# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 01:01 PM JST

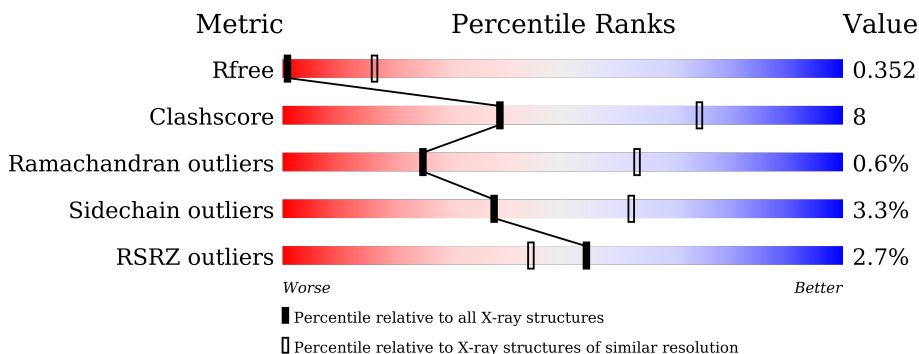|  |  |  |
|---|---|---|
| PDB ID | : | 6J4A |
| Title | : | Human H chain ferritin with an extension peptide |
| Authors | : | Zhang, X.; Zang, J.; Zhou, K.; Zhao, G. |
| Deposited on | : | 2019-01-08 |
| Resolution | : | 3.99 Å(reported) |

# 1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.99 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 | | 0.352 |
| Clashscore | | 8 |
| Ramachandran outliers | | 0.6% |
| Sidechain outliers | | 3.3% |
| RSRZ outliers | | 2.7% |

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)) |
|---|---|---|
| $R_{free}$ | 130704 | 1087 (4.30-3.70) |
| Clashscore | 141614 | 1148 (4.30-3.70) |
| Ramachandran outliers | 138981 | 1108 (4.30-3.70) |
| Sidechain outliers | 138945 | 1099 (4.30-3.70) |
| RSRZ outliers | 127900 | 1028 (4.34-3.66) |

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 of 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 |
|---|---|---|---|
| 1 | A | 183 | 4% — 67% · 23% · 6% |
| 1 | B | 183 | 3% — 70% · 22% · 6% |
| 1 | C | 183 | 2% — 76% · 17% · 6% |
| 1 | D | 183 | % — 76% · 18% · 6% |
| 1 | E | 183 | 3% — 71% · 22% · 6% |
| 1 | F | 183 | 2% — 75% · 18% · 6% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 183 | % 79% 14% · 6% |
| 1 | H | 183 | 3% 80% 14% · 6% |
| 1 | I | 183 | 3% 74% 19% · 6% |
| 1 | J | 183 | 2% 69% 25% 6% |
| 1 | K | 183 | 4% 78% 16% · 6% |
| 1 | L | 183 | % 84% 9% · 6% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16972 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 Ferritin heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | B | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | C | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | D | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | F | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | G | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | H | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | I | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | J | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | K | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |
| 1 | L | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1413 | 885 | 248 | 273 | 7 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 86 | GLN | LYS | conflict | UNP P02794 |
| B | 86 | GLN | LYS | conflict | UNP P02794 |
| C | 86 | GLN | LYS | conflict | UNP P02794 |
| D | 86 | GLN | LYS | conflict | UNP P02794 |
| E | 86 | GLN | LYS | conflict | UNP P02794 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| F | 86 | GLN | LYS | conflict | UNP P02794 |
| G | 86 | GLN | LYS | conflict | UNP P02794 |
| H | 86 | GLN | LYS | conflict | UNP P02794 |
| I | 86 | GLN | LYS | conflict | UNP P02794 |
| J | 86 | GLN | LYS | conflict | UNP P02794 |
| K | 86 | GLN | LYS | conflict | UNP P02794 |
| L | 86 | GLN | LYS | conflict | UNP P02794 |

- Molecule 2 is water.

