# Full wwPDB X-ray Structure Validation Report ⓘ

| | | |
|---|---|---|
| PDB ID | : | 5CCI |
| Title | : | Structure of the Mg2+-bound synaptotagmin-1 SNARE complex (short unit cell form) |
| Authors | : | Zhou, Q.; Zhao, M.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Weis, W.I.; Brunger, A.T. |
| Deposited on | : | 2015-07-02 |
| Resolution | : | 4.10 Å(reported) |

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

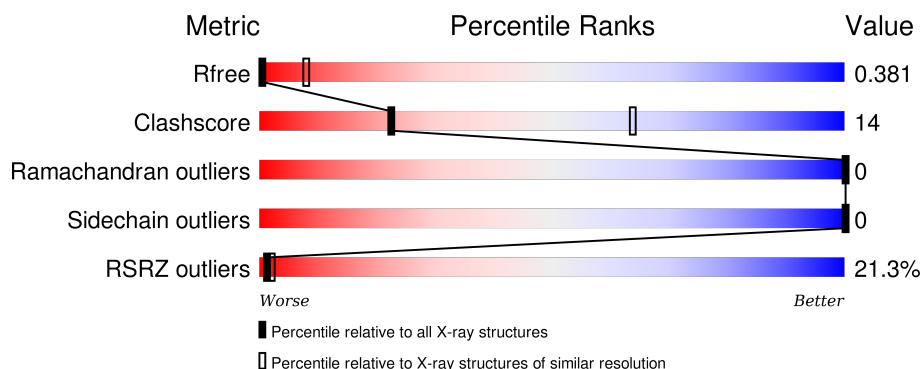| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026982 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20026982 |

# 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 4.10 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 | | 0.381 |
| Clashscore | | 14 |
| Ramachandran outliers | | 0 |
| Sidechain outliers | | 0 |
| RSRZ outliers | | 21.3% |

*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)) |
|---|---|---|
| $R_{free}$ | 91344 | 1018 (4.60-3.60) |
| Clashscore | 102246 | 1117 (4.60-3.60) |
| Ramachandran outliers | 100387 | 1063 (4.60-3.60) |
| Sidechain outliers | 100360 | 1049 (4.60-3.60) |
| RSRZ outliers | 91569 | 1022 (4.60-3.60) |

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 | 63 | 5% — 76% green, 22% yellow, • |
| 2 | B | 67 | 10% — 78% green, 22% yellow |
| 3 | C | 77 | 19% — 81% green, 14% yellow, 5% |
| 4 | D | 65 | 3% — 80% green, 18% yellow, • |
| 5 | E | 281 | 19% — 79% green, 21% yellow |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5 | F | 281 | |

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6406 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 Vesicle-associated membrane protein 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 1 | A | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 503 | 306 | 95 | 101 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 27 | GLY | - | expression tag | UNP P63045 |

- Molecule 2 is a protein called Syntaxin-1A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 2 | B | 67 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 541 | 334 | 92 | 110 | 5 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| B | 190 | MET | - | initiating methionine | UNP P32851 |

- Molecule 3 is a protein called Synaptosomal-associated protein 25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 3 | C | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 350 | 106 | 127 | 5 | | | |

- Molecule 4 is a protein called Synaptosomal-associated protein 25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 4 | D | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 499 | 294 | 98 | 102 | 5 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| D | 140 | MET | - | initiating methionine | UNP P60881 |

- Molecule 5 is a protein called Synaptotagmin-1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 5 | E | 280 | 2190 | 1405 | 367 | 410 | 8 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 5 | F | 268 | 2081 | 1337 | 350 | 387 | 7 | 0 | 0 | 0 |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| | | | Total | Mg | | |
| 6 | F | 2 | 2 | 2 | 0 | 0 |
| | | | Total | Mg | | |
| 6 | E | 2 | 2 | 2 | 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 errors 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.

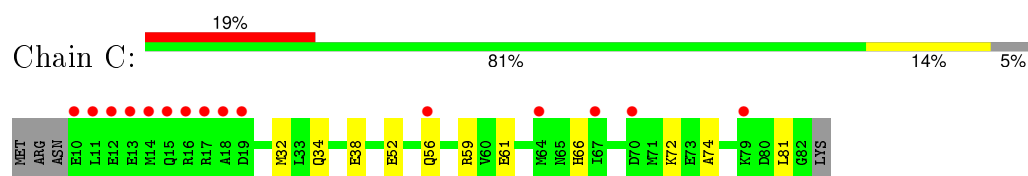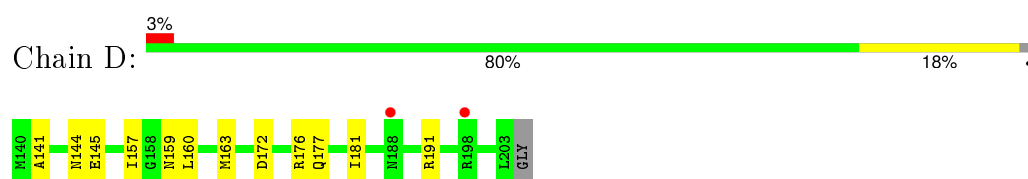- Molecule 1: Vesicle-associated membrane protein 2
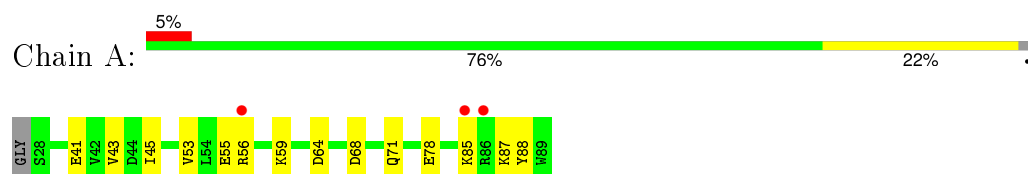
Chain A:

