



## Full wwPDB EM Validation Report ⓘ

Nov 25, 2023 – 07:17 am GMT

PDB ID : 8Q6T  
EMDB ID : EMD-18198  
Title : Helical reconstruction of the relaxed thick filament from FIB milled left ventricular mouse myofibrils  
Authors : Tamborrini, D.; Raunser, S.  
Deposited on : 2023-08-14  
Resolution : 18.00 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

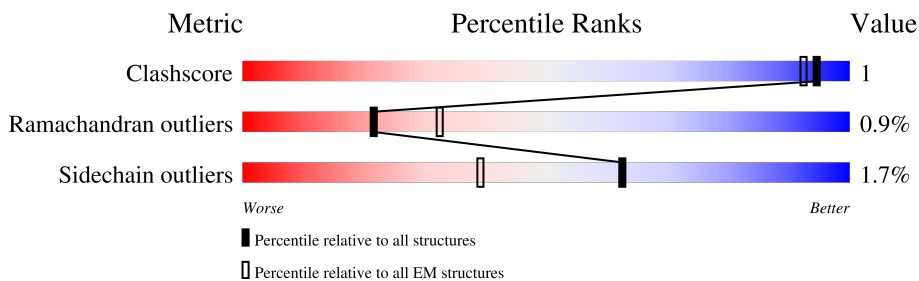
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 18.00 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) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| Ramachandran outliers | 154571                   | 4023                     |
| Sidechain outliers    | 154315                   | 3826                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1935   |                  |
| 1   | B     | 1935   |                  |
| 1   | H     | 1935   |                  |
| 1   | N     | 1935   |                  |
| 1   | O     | 1935   |                  |
| 1   | Q     | 1935   |                  |
| 2   | C     | 152    |                  |
| 2   | D     | 152    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | J     | 152    | <br>5% 95% 5%    |
| 2   | K     | 152    | <br>93% 6%       |
| 2   | R     | 152    | <br>94% 6%       |
| 2   | S     | 152    | <br>11% 95%      |
| 3   | E     | 160    | <br>16% 94% 5%   |
| 3   | F     | 160    | <br>12% 94% 5%   |
| 3   | L     | 160    | <br>8% 92% 7%    |
| 3   | M     | 160    | <br>96%          |
| 3   | T     | 160    | <br>12% 93% 6%   |
| 3   | U     | 160    | <br>92% 7%       |
| 4   | G     | 400    | <br>96%          |
| 4   | V     | 400    | <br>94% 6%       |
| 5   | I     | 1079   | <br>97%          |
| 5   | P     | 1079   | <br>95%          |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 131418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Myosin-7.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |       |
| 1   | A     | 1926     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15571 | 9670 | 2761 | 3076 | 64 |         |       |
| 1   | B     | 1926     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15571 | 9670 | 2761 | 3076 | 64 |         |       |
| 1   | H     | 1930     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15600 | 9690 | 2765 | 3080 | 65 |         |       |
| 1   | N     | 1930     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15600 | 9690 | 2765 | 3080 | 65 |         |       |
| 1   | O     | 1926     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15571 | 9670 | 2761 | 3076 | 64 |         |       |
| 1   | Q     | 1926     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15571 | 9670 | 2761 | 3076 | 64 |         |       |

- Molecule 2 is a protein called Myosin light chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 2   | C     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 758 | 200 | 239 | 9 |         |       |
| 2   | D     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 758 | 200 | 239 | 9 |         |       |
| 2   | J     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 758 | 200 | 239 | 9 |         |       |
| 2   | K     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 758 | 200 | 239 | 9 |         |       |
| 2   | R     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 758 | 200 | 239 | 9 |         |       |
| 2   | S     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 758 | 200 | 239 | 9 |         |       |

- Molecule 3 is a protein called Myosin regulatory light chain 2, ventricular/cardiac muscle isoform.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | E     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 811 | 211 | 255 | 6 |         |       |
| 3   | F     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 811 | 211 | 255 | 6 |         |       |
| 3   | L     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 811 | 211 | 255 | 6 |         |       |
| 3   | M     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 811 | 211 | 255 | 6 |         |       |
| 3   | T     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 811 | 211 | 255 | 6 |         |       |
| 3   | U     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 811 | 211 | 255 | 6 |         |       |