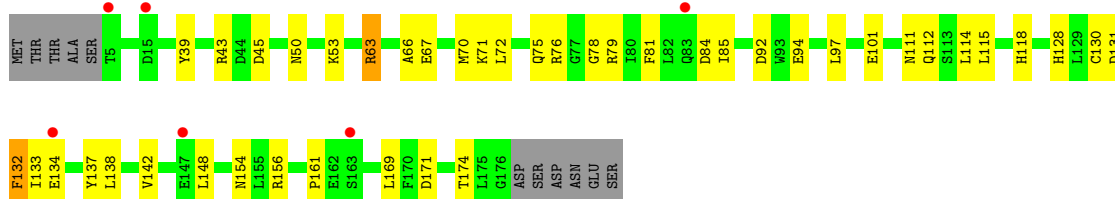| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2 | A | 3 | Total 3 | O 3 | 0 | 0 |
| 2 | B | 1 | Total 1 | O 1 | 0 | 0 |
| 2 | D | 2 | Total 2 | O 2 | 0 | 0 |
| 2 | E | 1 | Total 1 | O 1 | 0 | 0 |
| 2 | F | 2 | Total 2 | O 2 | 0 | 0 |
| 2 | G | 1 | Total 1 | O 1 | 0 | 0 |
| 2 | H | 2 | Total 2 | O 2 | 0 | 0 |
| 2 | I | 1 | Total 1 | O 1 | 0 | 0 |
| 2 | J | 2 | Total 2 | O 2 | 0 | 0 |
| 2 | L | 1 | Total 1 | O 1 | 0 | 0 |

# 3 Residue-property plots ⓘ

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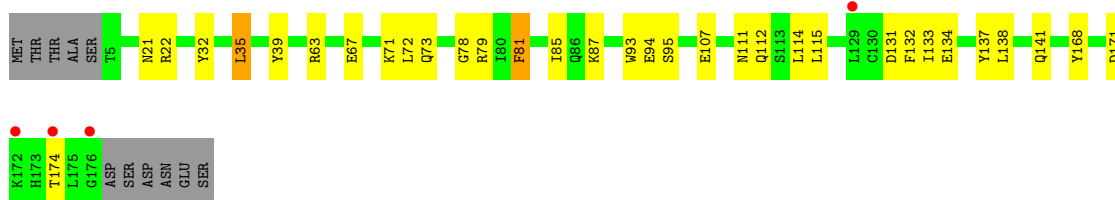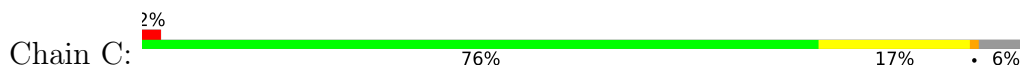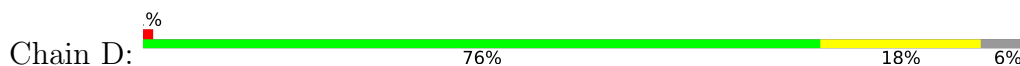
• Molecule 1: Ferritin heavy chain

Chain A:

• Molecule 1: Ferritin heavy chain
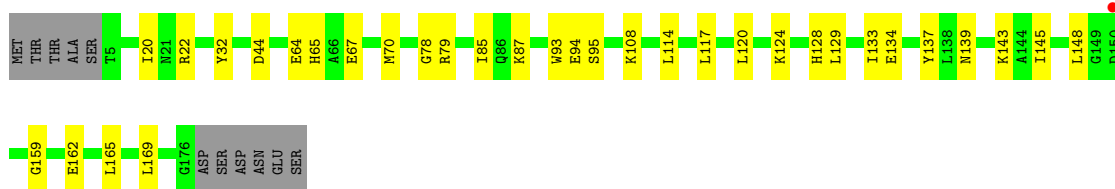
Chain B:

• Molecule 1: Ferritin heavy chain

Chain C:

• Molecule 1: Ferritin heavy chain

Chain D:

MET THR ALA SER T5 I20 N21 R22 Y32 D44 E64 H65 A66 E67 M70 G78 R79 I85 Q86 K87 W93 E94 S95 K108 L114 L117 L120 K124 H128 L129 I133 E134 Y137 L138 N139 K143 A144 I145 L148 G149 D150

G159 E162 L165 L169 G176 ASP SER ASP ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain E:

3%
71% 22% • 6%

MET THR ALA SER T5 S6 Q7 V8 R9 Q10 N11 Y12 I20 N21 R22 Y29 Y32 V33 D42 D45 R63 K71 L72 Q73 N74 Q75 R76 R79 I80 F81 L82 Q83 D84 I85 Q86 K87 P88 D89 C90 E94 L97 N109 L117 H118 D123 K124

D131 F132 I133 E134 T135 V142 L148 G149 D150 H151 V152 T153 N154 L155 R156 K157 M158 A166 L169 G176 ASP SER ASP ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain F:

2%
75% 18% • 6%

MET THR ALA SER T5 N21 I24 L28 Y29 A30 S31 Y32 V33 R43 D44 D45 V46 A47 N50 K53 H60 E61 E62 M70 K71 L72 Q73 N74 G78 R79 I80 F81 D84 I85 Q86 K87 E94 H105 L106 E107 Q112 S113 L114 F132 I133

E134 L138 Q141 N154 M158 E162 D171 T174 L175 G176 ASP SER ASP ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain G:

%
79% 14% • 6%

MET THR ALA SER T5 V8 Y12 I20 N21 R22 S31 Y32 D42 S59 Q73 N74 G78 R79 I80 F81 D84 K87 W93 E94 S95 D123 H128 L129 C130 D131 F132 I133 E134 L138 K143 E162 Y168 G176 ASP SER ASP

ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain H:

3%
80% 14% • 6%

MET THR ALA SER T5 Y29 Y32 V33 D42 K71 N74 Q75 R76 R79 L82 K87 E94 L114 H118 N125 D126 P127 H128 D131 F132 I133 E134 L138 N139 E140 Q141 V142 I145 K146 E147 H151 V152 T153 K157 P161
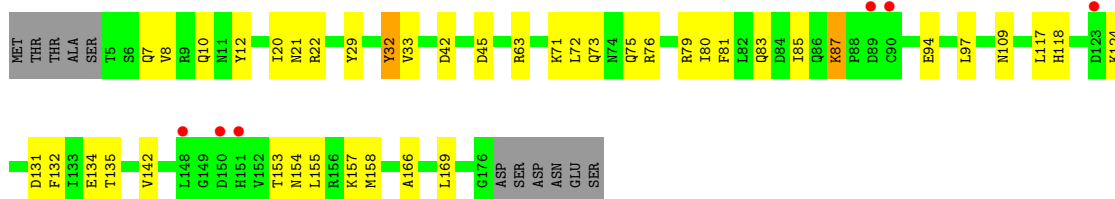
L169 K172 G176 ASP SER ASP ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain I:

Chain I residue bar: MET THR THR ALA SER T5 Y12 I24 Y29 Y32 V33 Y34 L35 S36 M37 D45 M70 Q73 N74 Q75 R76 G77 G78 R79 K87 W93 E94 L97 H105 L106 E107 Q112 S113 L117 H118 K119 L120 K124 N125 D126 C130 D131 E134 T135
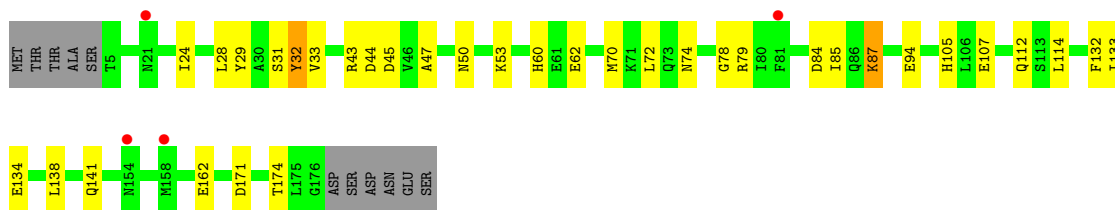
H136 Q141 I145 G149 D150 T153 N154 L155 M158 G176 ASP SER ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain J:

Chain J residue bar: MET THR THR ALA SER T5 V8 H13 I20 N21 R22 Q23 Y29 Y32 V33 D42 D45 V46 A47 R63 E64 H65 A66 L69 M70 K71 L72 Q75 I80 D84 K87 P88 D89 E94 S95 G96 K108 N111 Q112 S113 L114 L115 E116 L117

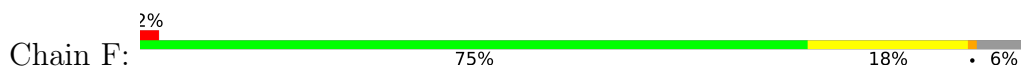K124 N125 L129 C130 D131 F132 I133 E134 T135 H136 Y137 L138 Q141 I145 K146 E147 D150 N154 M158 G159 Y168 L169 G176 ASP SER ASP ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain K:

Chain K residue bar: MET THR THR ALA SER T5 R22 Y32 Y40 F41 D42 R43 D44 D45 K49 H60 R63 E64 H65 A66 E67 K71 L72 Q73 N74 Q75 L82 K87 W93 E94 S95 N111 L115 H128 L129 F132 I133 E134 Y137 L138 E147 D150

N154 M158 Y168 D171 G176 ASP SER ASP ASN GLU SER

• Molecule 1: Ferritin heavy chain

Chain L:

Chain L residue bar: MET THR THR ALA SER T5 Y12 Y32 R63 Q73 N74 G78 R79 L82 I85 Q86 K87 W93 E94 S95 E101 C130 D131 E134 I145 R156 S163 G176 ASP SER ASP ASN GLU SER

# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 42 21 2 | Depositor |
| Cell constants <br> a, b, c, $\alpha$, $\beta$, $\gamma$ | 219.80Å    219.80Å    148.34Å <br> 90.00°     90.00°     90.00° | Depositor |
| Resolution (Å) | 107.31   –   3.99 <br> 107.31   –   3.99 | Depositor <br> EDS |
| % Data completeness <br> (in resolution range) | 95.1 (107.31-3.99) <br> 79.5 (107.31-3.99) | Depositor <br> EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.10 (at 4.01Å) | Xtriage |
| Refinement program | PHENIX (1.10.1_2155: ???) | Depositor |
| R, $R_{free}$ | 0.283   ,   0.351 <br> 0.283   ,   0.352 | Depositor <br> DCC |
| $R_{free}$ test set | 1536 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 32.8 | Xtriage |
| Anisotropy | 0.439 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 37.5 | EDS |
| L-test for twinning[2] | $< |L| > = 0.49, < L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o,F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 16972 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 43.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2702e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 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 | A | 0.29 | 0/1442 | 0.45 | 0/1943 |
| 1 | B | 0.27 | 0/1442 | 0.41 | 0/1943 |
| 1 | C | 0.27 | 0/1442 | 0.40 | 0/1943 |
| 1 | D | 0.25 | 0/1442 | 0.38 | 0/1943 |
| 1 | E | 0.26 | 0/1442 | 0.40 | 0/1943 |
| 1 | F | 0.26 | 0/1442 | 0.37 | 0/1943 |
| 1 | G | 0.26 | 0/1442 | 0.40 | 0/1943 |
| 1 | H | 0.25 | 0/1442 | 0.39 | 0/1943 |
| 1 | I | 0.26 | 0/1442 | 0.39 | 0/1943 |
| 1 | J | 0.26 | 0/1442 | 0.39 | 0/1943 |
| 1 | K | 0.26 | 0/1442 | 0.38 | 0/1943 |
| 1 | L | 0.26 | 0/1442 | 0.38 | 0/1943 |
| All | All | 0.26 | 0/17304 | 0.40 | 0/23316 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2   Too-close contacts  ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1413 | 0 | 1352 | 36 | 0 |
| 1 | B | 1413 | 0 | 1352 | 35 | 0 |
| 1 | C | 1413 | 0 | 1352 | 19 | 0 |
| 1 | D | 1413 | 0 | 1352 | 21 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | E | 1413 | 0 | 1352 | 38 | 0 |
| 1 | F | 1413 | 0 | 1352 | 27 | 1 |
| 1 | G | 1413 | 0 | 1352 | 22 | 1 |
| 1 | H | 1413 | 0 | 1352 | 16 | 0 |
| 1 | I | 1413 | 0 | 1352 | 25 | 0 |
| 1 | J | 1413 | 0 | 1352 | 32 | 0 |
| 1 | K | 1413 | 0 | 1352 | 21 | 0 |
| 1 | L | 1413 | 0 | 1352 | 12 | 0 |
| 2 | A | 3 | 0 | 0 | 1 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 2 | 0 | 0 | 1 | 0 |
| 2 | E | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 2 | G | 1 | 0 | 0 | 0 | 0 |
| 2 | H | 2 | 0 | 0 | 0 | 0 |
| 2 | I | 1 | 0 | 0 | 0 | 0 |
| 2 | J | 2 | 0 | 0 | 0 | 0 |
| 2 | L | 1 | 0 | 0 | 0 | 0 |
| All | All | 16972 | 0 | 16224 | 249 | 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 8.

