# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:21 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 3EAB |
| Title | : | Crystal structure of Spastin MIT in complex with ESCRT III |
| Authors | : | Yang, D.; Rimanchi, N.; Renvoise, B.; Lippincott-Schwartz, J.; Blackstone, C.; Hurley, J.H. |
| Deposited on | : | 2008-08-25 |
| Resolution | : | 2.50 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 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.
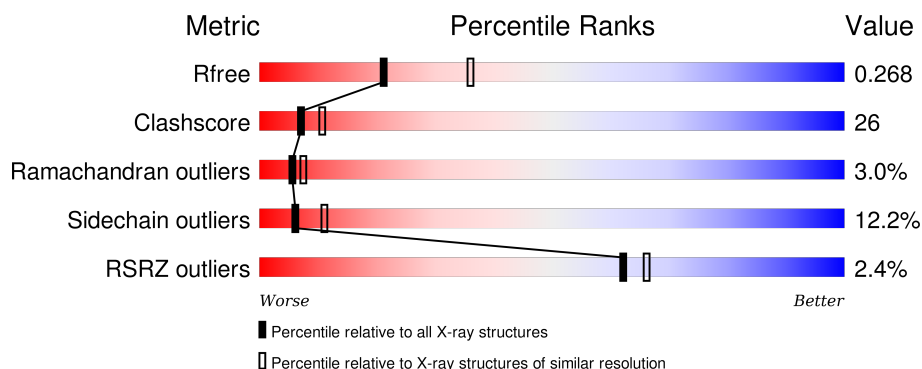


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 3553 (2.50-2.50) |
| Clashscore | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (2.50-2.50) |
| RSRZ outliers | 91569 | 3562 (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. 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 | 89 | 4%  55%  35%  8% • |
| 1 | B | 89 | %  57%  33%  7% •• |
| 1 | C | 89 | 3%  58%  37% •• |
| 1 | D | 89 | 4%  55%  33%  10% •• |
| 1 | E | 89 | 2%  71%  21% • • |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 89 | 3%  54%  37% |
| 2 | G | 50 | 54%  24%  20% |
| 2 | H | 50 | 50%  14%  14%  22% |
| 2 | I | 50 | 58%  14%  8%  18% |
| 2 | J | 50 | 2%  46%  18%  8%  26% |
| 2 | K | 50 | 44%  22%  8%  24% |
| 2 | L | 50 | 40%  30%  26% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5977 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 Spastin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 89 | Total 719 | C 448 | N 129 | O 136 | S 6 | 0 | 0 | 0 |
| 1 | B | 88 | Total 711 | C 443 | N 128 | O 135 | S 5 | 0 | 0 | 0 |
| 1 | C | 89 | Total 719 | C 448 | N 129 | O 136 | S 6 | 0 | 0 | 0 |
| 1 | D | 88 | Total 709 | C 443 | N 128 | O 132 | S 6 | 0 | 0 | 0 |
| 1 | E | 86 | Total 701 | C 438 | N 126 | O 132 | S 5 | 0 | 0 | 0 |
| 1 | F | 87 | Total 701 | C 437 | N 127 | O 131 | S 6 | 0 | 0 | 0 |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 108 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| A | 109 | GLY | - | EXPRESSION TAG | UNP Q9UBP0 |
| A | 110 | SER | - | EXPRESSION TAG | UNP Q9UBP0 |
| A | 111 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| B | 108 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| B | 109 | GLY | - | EXPRESSION TAG | UNP Q9UBP0 |
| B | 110 | SER | - | EXPRESSION TAG | UNP Q9UBP0 |
| B | 111 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| C | 108 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| C | 109 | GLY | - | EXPRESSION TAG | UNP Q9UBP0 |
| C | 110 | SER | - | EXPRESSION TAG | UNP Q9UBP0 |
| C | 111 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| D | 108 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| D | 109 | GLY | - | EXPRESSION TAG | UNP Q9UBP0 |
| D | 110 | SER | - | EXPRESSION TAG | UNP Q9UBP0 |
| D | 111 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| E | 108 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| E | 109 | GLY | - | EXPRESSION TAG | UNP Q9UBP0 |
| E | 110 | SER | - | EXPRESSION TAG | UNP Q9UBP0 |
| E | 111 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| F | 108 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |
| F | 109 | GLY | - | EXPRESSION TAG | UNP Q9UBP0 |
| F | 110 | SER | - | EXPRESSION TAG | UNP Q9UBP0 |
| F | 111 | MET | - | EXPRESSION TAG | UNP Q9UBP0 |