- Molecule 4 is a protein called Myosin binding protein C, cardiac.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | G     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3151  | 2002 | 556 | 579 | 14 |         |       |
| 4   | V     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3151  | 2002 | 556 | 579 | 14 |         |       |

- Molecule 5 is a protein called Titin.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 5   | I     | 1079     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8349  | 5261 | 1424 | 1637 | 27 |         |       |
| 5   | P     | 1079     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8349  | 5261 | 1424 | 1637 | 27 |         |       |

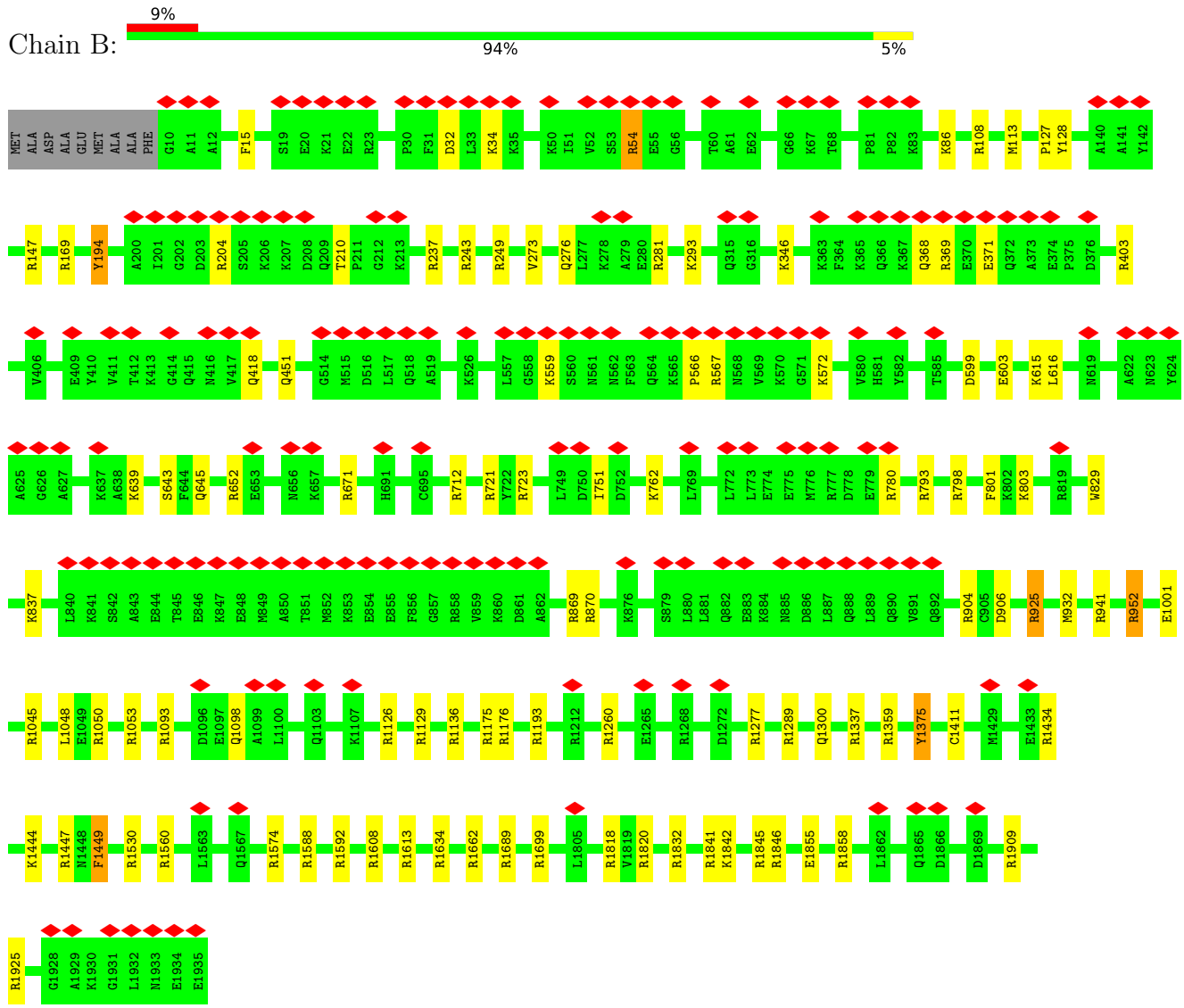
### 3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