- Molecule 2: Syntaxin-1A
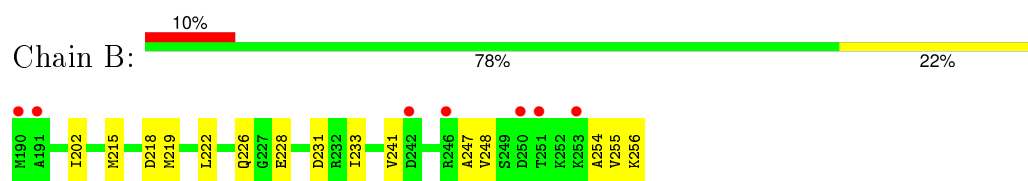
Chain B:

- Molecule 3: Synaptosomal-associated protein 25

Chain C:

- Molecule 4: Synaptosomal-associated protein 25

Chain D:

- Molecule 5: Synaptotagmin-1

Chain E:

K375 V376 F377 V378 G379 E386 R398 R399 P400 W404 H405 E410 L417 K420 LYS
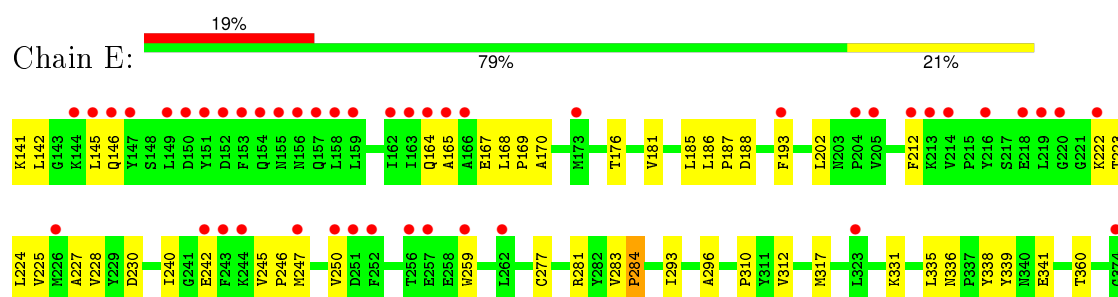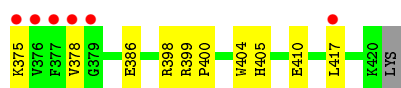
• Molecule 5: Synaptotagmin-1

Chain F:

33%

74%    21%    5%

K141 K144 L145 Q146 Y147 L158 L159 V160 G161 I162 A166 E167 L171 D172 M173 G174 G175 T176 P179 Y180 V181 K182 V183 F184 L185 L186 P187 D188 F193 E194 V197 H198 R199 V205 P206 N207 E208 Q209 F210 T211 F212 K213 V214 S217 E218 L219 K222 T223 M226

A227 V228 Y229 R233 F234 S235 K236 I239 I240 G241 E242 F243 K244 M247 N248 D251 F252 W259 L262 K267 GLU GLU GLN GLU LYS LEU G274 D275 I276 C277 F278 S279 L280 R281 Y282 V283 K288 L289 T290 I293 L294 E295 A296 L299 M302 ASP VAL GLY GLY

LEU S308 V312 K313 I314 H315 L316 M317 Q318 K321 R322 L323 K324 T334 P337 Y338 Y339 N340 E341 S344 F345 E346 V347 P348 I352 V355 Q356 V357 V358 V359 T360 V361 L362 D363 K366 ILE G368 D371 A372 I373 G374 K375 V376 F377 V378 G379 Y380 A385 E386 L387

R388 H389 W390 M393 R398 R399 P400 I401 A402 Q403 W404 L407 Q408 V409 L417 K420 LYS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|----------|-------|--------|
| Space group | P 21 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 69.06Å    171.76Å    146.56Å<br>90.00°    90.00°    90.00° | Depositor |
| Resolution (Å) | 48.24   –   4.10<br>74.10   –   4.10 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 95.7 (48.24-4.10)<br>94.9 (74.10-4.10) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.12 | Depositor |
| $<I/\sigma(I)>$ [1] | 2.07 (at 4.15Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.276   ,   0.323<br>0.327   ,   0.381 | Depositor<br>DCC |
| $R_{free}$ test set | 676 reflections (4.99%) | DCC |
| Wilson B-factor (Å$^2$) | 135.5 | Xtriage |
| Anisotropy | 0.803 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.40 , 231.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $<|L|> = 0.41, <L^2> = 0.24$ | Xtriage |
| Outliers | 3 of 13567 reflections (0.022%) | Xtriage |
| $F_o,F_c$ correlation | 0.86 | EDS |
| Total number of atoms | 6406 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 193.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

