | expression tag | UNP B1VB62 |
| F | 109 | LEU | - | expression tag | UNP B1VB62 |
| F | 110 | ALA | - | expression tag | UNP B1VB62 |
| F | 111 | ALA | - | expression tag | UNP B1VB62 |
| F | 112 | ALA | - | expression tag | UNP B1VB62 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| F | 113 | THR | - | expression tag | UNP B1VB62 |

- Molecule 2 is water.

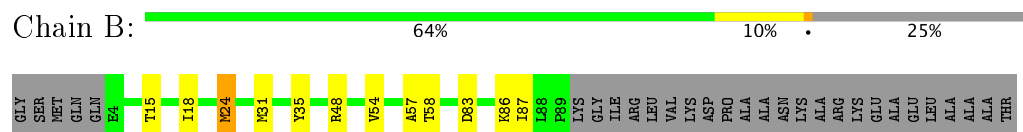| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2 | A | 52 | Total<br>52 | O<br>52 | 0 | 0 |
| 2 | B | 41 | Total<br>41 | O<br>41 | 0 | 0 |
| 2 | C | 35 | Total<br>35 | O<br>35 | 0 | 0 |
| 2 | D | 53 | Total<br>53 | O<br>53 | 0 | 0 |
| 2 | E | 76 | Total<br>76 | O<br>76 | 0 | 0 |
| 2 | F | 60 | Total<br>60 | O<br>60 | 0 | 0 |

# 3  Residue-property plots ⓘ

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.
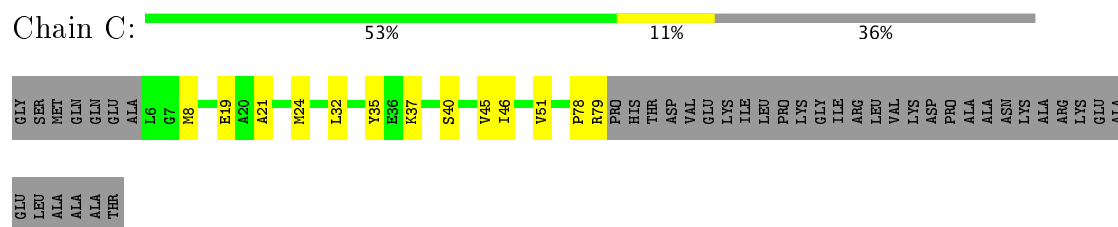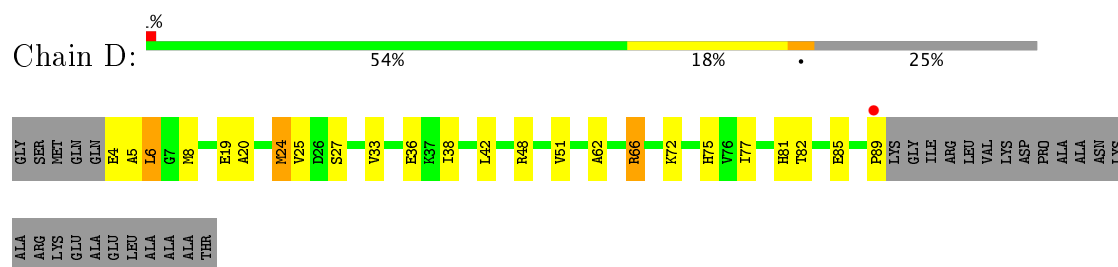
- Molecule 1: Polyhedral bodies

Chain A:



- Molecule 1: Polyhedral bodies

Chain B:



- Molecule 1: Polyhedral bodies

Chain C:



- Molecule 1: Polyhedral bodies

Chain D:



- Molecule 1: Polyhedral bodies

**Chain E:**

58%    15%    •    25%

GLY SER MET GLN GLN **E4** M8 V9 E10 L14 T15 A16 E19 M24 G41 R48 V51 K55 A56 A57 T58 R66 N67 V68 K72 I77 K86 P89 LYS GLY ILE ARG LEU VAL LYS ASP PRO ALA ALA ASN LYS ALA ARG LYS GLU ALA GLU

LEU ALA ALA THR

• Molecule 1: Polyhedral bodies

**Chain F:**

60%    11%    •    27%

GLY SER MET GLN GLN GLU **A5** E10 T11 K12 I18 E19 A20 M24 V25 D26 M31 A57 V71 H75 V76 I77 P78 R79 P80 H81 T82 L88 PRO LYS GLY ILE ARG LEU VAL LYS ASP PRO ALA ALA ASN LYS ALA ARG LYS GLU ALA GLU LEU ALA ALA ALA

THR

## GLOBAL-STATISTICS INFOmissingINFO

# 4 Model quality ⓘ

## 4.1 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 | A | 1.18 | 0/604 | 1.25 | 6/819 (0.7%) |
| 1 | B | 1.17 | 0/611 | 1.19 | 2/830 (0.2%) |
| 1 | C | 1.06 | 0/514 | 1.22 | 1/696 (0.1%) |
| 1 | D | 1.27 | 1/611 (0.2%) | 1.46 | 4/830 (0.5%) |
| 1 | E | 1.36 | 2/611 (0.3%) | 1.31 | 6/830 (0.7%) |
| 1 | F | 1.36 | 1/594 (0.2%) | 1.50 | 7/806 (0.9%) |
| All | All | 1.24 | 4/3545 (0.1%) | 1.33 | 26/4811 (0.5%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | F | 10 | GLU | CG-CD | 5.58 | 1.60 | 1.51 |
| 1 | D | 27 | SER | CB-OG | 5.56 | 1.49 | 1.42 |
| 1 | E | 4 | GLU | N-CA | 5.55 | 1.57 | 1.46 |
| 1 | E | 10 | GLU | CG-CD | 5.46 | 1.60 | 1.51 |