- Molecule 2 is a protein called CHMP1b.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 2 | G | 40 | Total 297 | C 176 | N 53 | O 66 | S 2 | 0 | 0 | 0 |
| 2 | H | 39 | Total 290 | C 170 | N 51 | O 67 | S 2 | 0 | 0 | 0 |
| 2 | I | 41 | Total 307 | C 182 | N 54 | O 69 | S 2 | 0 | 0 | 0 |
| 2 | J | 37 | Total 271 | C 160 | N 47 | O 62 | S 2 | 0 | 0 | 0 |
| 2 | K | 38 | Total 281 | C 167 | N 50 | O 62 | S 2 | 0 | 0 | 0 |
| 2 | L | 37 | Total 271 | C 162 | N 47 | O 60 | S 2 | 0 | 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 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: Spastin



- Molecule 1: Spastin



- Molecule 1: Spastin



- Molecule 1: Spastin



- Molecule 1: Spastin

Chain E:

2%

71%

21%

MET GLY SER M111 E114 R115 V118 F119 E125 E137 K138 Q141 K142 E143 K150 I153 T165 G166 Q167 G168 C171 A174 L177 M184 L185 R191 L192 E196

● Molecule 1: Spastin

Chain F:

3%

54%

37%

M108 G109 S110 M111 E114 R115 V118 F119 H120 K121 S128 L131 E137 K138 Q141 K142 E143 Q144 A145 V146 E147 W148 Y149 K150 K151 G152 I153 L156 E157 I160 A161 V162 I163 V164 T165 G166 Q167 G168 E169 Q170 C171 E172 R173 M181 L185 A188 K189 D190 R191

L192 Q193 L194 LEU GLU

● Molecule 2: CHMP1b

Chain G:

54%

24%

20%

Q148 L152 L153 Q154 E155 M156 D163 LEU ASN MET GLU LEU PRO GLN GLY GLN T173 V176 E184 Q185 D186 E187 L188 R191 L192 L195 R196 ASP

● Molecule 2: CHMP1b

Chain H:

50%

14%

14%

22%

GLN VAL D150 A160 G161 L162 D163 LEU ASN MET GLU LEU PRO GLN GLY GLN T173 G174 S175 V176 G177 S182 L188 R191 L192 L195 R196 D197

● Molecule 2: CHMP1b

Chain I:

58%

14%

8%

18%

Q148 M151 L152 L153 Q154 E155 M156 A157 D158 E159 L164 ASN MET GLU LEU PRO GLN GLY GLN THR G174 E184 Q185 D186 R191 L195 R196 D197

● Molecule 2: CHMP1b

Chain J:

2%

46%

18%

8%

26%

Q148 V149 D150 M151 L152 M156 A157 D158 E159 A160 D163 LEU ASN MET GLU LEU PRO GLN GLY GLN THR G174 S175 V176 V180 E184 Q185 A193 R194 LEU ARG ASP

● Molecule 2: CHMP1b

Chain K:

44%

22%

8%

24%

GLN V149 D150 M151 L152 L153 Q154 E159 A160 G161 L162 D163 LEU ASN MET GLU LEU PRO GLN GLY GLN THR G174 S175 V176 G177 Q185 D186 E187 R191 L192 A193 R194 L195 R196 ASP

● Molecule 2: CHMP1b

Chain L:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|----------|-------|--------|
| Space group | P 21 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 151.97Å    95.49Å    100.36Å<br>90.00°    90.00°    90.00° | Depositor |
| Resolution (Å) | 47.65   –   2.50<br>47.65   –   2.30 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.7 (47.65-2.50)<br>84.6 (47.65-2.30) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.17 (at 2.29Å) | Xtriage |
| Refinement program | CNS1.1 and Refmac | Depositor |
| R, $R_{free}$ | 0.232   ,   0.268<br>0.232   ,   0.268 | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | DCC |
| Wilson B-factor (Å$^2$) | 37.5 | Xtriage |
| Anisotropy | 0.834 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 56.8 | EDS |
| Estimated twinning fraction | 0.029 for -h,l,k | Xtriage |
| L-test for twinning[2] | $< |L| > = 0.47, < L^2 > = 0.29$ | Xtriage |
| Outliers | 1 of 59568 reflections (0.002%) | Xtriage |
| $F_o,F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 5977 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 53.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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 (i)