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

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 | 0.25 | 0/506 | 0.35 | 0/677 |
| 2 | B | 0.25 | 0/546 | 0.34 | 0/730 |
| 3 | C | 0.24 | 0/588 | 0.33 | 0/782 |
| 4 | D | 0.24 | 0/499 | 0.40 | 0/664 |
| 5 | E | 0.30 | 1/2239 (0.0%) | 0.43 | 0/3029 |
| 5 | F | 0.26 | 1/2127 (0.0%) | 0.41 | 0/2875 |
| All | All | 0.27 | 2/6505 (0.0%) | 0.40 | 0/8757 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 5 | E | 284 | PRO | N-CD | -7.69 | 1.37 | 1.47 |
| 5 | F | 187 | PRO | N-CD | 5.11 | 1.55 | 1.47 |

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 | 503 | 0 | 502 | 12 | 0 |
| 2 | B | 541 | 0 | 529 | 12 | 0 |
| 3 | C | 588 | 0 | 573 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | D | 499 | 0 | 486 | 11 | 0 |
| 5 | E | 2190 | 0 | 2133 | 90 | 0 |
| 5 | F | 2081 | 0 | 2015 | 55 | 0 |
| 6 | E | 2 | 0 | 0 | 0 | 0 |
| 6 | F | 2 | 0 | 0 | 0 | 0 |
| All | All | 6406 | 0 | 6238 | 173 | 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 14.