The worst 5 of 249 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:A:33:VAL:HG12 | 1:A:88:PRO:HB3 | 1.63 | 0.80 |
| 1:C:21:ASN:HD21 | 1:C:81:PHE:H | 1.30 | 0.79 |
| 1:F:107:GLU:OE1 | 1:F:141:GLN:NE2 | 2.18 | 0.77 |
| 1:B:174:THR:HG1 | 1:J:168:TYR:HH | 1.35 | 0.75 |
| 1:B:67:GLU:O | 1:B:71:LYS:N | 2.16 | 0.74 |

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) |
|--------|--------|--------------------------|-------------------|
| 1:F:174:THR:OG1 | 1:G:168:TYR:OH[8_777] | 2.18 | 0.02 |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 | 170/183 (93%) | 158 (93%) | 11 (6%) | 1 (1%) | 25 | 63 |
| 1 | B | 170/183 (93%) | 161 (95%) | 8 (5%) | 1 (1%) | 25 | 63 |
| 1 | C | 170/183 (93%) | 165 (97%) | 4 (2%) | 1 (1%) | 25 | 63 |
| 1 | D | 170/183 (93%) | 164 (96%) | 5 (3%) | 1 (1%) | 25 | 63 |
| 1 | E | 170/183 (93%) | 160 (94%) | 9 (5%) | 1 (1%) | 25 | 63 |
| 1 | F | 170/183 (93%) | 164 (96%) | 5 (3%) | 1 (1%) | 25 | 63 |
| 1 | G | 170/183 (93%) | 164 (96%) | 5 (3%) | 1 (1%) | 25 | 63 |
| 1 | H | 170/183 (93%) | 165 (97%) | 4 (2%) | 1 (1%) | 25 | 63 |
| 1 | I | 170/183 (93%) | 168 (99%) | 1 (1%) | 1 (1%) | 25 | 63 |
| 1 | J | 170/183 (93%) | 163 (96%) | 5 (3%) | 2 (1%) | 13 | 49 |
| 1 | K | 170/183 (93%) | 161 (95%) | 8 (5%) | 1 (1%) | 25 | 63 |
| 1 | L | 170/183 (93%) | 165 (97%) | 4 (2%) | 1 (1%) | 25 | 63 |
| All | All | 2040/2196 (93%) | 1958 (96%) | 69 (3%) | 13 (1%) | 25 | 63 |