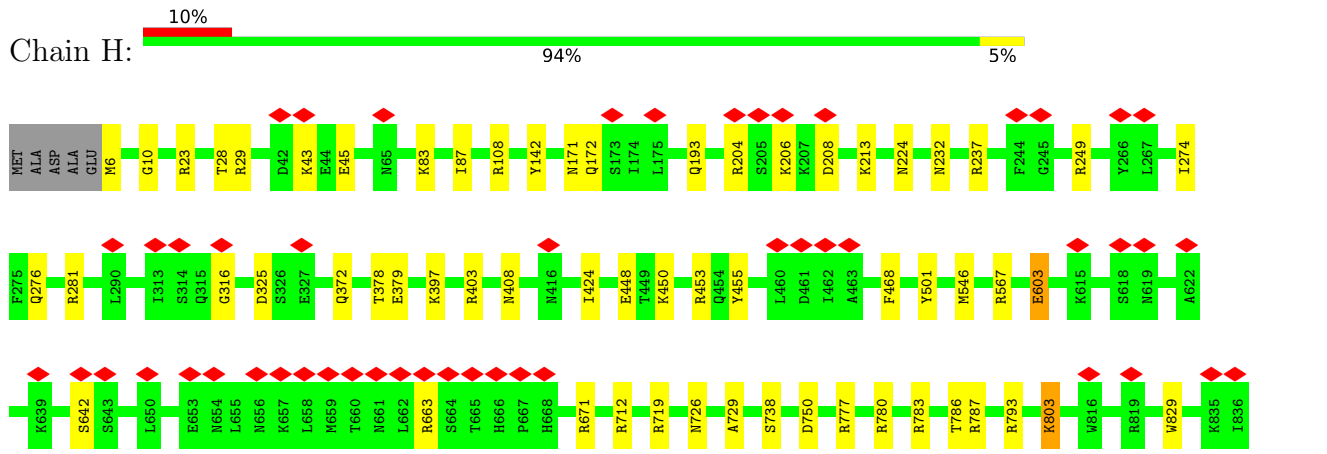
- Molecule 1: Myosin-7

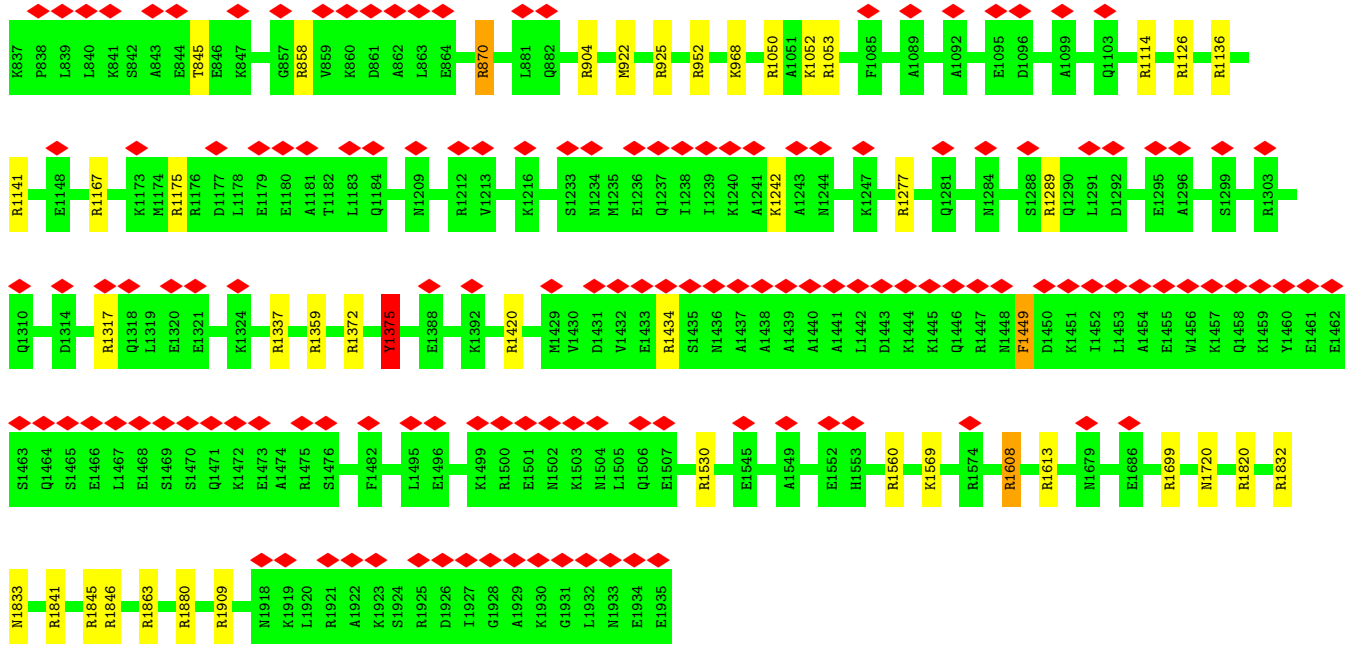


• Molecule 1: Myosin-7

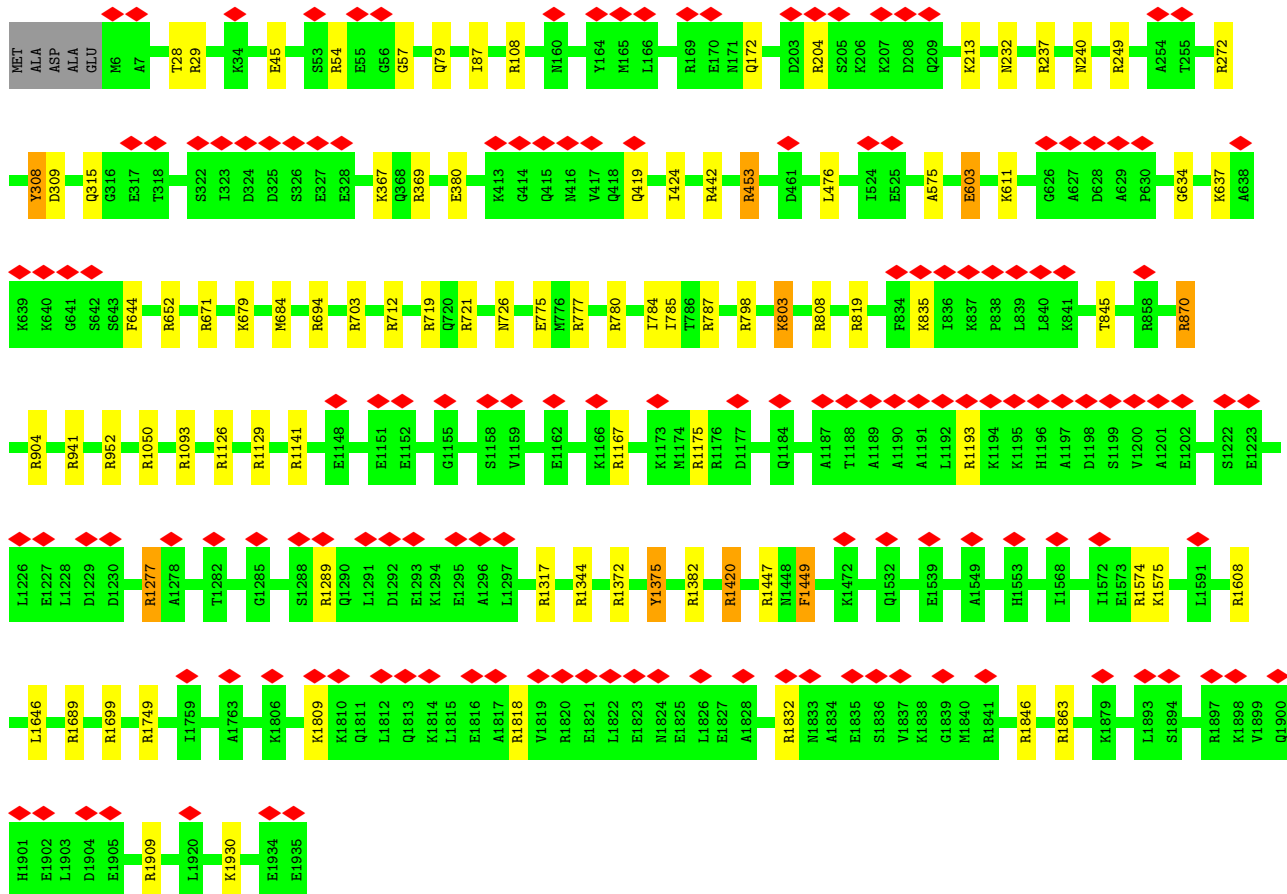


• Molecule 1: Myosin-7



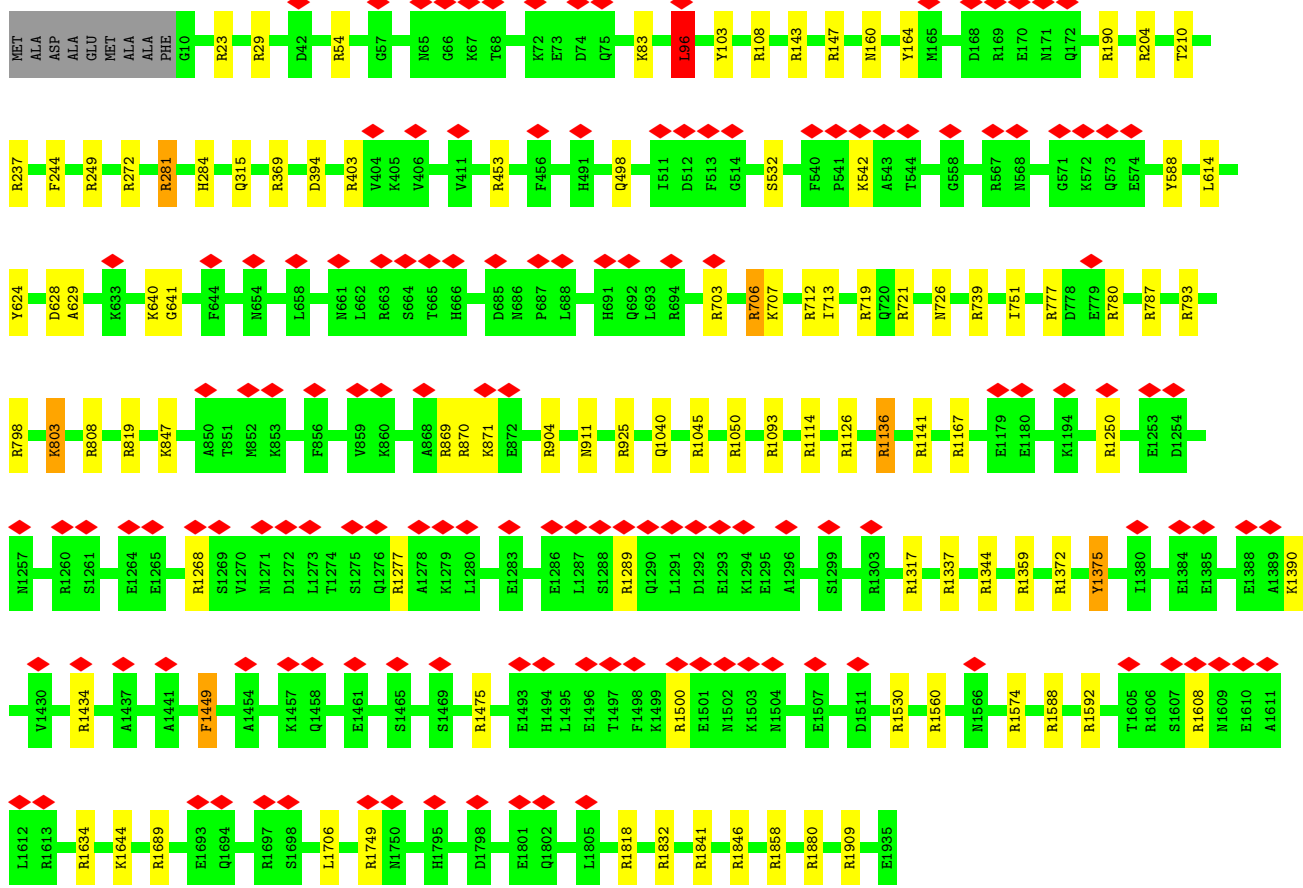


• Molecule 1: Myosin-7