All (173) 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) |
|--------|--------|--------------------------|-------------------|
| 5:F:187:PRO:CG | 5:F:222:LYS:HG3 | 1.46 | 1.45 |
| 5:E:142:LEU:CD2 | 5:E:169:PRO:HG3 | 1.47 | 1.42 |
| 5:F:187:PRO:HG3 | 5:F:222:LYS:CG | 1.53 | 1.39 |
| 5:E:222:LYS:O | 5:E:247:MET:HG2 | 1.37 | 1.21 |
| 5:E:142:LEU:CD2 | 5:E:169:PRO:CG | 2.22 | 1.18 |
| 5:E:142:LEU:HD23 | 5:E:169:PRO:CG | 1.82 | 1.07 |
| 5:E:222:LYS:O | 5:E:247:MET:CG | 2.01 | 1.07 |
| 5:E:142:LEU:HA | 5:E:169:PRO:HD3 | 1.37 | 1.06 |
| 5:E:142:LEU:CA | 5:E:169:PRO:HD3 | 1.87 | 1.04 |
| 5:E:142:LEU:HD22 | 5:E:169:PRO:CG | 1.86 | 1.03 |
| 5:E:142:LEU:CD1 | 5:E:240:ILE:O | 2.08 | 1.00 |
| 5:F:187:PRO:CD | 5:F:222:LYS:HG3 | 1.94 | 0.98 |
| 4:D:141:ALA:HA | 4:D:144:ASN:ND2 | 1.79 | 0.97 |
| 5:F:193:PHE:CE1 | 5:F:212:PHE:CE1 | 2.55 | 0.94 |
| 5:E:185:LEU:HD21 | 5:E:212:PHE:CG | 2.01 | 0.94 |
| 5:E:142:LEU:O | 5:E:169:PRO:HD3 | 1.68 | 0.93 |
| 5:E:142:LEU:O | 5:E:168:LEU:HA | 1.69 | 0.92 |
| 5:E:142:LEU:HD22 | 5:E:169:PRO:HG2 | 1.54 | 0.87 |
| 5:F:187:PRO:HG3 | 5:F:222:LYS:CD | 2.04 | 0.86 |
| 5:E:142:LEU:HD23 | 5:E:169:PRO:HG3 | 0.86 | 0.85 |
| 5:E:142:LEU:C | 5:E:169:PRO:HD3 | 1.97 | 0.84 |
| 4:D:144:ASN:OD1 | 4:D:145:GLU:N | 2.11 | 0.84 |
| 5:E:187:PRO:CG | 5:E:222:LYS:HA | 2.09 | 0.83 |
| 5:E:142:LEU:HD11 | 5:E:240:ILE:O | 1.79 | 0.82 |
| 5:E:186:LEU:N | 5:E:223:THR:O | 2.12 | 0.82 |
| 4:D:141:ALA:HA | 4:D:144:ASN:HD21 | 1.44 | 0.82 |
| 5:F:186:LEU:HB3 | 5:F:223:THR:HB | 1.62 | 0.81 |
| 5:E:187:PRO:HG2 | 5:E:222:LYS:HG2 | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:142:LEU:O | 5:E:167:GLU:O | 1.98 | 0.81 |
| 5:E:142:LEU:HA | 5:E:169:PRO:CD | 2.11 | 0.80 |
| 5:E:185:LEU:HD21 | 5:E:212:PHE:CD1 | 2.17 | 0.78 |
| 5:E:193:PHE:HE2 | 5:E:212:PHE:CE1 | 2.01 | 0.78 |
| 5:F:187:PRO:HG3 | 5:F:222:LYS:HG3 | 0.78 | 0.77 |
| 5:E:142:LEU:HD13 | 5:E:240:ILE:O | 1.86 | 0.76 |
| 5:E:187:PRO:HG2 | 5:E:222:LYS:HA | 1.67 | 0.75 |
| 5:F:356:GLN:HE22 | 5:F:380:TYR:HB3 | 1.51 | 0.74 |
| 5:E:141:LYS:HD3 | 5:E:141:LYS:N | 2.03 | 0.72 |
| 5:E:142:LEU:O | 5:E:169:PRO:CD | 2.36 | 0.72 |
| 5:E:193:PHE:CE2 | 5:E:212:PHE:CE1 | 2.78 | 0.72 |
| 5:E:142:LEU:CA | 5:E:169:PRO:CD | 2.66 | 0.72 |
| 5:F:193:PHE:HE1 | 5:F:212:PHE:CE1 | 2.06 | 0.71 |
| 5:E:187:PRO:HG2 | 5:E:222:LYS:CB | 2.20 | 0.71 |
| 5:F:317:MET:HB2 | 5:F:356:GLN:HB2 | 1.71 | 0.71 |
| 5:E:223:THR:HG23 | 5:E:245:VAL:O | 1.91 | 0.70 |
| 5:F:187:PRO:CG | 5:F:222:LYS:CG | 2.33 | 0.70 |
| 5:E:142:LEU:HD13 | 5:E:240:ILE:HG22 | 1.72 | 0.69 |
| 5:E:296:ALA:O | 5:E:336:ASN:ND2 | 2.26 | 0.68 |
| 5:E:186:LEU:CB | 5:E:223:THR:HB | 2.24 | 0.68 |
| 5:E:187:PRO:HG2 | 5:E:222:LYS:CG | 2.23 | 0.68 |
| 5:E:187:PRO:HG3 | 5:E:222:LYS:HA | 1.76 | 0.68 |
| 5:F:187:PRO:HD3 | 5:F:223:THR:H | 1.58 | 0.68 |
| 5:F:186:LEU:CB | 5:F:223:THR:HB | 2.26 | 0.65 |
| 5:F:288:LYS:NZ | 5:F:290:THR:OG1 | 2.30 | 0.65 |
| 5:E:187:PRO:HG2 | 5:E:222:LYS:CA | 2.26 | 0.65 |
| 5:F:281:ARG:HB3 | 5:F:290:THR:HB | 1.78 | 0.65 |
| 5:F:193:PHE:HE1 | 5:F:212:PHE:HE1 | 1.44 | 0.64 |
| 5:E:187:PRO:HD3 | 5:E:223:THR:H | 1.63 | 0.64 |
| 5:F:187:PRO:CD | 5:F:222:LYS:CG | 2.71 | 0.64 |
| 5:F:193:PHE:CE1 | 5:F:212:PHE:HE1 | 2.15 | 0.62 |
| 5:E:146:GLN:HB2 | 5:E:259:TRP:CE2 | 2.35 | 0.62 |
| 5:E:187:PRO:HD3 | 5:E:223:THR:N | 2.15 | 0.62 |
| 2:B:248:VAL:HG22 | 3:C:74:ALA:HB2 | 1.81 | 0.61 |
| 5:F:316:LEU:HB3 | 5:F:324:LYS:HB2 | 1.82 | 0.61 |
| 5:E:360:THR:HG23 | 5:E:375:LYS:HB3 | 1.83 | 0.60 |