5 of 13 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 94 | GLU |
| 1 | D | 94 | GLU |
| 1 | H | 94 | GLU |
| 1 | B | 94 | GLU |
| 1 | E | 94 | GLU |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|-------------|---|
| 1 | A | 153/163 (94%) | 145 (95%) | 8 (5%) | 23 | 51 |
| 1 | B | 153/163 (94%) | 148 (97%) | 5 (3%) | 38 | 62 |
| 1 | C | 153/163 (94%) | 144 (94%) | 9 (6%) | 19 | 48 |
| 1 | D | 153/163 (94%) | 147 (96%) | 6 (4%) | 32 | 58 |
| 1 | E | 153/163 (94%) | 149 (97%) | 4 (3%) | 46 | 67 |
| 1 | F | 153/163 (94%) | 149 (97%) | 4 (3%) | 46 | 67 |
| 1 | G | 153/163 (94%) | 149 (97%) | 4 (3%) | 46 | 67 |
| 1 | H | 153/163 (94%) | 148 (97%) | 5 (3%) | 38 | 62 |
| 1 | I | 153/163 (94%) | 148 (97%) | 5 (3%) | 38 | 62 |
| 1 | J | 153/163 (94%) | 149 (97%) | 4 (3%) | 46 | 67 |
| 1 | K | 153/163 (94%) | 148 (97%) | 5 (3%) | 38 | 62 |
| 1 | L | 153/163 (94%) | 151 (99%) | 2 (1%) | 69 | 82 |
| All | All | 1836/1956 (94%) | 1775 (97%) | 61 (3%) | 38 | 62 |

5 of 61 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 22 | ARG |
| 1 | K | 42 | ASP |
| 1 | F | 162 | GLU |
| 1 | K | 22 | ARG |
| 1 | L | 32 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 111 | ASN |
| 1 | J | 154 | ASN |
| 1 | L | 74 | ASN |
| 1 | F | 60 | HIS |
| 1 | E | 10 | GLN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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 | 172/183 (93%) | 0.48 | 8 (4%) | 31 | 26 | 27, 44, 61, 77 | 0 |
| 1 | B | 172/183 (93%) | 0.57 | 6 (3%) | 44 | 35 | 28, 44, 65, 75 | 0 |
| 1 | C | 172/183 (93%) | 0.38 | 4 (2%) | 60 | 51 | 28, 44, 66, 91 | 0 |
| 1 | D | 172/183 (93%) | 0.38 | 1 (0%) | 89 | 84 | 27, 43, 64, 78 | 0 |
| 1 | E | 172/183 (93%) | 0.46 | 6 (3%) | 44 | 35 | 22, 42, 63, 83 | 0 |
| 1 | F | 172/183 (93%) | 0.33 | 4 (2%) | 60 | 51 | 21, 40, 59, 68 | 0 |
| 1 | G | 172/183 (93%) | 0.28 | 1 (0%) | 89 | 84 | 21, 40, 60, 70 | 0 |
| 1 | H | 172/183 (93%) | 0.47 | 6 (3%) | 44 | 35 | 21, 41, 62, 84 | 0 |
| 1 | I | 172/183 (93%) | 0.38 | 5 (2%) | 51 | 41 | 23, 39, 57, 71 | 0 |
| 1 | J | 172/183 (93%) | 0.45 | 4 (2%) | 60 | 51 | 21, 40, 59, 75 | 0 |
| 1 | K | 172/183 (93%) | 0.45 | 8 (4%) | 31 | 26 | 20, 41, 59, 68 | 0 |
| 1 | L | 172/183 (93%) | 0.37 | 2 (1%) | 79 | 70 | 20, 41, 60, 70 | 0 |
| All | All | 2064/2196 (93%) | 0.42 | 55 (2%) | 54 | 44 | 20, 42, 62, 91 | 0 |

The worst 5 of 55 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 150 | ASP | 3.2 |
| 1 | I | 158 | MET | 3.2 |
| 1 | H | 161 | PRO | 3.1 |
| 1 | I | 131 | ASP | 2.8 |
| 1 | E | 89 | ASP | 2.8 |

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.