## 5.1 Standard geometry (i)

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 | 0.50 | 0/725 | 0.48 | 0/963 |
| 1 | B | 0.81 | 3/717 (0.4%) | 0.62 | 1/953 (0.1%) |
| 1 | C | 0.76 | 1/725 (0.1%) | 0.56 | 1/963 (0.1%) |
| 1 | D | 0.47 | 0/715 | 0.54 | 0/951 |
| 1 | E | 0.48 | 0/707 | 0.52 | 0/940 |
| 1 | F | 0.76 | 2/707 (0.3%) | 0.63 | 1/940 (0.1%) |
| 2 | G | 0.35 | 0/295 | 0.51 | 0/394 |
| 2 | H | 0.43 | 0/288 | 0.56 | 0/383 |
| 2 | I | 0.36 | 0/305 | 0.52 | 0/406 |
| 2 | J | 0.42 | 0/269 | 0.55 | 0/359 |
| 2 | K | 0.44 | 0/279 | 0.60 | 0/372 |
| 2 | L | 0.34 | 0/269 | 0.52 | 0/359 |
| All | All | 0.59 | 6/6001 (0.1%) | 0.56 | 3/7983 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | C | 0 | 2 |
| 1 | E | 0 | 2 |
| 1 | F | 0 | 1 |
| 2 | J | 0 | 2 |
| All | All | 0 | 9 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | C | 150 | LYS | CE-NZ | 15.49 | 1.87 | 1.49 |
| 1 | B | 150 | LYS | CE-NZ | 14.85 | 1.86 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | F | 121 | LYS | CE-NZ | 11.64 | 1.78 | 1.49 |
| 1 | F | 121 | LYS | CD-CE | 8.19 | 1.71 | 1.51 |
| 1 | B | 121 | LYS | CE-NZ | 7.81 | 1.68 | 1.49 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | F | 121 | LYS | CD-CE-NZ | -7.89 | 93.55 | 111.70 |
| 1 | B | 150 | LYS | CD-CE-NZ | -7.62 | 94.19 | 111.70 |
| 1 | C | 150 | LYS | CD-CE-NZ | -6.81 | 96.03 | 111.70 |

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 167 | GLN | Peptide |
| 1 | B | 138 | LYS | Peptide |
| 1 | C | 138 | LYS | Peptide |
| 1 | C | 166 | GLY | Peptide |
| 1 | E | 166 | GLY | Peptide |

## 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 | A | 719 | 0 | 733 | 41 | 0 |
| 1 | B | 711 | 0 | 724 | 65 | 1 |
| 1 | C | 719 | 0 | 733 | 27 | 0 |
| 1 | D | 709 | 0 | 727 | 42 | 1 |
| 1 | E | 701 | 0 | 716 | 30 | 0 |
| 1 | F | 701 | 0 | 716 | 46 | 1 |
| 2 | G | 297 | 0 | 288 | 17 | 0 |
| 2 | H | 290 | 0 | 275 | 19 | 0 |
| 2 | I | 307 | 0 | 296 | 15 | 0 |
| 2 | J | 271 | 0 | 257 | 19 | 0 |
| 2 | K | 281 | 0 | 273 | 15 | 0 |
| 2 | L | 271 | 0 | 264 | 23 | 1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 5977 | 0 | 6002 | 315 | 3 |

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 26.

The worst 5 of 315 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:B:121:LYS:CE | 1:B:121:LYS:NZ | 1.68 | 1.51 |
| 1:F:121:LYS:NZ | 1:F:121:LYS:CE | 1.78 | 1.46 |
| 1:B:150:LYS:CE | 1:B:150:LYS:NZ | 1.86 | 1.39 |
| 1:C:150:LYS:CE | 1:C:150:LYS:NZ | 1.87 | 1.37 |
| 2:J:194:ARG:N | 2:J:194:ARG:HD3 | 1.12 | 1.21 |

All (3) 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:L:156:MET:CE | 2:L:156:MET:CE[2_555] | 1.72 | 0.48 |
| 1:B:147:GLU:OE2 | 1:D:144:GLN:NE2[4_457] | 1.89 | 0.31 |
| 1:F:144:GLN:NE2 | 1:F:147:GLU:OE2[2_555] | 2.17 | 0.03 |

## 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 | 87/89 (98%) | 78 (90%) | 6 (7%) | 3 (3%) | 5 | 6 |
| 1 | B | 86/89 (97%) | 81 (94%) | 4 (5%) | 1 (1%) | 16 | 29 |
| 1 | C | 87/89 (98%) | 85 (98%) | 0 | 2 (2%) | 8 | 12 |
| 1 | D | 86/89 (97%) | 76 (88%) | 6 (7%) | 4 (5%) | 3 | 3 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|------|------|
| 1 | E | 84/89 (94%) | 82 (98%) | 1 (1%) | 1 (1%) | 16 | 29 |
| 1 | F | 85/89 (96%) | 79 (93%) | 3 (4%) | 3 (4%) | 4 | 6 |
| 2 | G | 36/50 (72%) | 33 (92%) | 3 (8%) | 0 | 100 | 100 |
| 2 | H | 35/50 (70%) | 30 (86%) | 3 (9%) | 2 (6%) | 2 | 2 |
| 2 | I | 37/50 (74%) | 33 (89%) | 3 (8%) | 1 (3%) | 6 | 9 |
| 2 | J | 33/50 (66%) | 30 (91%) | 2 (6%) | 1 (3%) | 5 | 7 |
| 2 | K | 34/50 (68%) | 29 (85%) | 3 (9%) | 2 (6%) | 2 | 2 |
| 2 | L | 33/50 (66%) | 29 (88%) | 2 (6%) | 2 (6%) | 2 | 1 |
| All | All | 723/834 (87%) | 665 (92%) | 36 (5%) | 22 (3%) | 5 | 7 |