| 5:F:193:PHE:CD1 | 5:F:212:PHE:CZ | 2.90 | 0.60 |
| 5:E:142:LEU:O | 5:E:168:LEU:CA | 2.48 | 0.59 |
| 5:E:188:ASP:OD1 | 5:E:188:ASP:O | 2.21 | 0.59 |
| 5:F:185:LEU:HB2 | 5:F:188:ASP:OD1 | 2.03 | 0.59 |
| 5:E:185:LEU:CD2 | 5:E:212:PHE:CD1 | 2.86 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:277:CYS:HB2 | 5:E:404:TRP:CD2 | 2.38 | 0.58 |
| 5:E:223:THR:HG22 | 5:E:224:LEU:N | 2.19 | 0.58 |
| 5:F:315:HIS:HB3 | 5:F:322:ARG:HD2 | 1.85 | 0.58 |
| 3:C:34:GLN:NE2 | 3:C:38:GLU:OE2 | 2.38 | 0.57 |
| 1:A:55:GLU:HG2 | 1:A:59:LYS:HE2 | 1.87 | 0.57 |
| 5:E:223:THR:HG23 | 5:E:245:VAL:C | 2.25 | 0.56 |
| 5:F:312:VAL:HG22 | 5:F:361:VAL:HG22 | 1.87 | 0.56 |
| 5:F:283:VAL:HG13 | 5:F:398:ARG:HG2 | 1.87 | 0.55 |
| 5:F:363:ASP:HB3 | 5:F:371:ASP:HB2 | 1.90 | 0.54 |
| 5:E:187:PRO:HD3 | 5:E:223:THR:O | 2.08 | 0.54 |
| 1:A:78:GLU:HA | 2:B:247:ALA:HB2 | 1.90 | 0.54 |
| 5:F:219:LEU:HA | 5:F:222:LYS:HE3 | 1.89 | 0.53 |
| 5:F:374:GLY:HA3 | 5:F:407:LEU:HD13 | 1.89 | 0.53 |
| 5:E:335:LEU:HD23 | 5:E:335:LEU:H | 1.73 | 0.53 |
| 1:A:56:ARG:NH1 | 2:B:226:GLN:OE1 | 2.42 | 0.53 |
| 1:A:88:TYR:CD2 | 3:C:81:LEU:HD21 | 2.44 | 0.52 |
| 5:F:187:PRO:HD3 | 5:F:222:LYS:HG3 | 1.90 | 0.51 |
| 1:A:85:LYS:HA | 2:B:254:ALA:HB2 | 1.93 | 0.51 |
| 2:B:218:ASP:O | 2:B:222:LEU:HG | 2.12 | 0.50 |
| 5:E:378:VAL:HG12 | 5:E:386:GLU:HB3 | 1.93 | 0.49 |
| 4:D:157:ILE:HD13 | 4:D:160:LEU:HD12 | 1.94 | 0.49 |
| 5:F:318:GLN:O | 5:F:321:LYS:HG2 | 2.12 | 0.49 |
| 5:E:331:LYS:NZ | 5:E:338:TYR:O | 2.45 | 0.49 |
| 5:E:142:LEU:HA | 5:E:169:PRO:CG | 2.42 | 0.49 |
| 5:F:146:GLN:HB2 | 5:F:259:TRP:CE2 | 2.48 | 0.49 |
| 5:E:283:VAL:HG12 | 5:E:398:ARG:HA | 1.94 | 0.48 |
| 5:F:356:GLN:NE2 | 5:F:380:TYR:HB3 | 2.24 | 0.48 |
| 5:E:187:PRO:CD | 5:E:223:THR:H | 2.27 | 0.48 |
| 2:B:255:VAL:HG13 | 2:B:256:LYS:HG3 | 1.96 | 0.48 |
| 5:F:193:PHE:CD1 | 5:F:212:PHE:CE1 | 3.00 | 0.48 |
| 5:E:223:THR:CG2 | 5:E:224:LEU:N | 2.76 | 0.48 |
| 5:E:187:PRO:CG | 5:E:222:LYS:CA | 2.85 | 0.47 |
| 5:F:166:ALA:O | 5:F:167:GLU:HG2 | 2.13 | 0.47 |
| 4:D:177:GLN:O | 4:D:181:ILE:HG12 | 2.14 | 0.47 |
| 5:F:218:GLU:N | 5:F:218:GLU:OE1 | 2.45 | 0.47 |
| 5:F:185:LEU:HD11 | 5:F:212:PHE:HB3 | 1.96 | 0.47 |
| 5:E:181:VAL:HG22 | 5:E:228:VAL:HG22 | 1.96 | 0.47 |
| 1:A:64:ASP:HA | 2:B:233:ILE:HG12 | 1.96 | 0.47 |
| 5:F:186:LEU:HD13 | 5:F:223:THR:HG21 | 1.98 | 0.46 |
| 5:E:230:ASP:HB2 | 5:E:240:ILE:HD11 | 1.97 | 0.46 |
| 1:A:43:VAL:HA | 2:B:215:MET:HE1 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:F:181:VAL:HG22 | 5:F:228:VAL:HG22 | 1.98 | 0.46 |
| 5:E:222:LYS:O | 5:E:247:MET:HG3 | 2.05 | 0.46 |
| 5:E:227:ALA:HA | 5:E:242:GLU:HA | 1.98 | 0.46 |
| 5:E:283:VAL:CG1 | 5:E:398:ARG:HA | 2.46 | 0.46 |
| 5:E:165:ALA:HB1 | 5:E:168:LEU:HD21 | 1.98 | 0.46 |
| 5:E:142:LEU:HD13 | 5:E:240:ILE:CG2 | 2.44 | 0.45 |
| 5:E:141:LYS:CD | 5:E:141:LYS:N | 2.73 | 0.45 |
| 5:E:386:GLU:HA | 5:E:405:HIS:HE1 | 1.82 | 0.45 |
| 5:E:310:PRO:HD2 | 5:E:331:LYS:O | 2.16 | 0.45 |
| 5:E:186:LEU:CB | 5:E:223:THR:CB | 2.94 | 0.45 |
| 5:E:186:LEU:CB | 5:E:223:THR:C | 2.86 | 0.44 |
| 5:E:186:LEU:CB | 5:E:225:VAL:HG23 | 2.47 | 0.44 |
| 5:F:182:LYS:HG3 | 5:F:194:GLU:HG2 | 1.98 | 0.44 |
| 5:F:217:SER:OG | 5:F:218:GLU:OE1 | 2.31 | 0.44 |
| 5:F:214:VAL:HG21 | 5:F:222:LYS:HE2 | 1.98 | 0.44 |
| 3:C:56:GLN:HG2 | 3:C:59:ARG:NH2 | 2.33 | 0.44 |
| 5:F:187:PRO:CG | 5:F:222:LYS:CD | 2.87 | 0.44 |
| 5:E:185:LEU:HG | 5:E:212:PHE:CE1 | 2.52 | 0.44 |
| 5:F:366:LYS:O | 5:F:368:GLY:HA3 | 2.18 | 0.44 |