The worst 5 of 26 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1 | D | 24 | MET | CG-SD-CE | -22.84 | 63.66 | 100.20 |
| 1 | C | 24 | MET | CG-SD-CE | -12.93 | 79.51 | 100.20 |
| 1 | A | 24 | MET | CG-SD-CE | -12.23 | 80.63 | 100.20 |
| 1 | F | 31 | MET | CG-SD-CE | -11.98 | 81.03 | 100.20 |
| 1 | F | 24 | MET | CG-SD-CE | -11.98 | 81.04 | 100.20 |

There are no chirality outliers.

There are no planarity outliers.

## 4.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 600 | 0 | 620 | 38 | 0 |
| 1 | B | 606 | 0 | 630 | 12 | 0 |
| 1 | C | 512 | 0 | 537 | 20 | 0 |
| 1 | D | 606 | 0 | 630 | 36 | 0 |
| 1 | E | 606 | 0 | 630 | 22 | 0 |
| 1 | F | 590 | 0 | 617 | 17 | 0 |
| 2 | A | 52 | 0 | 0 | 10 | 0 |
| 2 | B | 41 | 0 | 0 | 2 | 0 |
| 2 | C | 35 | 0 | 0 | 7 | 0 |
| 2 | D | 53 | 0 | 0 | 5 | 0 |
| 2 | E | 76 | 0 | 0 | 7 | 1 |
| 2 | F | 60 | 0 | 0 | 3 | 1 |
| All | All | 3837 | 0 | 3664 | 126 | 1 |

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 18.

The worst 5 of 126 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:D:6:LEU:HD23 | 1:D:48:ARG:CD | 1.66 | 1.25 |
| 1:E:24:MET:CE | 1:E:58:THR:HA | 1.70 | 1.19 |
| 1:B:15:THR:HG23 | 1:C:8:MET:CE | 1.74 | 1.18 |
| 1:A:87:ILE:HD12 | 1:A:87:ILE:O | 1.42 | 1.17 |
| 1:E:24:MET:HE2 | 1:E:58:THR:CA | 1.84 | 1.07 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 2:E:232:HOH:O | 2:F:204:HOH:O[2_756] | 2.17 | 0.03 |

## 4.3 Torsion angles (i)

### 4.3.1 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 | 83/115 (72%) | 82 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | B | 84/115 (73%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 1 | C | 72/115 (63%) | 72 (100%) | 0 | 0 | 100 | 100 |
| 1 | D | 84/115 (73%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 1 | E | 84/115 (73%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | F | 82/115 (71%) | 81 (99%) | 1 (1%) | 0 | 100 | 100 |
| All | All | 489/690 (71%) | 486 (99%) | 3 (1%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 4.3.2 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 | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | A | 60/81 (74%) | 59 (98%) | 1 (2%) | 66 | 49 |
| 1 | B | 61/81 (75%) | 60 (98%) | 1 (2%) | 68 | 51 |
| 1 | C | 50/81 (62%) | 49 (98%) | 1 (2%) | 60 | 41 |
| 1 | D | 61/81 (75%) | 61 (100%) | 0 | 100 | 100 |
| 1 | E | 61/81 (75%) | 61 (100%) | 0 | 100 | 100 |
| 1 | F | 59/81 (73%) | 58 (98%) | 1 (2%) | 66 | 49 |
| All | All | 352/486 (72%) | 348 (99%) | 4 (1%) | 78 | 67 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 87 | ILE |
| 1 | B | 83 | ASP |
| 1 | C | 40 | SER |
| 1 | F | 82 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 81 | HIS |
| 1 | B | 81 | HIS |
| 1 | C | 67 | ASN |

### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 4.6 Ligand geometry (i)

There are no ligands in this entry.

## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 5 Fit of model and data (i)

## 5.1 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, $95^{th}$ 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 | 85/115 (73%) | -0.09 | 2 (2%) | 59 | 65 | 19, 27, 47, 78 | 0 |
| 1 | B | 86/115 (74%) | -0.16 | 0 | 100 | 100 | 20, 27, 47, 54 | 0 |
| 1 | C | 74/115 (64%) | -0.15 | 0 | 100 | 100 | 21, 31, 45, 59 | 0 |
| 1 | D | 86/115 (74%) | -0.12 | 1 (1%) | 79 | 83 | 16, 23, 43, 54 | 0 |
| 1 | E | 86/115 (74%) | -0.34 | 0 | 100 | 100 | 16, 22, 32, 39 | 0 |
| 1 | F | 84/115 (73%) | -0.27 | 0 | 100 | 100 | 15, 21, 36, 50 | 0 |
| All | All | 501/690 (72%) | -0.19 | 3 (0%) | 89 | 92 | 15, 25, 44, 78 | 0 |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 86 | LYS | 4.0 |
| 1 | A | 87 | ILE | 3.4 |
| 1 | D | 89 | PRO | 2.3 |

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

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

## 5.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.4 Ligands (i)

There are no ligands in this entry.

## 5.5 Other polymers (i)

There are no such residues in this entry.