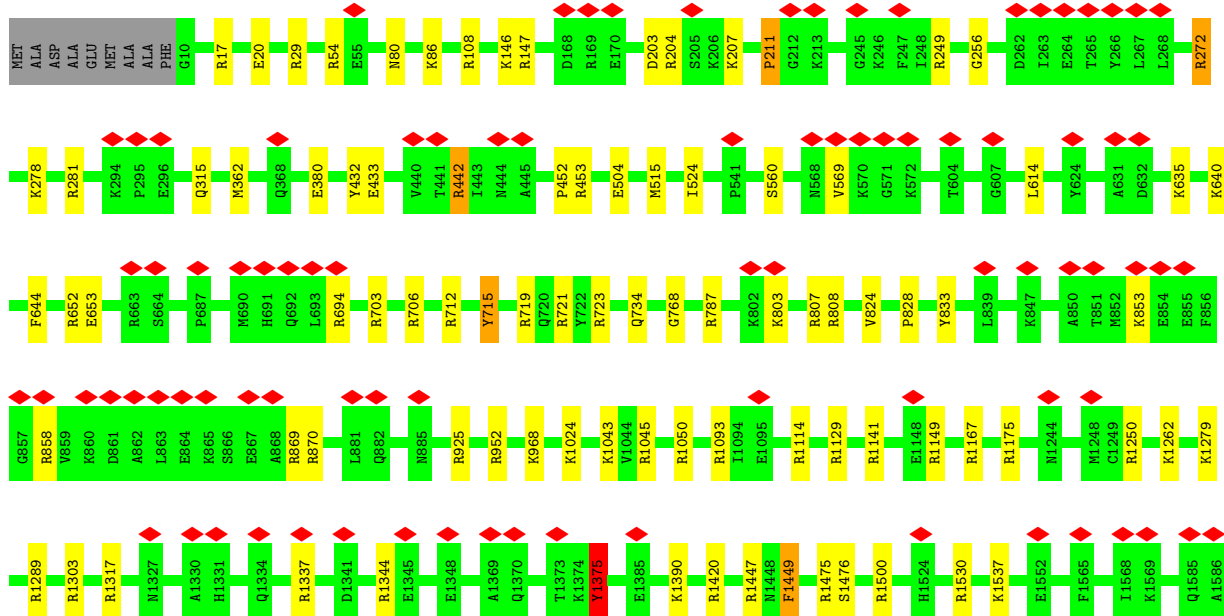


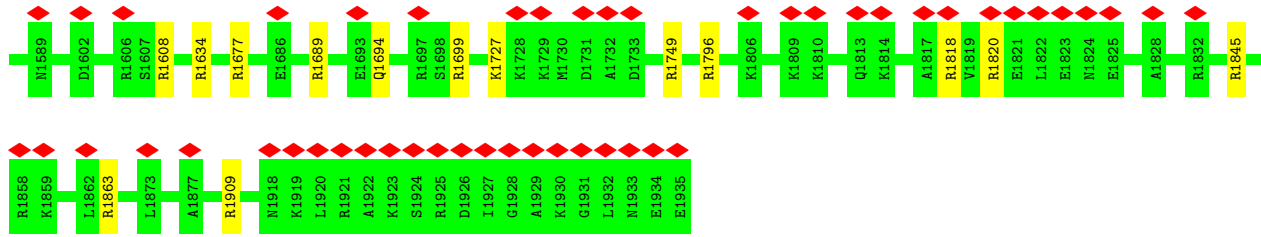
• Molecule 1: Myosin-7



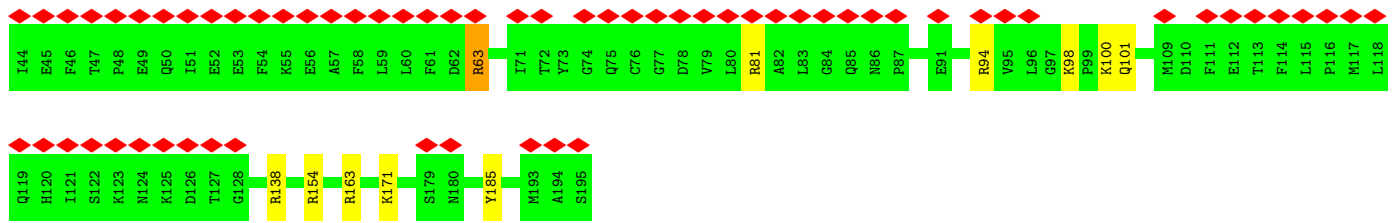
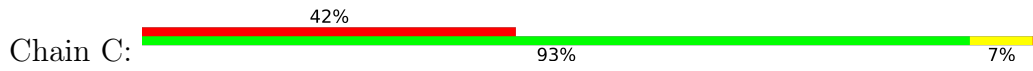


• Molecule 1: Myosin-7

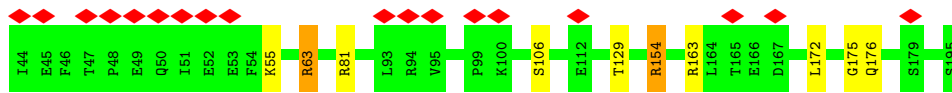