| 4:D:163:MET:HG2 | 5:E:338:TYR:CZ | 2.53 | 0.43 |
| 4:D:163:MET:HG2 | 5:E:338:TYR:CE1 | 2.53 | 0.43 |
| 5:F:229:TYR:CE1 | 5:F:239:ILE:HG22 | 2.54 | 0.43 |
| 1:A:41:GLU:O | 1:A:45:ILE:HG12 | 2.17 | 0.43 |
| 5:F:277:CYS:HB3 | 5:F:404:TRP:CE3 | 2.54 | 0.43 |
| 1:A:53:VAL:HG21 | 2:B:219:MET:SD | 2.57 | 0.43 |
| 4:D:172:ASP:O | 4:D:176:ARG:HG2 | 2.19 | 0.43 |
| 5:E:339:TYR:HB3 | 5:E:341:GLU:HG3 | 2.00 | 0.43 |
| 2:B:241:VAL:HG13 | 3:C:66:HIS:HD2 | 1.84 | 0.42 |
| 5:E:142:LEU:CB | 5:E:169:PRO:CD | 2.97 | 0.42 |
| 5:F:185:LEU:HD11 | 5:F:212:PHE:CB | 2.49 | 0.42 |
| 5:F:241:GLY:HA3 | 5:F:262:LEU:HD13 | 2.00 | 0.42 |
| 1:A:68:ASP:O | 1:A:71:GLN:HG3 | 2.19 | 0.42 |
| 5:F:187:PRO:HG3 | 5:F:222:LYS:HD3 | 1.96 | 0.42 |
| 5:E:185:LEU:CG | 5:E:212:PHE:CD1 | 3.03 | 0.42 |
| 5:E:246:PRO:O | 5:E:250:VAL:HG23 | 2.19 | 0.42 |
| 5:E:283:VAL:HA | 5:E:284:PRO:HD3 | 1.68 | 0.42 |
| 5:F:159:LEU:HD12 | 5:F:211:THR:HG22 | 2.02 | 0.42 |
| 5:F:227:ALA:HB2 | 5:F:242:GLU:HG3 | 2.01 | 0.42 |
| 2:B:202:ILE:HG23 | 3:C:32:MET:HE1 | 2.02 | 0.42 |
| 5:E:281:ARG:HB2 | 5:E:400:PRO:HB3 | 2.01 | 0.42 |
| 5:E:317:MET:SD | 5:E:417:LEU:HD13 | 2.60 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:159:ASN:ND2 | 5:E:336:ASN:OD1 | 2.52 | 0.41 |
| 5:F:277:CYS:HB3 | 5:F:404:TRP:CD2 | 2.55 | 0.41 |
| 5:E:146:GLN:HB2 | 5:E:259:TRP:CD2 | 2.54 | 0.41 |
| 3:C:61:GLU:HB2 | 4:D:181:ILE:HD11 | 2.03 | 0.41 |
| 5:E:176:THR:HG22 | 5:E:202:LEU:HG | 2.02 | 0.41 |
| 5:E:145:LEU:HD12 | 5:E:164:GLN:O | 2.20 | 0.41 |
| 5:F:219:LEU:HD21 | 5:F:252:PHE:HE2 | 1.85 | 0.41 |
| 5:E:142:LEU:HA | 5:E:169:PRO:HG3 | 2.02 | 0.41 |
| 1:A:87:LYS:HE3 | 1:A:88:TYR:CE1 | 2.55 | 0.41 |
| 5:F:399:ARG:HA | 5:F:400:PRO:HD3 | 1.91 | 0.41 |
| 1:A:88:TYR:CE2 | 3:C:81:LEU:HD21 | 2.56 | 0.41 |
| 3:C:52:GLU:CD | 5:E:399:ARG:HE | 2.24 | 0.41 |
| 5:F:347:VAL:HA | 5:F:348:PRO:HD2 | 1.90 | 0.41 |
| 2:B:228:GLU:O | 2:B:231:ASP:HB2 | 2.20 | 0.41 |
| 5:E:170:ALA:HB2 | 5:E:202:LEU:HD11 | 2.04 | 0.40 |
| 5:E:293:ILE:HG21 | 5:E:312:VAL:HG21 | 2.02 | 0.40 |
| 3:C:72:LYS:HG3 | 4:D:191:ARG:HH22 | 1.86 | 0.40 |
| 5:F:219:LEU:HD21 | 5:F:252:PHE:CE2 | 2.57 | 0.40 |
| 5:E:142:LEU:HB3 | 5:E:169:PRO:CD | 2.51 | 0.40 |
| 5:E:185:LEU:HG | 5:E:212:PHE:CD1 | 2.56 | 0.40 |
| 5:F:362:LEU:HD22 | 5:F:372:ALA:HA | 2.03 | 0.40 |
| 5:E:375:LYS:HD3 | 5:E:410:GLU:HA | 2.02 | 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 | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 60/63 (95%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 2 | B | 65/67 (97%) | 64 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | C | 71/77 (92%) | 71 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-----|-----|
| 4 | D | 62/65 (95%) | 60 (97%) | 2 (3%) | 0 | 100 | 100 |
| 5 | E | 278/281 (99%) | 270 (97%) | 8 (3%) | 0 | 100 | 100 |
| 5 | F | 260/281 (92%) | 253 (97%) | 7 (3%) | 0 | 100 | 100 |
| All | All | 796/834 (95%) | 778 (98%) | 18 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | Percentiles | |
|-----|-------|----------|-----------|----------|-----|-----|
| 1 | A | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 2 | B | 60/61 (98%) | 60 (100%) | 0 | 100 | 100 |
| 3 | C | 65/69 (94%) | 65 (100%) | 0 | 100 | 100 |
| 4 | D | 53/56 (95%) | 53 (100%) | 0 | 100 | 100 |
| 5 | E | 233/251 (93%) | 233 (100%) | 0 | 100 | 100 |
| 5 | F | 221/251 (88%) | 221 (100%) | 0 | 100 | 100 |
| All | All | 686/742 (92%) | 686 (100%) | 0 | 100 | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | F | 356 | GLN |