5 of 22 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 109 | GLY |
| 1 | A | 138 | LYS |
| 1 | B | 138 | LYS |
| 1 | C | 138 | LYS |
| 1 | D | 193 | GLN |

### 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 | 74/74 (100%) | 62 (84%) | 12 (16%) | 3 | 5 |
| 1 | B | 73/74 (99%) | 64 (88%) | 9 (12%) | 6 | 11 |
| 1 | C | 74/74 (100%) | 67 (90%) | 7 (10%) | 11 | 20 |
| 1 | D | 73/74 (99%) | 64 (88%) | 9 (12%) | 6 | 11 |
| 1 | E | 72/74 (97%) | 68 (94%) | 4 (6%) | 26 | 47 |
| 1 | F | 72/74 (97%) | 63 (88%) | 9 (12%) | 6 | 10 |
| 2 | G | 32/41 (78%) | 28 (88%) | 4 (12%) | 6 | 10 |
| 2 | H | 31/41 (76%) | 26 (84%) | 5 (16%) | 3 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|----|----|
| 2 | I | 33/41 (80%) | 27 (82%) | 6 (18%) | 2 | 3 |
| 2 | J | 29/41 (71%) | 25 (86%) | 4 (14%) | 4 | 8 |
| 2 | K | 30/41 (73%) | 24 (80%) | 6 (20%) | 1 | 3 |
| 2 | L | 29/41 (71%) | 28 (97%) | 1 (3%) | 44 | 72 |
| All | All | 622/690 (90%) | 546 (88%) | 76 (12%) | 6 | 11 |

5 of 76 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 190 | ASP |
| 1 | F | 110 | SER |
| 2 | K | 159 | GLU |
| 1 | D | 194 | LEU |
| 1 | E | 125 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 184 | ASN |
| 1 | F | 144 | GLN |
| 2 | K | 185 | GLN |
| 1 | E | 178 | GLN |
| 1 | E | 184 | 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)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

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 | 89/89 (100%) | -0.18 | 4 (4%) | 37 | 42 | 30, 53, 106, 120 | 0 |
| 1 | B | 88/89 (98%) | -0.42 | 1 (1%) | 82 | 84 | 29, 46, 92, 121 | 0 |
| 1 | C | 89/89 (100%) | -0.40 | 3 (3%) | 49 | 54 | 25, 44, 82, 119 | 0 |
| 1 | D | 88/89 (98%) | -0.13 | 4 (4%) | 37 | 42 | 34, 55, 92, 110 | 0 |
| 1 | E | 86/89 (96%) | -0.43 | 2 (2%) | 64 | 67 | 28, 47, 93, 124 | 0 |
| 1 | F | 87/89 (97%) | -0.29 | 3 (3%) | 49 | 54 | 37, 54, 85, 126 | 0 |
| 2 | G | 40/50 (80%) | -0.38 | 0 | 100 | 100 | 37, 50, 81, 95 | 0 |
| 2 | H | 39/50 (78%) | -0.50 | 0 | 100 | 100 | 28, 46, 88, 97 | 0 |
| 2 | I | 41/50 (82%) | -0.42 | 0 | 100 | 100 | 26, 45, 84, 94 | 0 |
| 2 | J | 37/50 (74%) | -0.02 | 1 (2%) | 58 | 62 | 34, 45, 89, 95 | 0 |
| 2 | K | 38/50 (76%) | -0.13 | 0 | 100 | 100 | 29, 43, 85, 98 | 0 |
| 2 | L | 37/50 (74%) | -0.51 | 0 | 100 | 100 | 34, 47, 69, 79 | 0 |
| All | All | 759/834 (91%) | -0.31 | 18 (2%) | 62 | 66 | 25, 49, 92, 126 | 0 |

The worst 5 of 18 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 111 | MET | 4.2 |
| 1 | F | 138 | LYS | 3.6 |
| 1 | A | 108 | MET | 3.5 |
| 1 | A | 167 | GLN | 3.0 |
| 1 | D | 163 | ILE | 2.8 |

## 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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.