### 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 4 ligands modelled in this entry, 4 are 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, $95^{th}$ 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(Å²) | Q<0.9 |
|-----|-------|----------|--------|---------|---|---|----------|-------|
| 1 | A | 62/63 (98%) | 0.52 | 3 (4%) | 34 | 26 | 145, 159, 185, 203 | 0 |
| 2 | B | 67/67 (100%) | 0.82 | 7 (10%) | 8 | 7 | 147, 159, 187, 189 | 0 |
| 3 | C | 73/77 (94%) | 1.34 | 15 (20%) | 1 | 2 | 149, 165, 208, 220 | 0 |
| 4 | D | 64/65 (98%) | 0.38 | 2 (3%) | 52 | 41 | 145, 164, 207, 211 | 0 |
| 5 | E | 280/281 (99%) | 0.94 | 52 (18%) | 2 | 3 | 144, 185, 215, 265 | 0 |
| 5 | F | 268/281 (95%) | 1.63 | 94 (35%) | 0 | 1 | 166, 228, 287, 302 | 0 |
| All | All | 814/834 (97%) | 1.12 | 173 (21%) | 1 | 2 | 144, 186, 272, 302 | 0 |

All (173) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | F | 375 | LYS | 8.6 |
| 5 | F | 403 | GLN | 8.2 |
| 3 | C | 12 | GLU | 7.6 |
| 5 | F | 377 | PHE | 7.3 |
| 5 | E | 153 | PHE | 7.3 |
| 2 | B | 190 | MET | 7.3 |
| 5 | F | 252 | PHE | 7.1 |
| 5 | F | 373 | ILE | 7.1 |
| 5 | E | 150 | ASP | 6.7 |
| 3 | C | 13 | GLU | 6.5 |
| 3 | C | 16 | ARG | 6.4 |
| 5 | F | 295 | GLU | 6.3 |
| 3 | C | 15 | GLN | 6.2 |
| 5 | E | 151 | TYR | 6.1 |
| 3 | C | 10 | GLU | 6.0 |
| 5 | E | 216 | TYR | 6.0 |
| 5 | F | 402 | ALA | 5.9 |
| 5 | F | 374 | GLY | 5.7 |
| 5 | F | 376 | VAL | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | F | 194 | GLU | 5.3 |
| 5 | F | 173 | MET | 5.3 |
| 5 | F | 182 | LYS | 5.2 |
| 5 | F | 378 | VAL | 5.1 |
| 5 | E | 219 | LEU | 5.1 |
| 5 | E | 164 | GLN | 5.0 |
| 5 | F | 296 | ALA | 4.9 |
| 5 | E | 212 | PHE | 4.9 |
| 5 | F | 278 | PHE | 4.9 |
| 5 | F | 359 | VAL | 4.8 |
| 5 | F | 358 | VAL | 4.7 |
| 5 | F | 337 | PRO | 4.7 |
| 5 | E | 146 | GLN | 4.7 |
| 5 | E | 154 | GLN | 4.7 |
| 5 | E | 144 | LYS | 4.6 |
| 5 | F | 226 | MET | 4.6 |
| 5 | E | 377 | PHE | 4.6 |
| 5 | F | 404 | TRP | 4.4 |
| 5 | F | 357 | VAL | 4.4 |
| 5 | F | 388 | ARG | 4.4 |
| 5 | E | 226 | MET | 4.3 |
| 3 | C | 11 | LEU | 4.3 |
| 3 | C | 17 | ARG | 4.2 |
| 3 | C | 14 | MET | 4.2 |
| 5 | E | 213 | LYS | 4.2 |
| 5 | F | 276 | ILE | 4.2 |
| 5 | F | 210 | PHE | 4.1 |
| 5 | F | 346 | GLU | 4.1 |
| 5 | F | 361 | VAL | 4.0 |
| 5 | E | 222 | LYS | 4.0 |
| 5 | F | 206 | PHE | 4.0 |
| 5 | E | 218 | GLU | 3.9 |
| 5 | E | 147 | TYR | 3.9 |
| 3 | C | 19 | ASP | 3.9 |
| 5 | E | 257 | GLU | 3.9 |
| 5 | E | 152 | ASP | 3.9 |
| 5 | F | 324 | LYS | 3.9 |
| 5 | F | 279 | SER | 3.8 |
| 5 | E | 252 | PHE | 3.7 |
| 5 | F | 372 | ALA | 3.7 |
| 5 | E | 259 | TRP | 3.7 |
| 5 | F | 385 | ALA | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | F | 227 | ALA | 3.7 |
| 5 | E | 157 | GLN | 3.7 |
| 5 | F | 316 | LEU | 3.6 |
| 5 | F | 389 | HIS | 3.6 |
| 5 | F | 179 | PRO | 3.6 |
| 5 | F | 338 | TYR | 3.6 |
| 5 | E | 173 | MET | 3.5 |
| 5 | E | 378 | VAL | 3.5 |
| 5 | F | 244 | LYS | 3.5 |
| 5 | E | 375 | LYS | 3.4 |
| 5 | E | 156 | ASN | 3.4 |
| 3 | C | 18 | ALA | 3.4 |
| 5 | E | 163 | ILE | 3.4 |
| 5 | F | 288 | LYS | 3.3 |
| 5 | F | 401 | ILE | 3.3 |
| 5 | E | 205 | VAL | 3.3 |
| 5 | E | 158 | LEU | 3.2 |
| 5 | F | 299 | LEU | 3.2 |
| 5 | F | 219 | LEU | 3.2 |
| 5 | E | 214 | VAL | 3.2 |
| 5 | E | 165 | ALA | 3.2 |
| 5 | F | 390 | TRP | 3.1 |
| 5 | F | 356 | GLN | 3.1 |
| 2 | B | 246 | ARG | 3.1 |
| 5 | F | 209 | GLN | 3.1 |
| 5 | E | 162 | ILE | 3.1 |
| 5 | F | 408 | GLN | 3.1 |
| 5 | F | 222 | LYS | 3.1 |
| 5 | F | 275 | ASP | 3.0 |
| 5 | F | 145 | LEU | 3.0 |
| 5 | F | 417 | LEU | 3.0 |
| 5 | F | 181 | VAL | 3.0 |
| 5 | E | 145 | LEU | 3.0 |
| 5 | F | 147 | TYR | 2.9 |
| 5 | E | 193 | PHE | 2.9 |
| 5 | F | 277 | CYS | 2.9 |
| 5 | F | 280 | LEU | 2.9 |
| 5 | E | 243 | PHE | 2.9 |
| 5 | F | 174 | GLY | 2.9 |
| 5 | E | 166 | ALA | 2.9 |
| 5 | F | 379 | GLY | 2.8 |
| 5 | F | 198 | HIS | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | F | 242 | GLU | 2.8 |
| 5 | E | 417 | LEU | 2.8 |
| 5 | F | 282 | TYR | 2.8 |
| 5 | F | 355 | VAL | 2.7 |
| 5 | E | 256 | THR | 2.7 |
| 5 | F | 180 | TYR | 2.7 |
| 3 | C | 79 | LYS | 2.7 |
| 5 | F | 248 | ASN | 2.7 |
| 5 | F | 199 | ARG | 2.7 |
| 5 | F | 160 | VAL | 2.6 |
| 5 | E | 149 | LEU | 2.6 |
| 5 | F | 208 | GLU | 2.6 |
| 5 | F | 314 | ILE | 2.6 |
| 5 | E | 220 | GLY | 2.6 |
| 5 | E | 244 | LYS | 2.6 |
| 4 | D | 198 | ARG | 2.6 |
| 5 | F | 176 | THR | 2.6 |
| 5 | F | 162 | ILE | 2.6 |
| 1 | A | 86 | ARG | 2.6 |
| 5 | F | 243 | PHE | 2.6 |
| 3 | C | 70 | ASP | 2.6 |
| 5 | F | 334 | THR | 2.6 |
| 5 | F | 352 | ILE | 2.5 |
| 5 | F | 158 | LEU | 2.5 |
| 5 | F | 233 | ARG | 2.5 |
| 5 | E | 159 | LEU | 2.5 |
| 4 | D | 188 | ASN | 2.4 |
| 5 | F | 360 | THR | 2.4 |
| 5 | E | 204 | PRO | 2.4 |
| 5 | F | 171 | LEU | 2.4 |
| 1 | A | 56 | ARG | 2.4 |
| 5 | F | 205 | VAL | 2.4 |
| 5 | F | 235 | SER | 2.4 |
| 1 | A | 85 | LYS | 2.4 |
| 5 | F | 240 | ILE | 2.4 |
| 5 | F | 144 | LYS | 2.4 |
| 5 | F | 197 | VAL | 2.4 |
| 5 | E | 376 | VAL | 2.3 |
| 5 | E | 379 | GLY | 2.3 |
| 5 | F | 293 | ILE | 2.3 |
| 5 | F | 386 | GLU | 2.3 |
| 5 | E | 374 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | F | 315 | HIS | 2.3 |
| 5 | F | 348 | PRO | 2.3 |
| 5 | F | 344 | SER | 2.2 |
| 5 | F | 340 | ASN | 2.2 |
| 5 | F | 393 | MET | 2.2 |
| 5 | F | 294 | LEU | 2.2 |
| 5 | E | 242 | GLU | 2.2 |
| 2 | B | 251 | THR | 2.2 |
| 3 | C | 67 | ILE | 2.2 |
| 5 | F | 236 | LYS | 2.2 |
| 5 | F | 251 | ASP | 2.2 |
| 2 | B | 191 | ALA | 2.1 |
| 5 | F | 183 | VAL | 2.1 |
| 2 | B | 253 | LYS | 2.1 |
| 2 | B | 242 | ASP | 2.1 |
| 5 | E | 323 | LEU | 2.1 |
| 5 | F | 409 | VAL | 2.1 |
| 3 | C | 56 | GLN | 2.1 |
| 5 | E | 155 | ASN | 2.1 |
| 5 | F | 228 | VAL | 2.1 |
| 5 | E | 247 | MET | 2.1 |
| 5 | E | 251 | ASP | 2.1 |
| 5 | F | 341 | GLU | 2.1 |
| 3 | C | 64 | MET | 2.0 |
| 2 | B | 250 | ASP | 2.0 |
| 5 | E | 262 | LEU | 2.0 |
| 5 | E | 250 | VAL | 2.0 |
| 5 | F | 247 | MET | 2.0 |

## 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors($Å^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|------------------|-------|
| 6 | MG | F | 502 | 1/1 | 0.29 | 0.12 | -1.74 | 283,283,283,283 | 0 |
| 6 | MG | E | 502 | 1/1 | 0.95 | 0.14 | -1.76 | 160,160,160,160 | 0 |
| 6 | MG | F | 501 | 1/1 | 0.89 | 0.17 | -1.91 | 167,167,167,167 | 0 |
| 6 | MG | E | 501 | 1/1 | 0.92 | 0.22 | - | 197,197,197,197 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.