• Molecule 2: Myosin light chain 3



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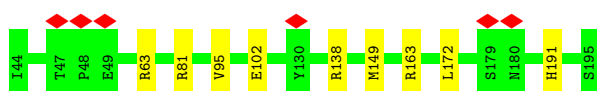
• Molecule 2: Myosin light chain 3



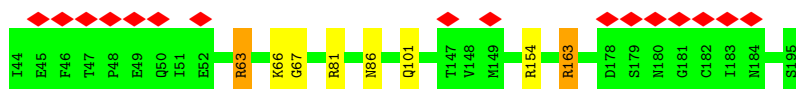
• Molecule 2: Myosin light chain 3



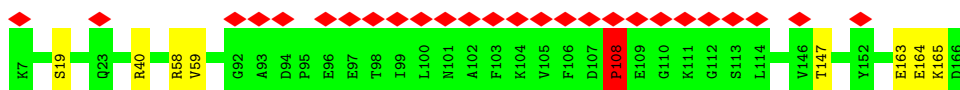
• Molecule 2: Myosin light chain 3



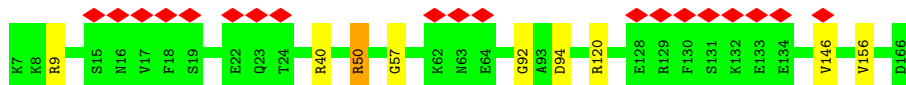
• Molecule 2: Myosin light chain 3



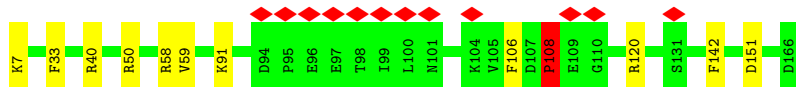
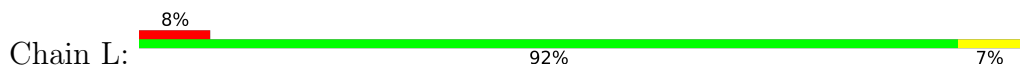
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform



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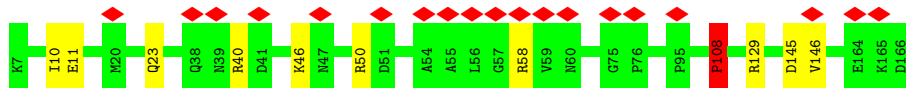
- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform



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- Molecule 3: Myosin regulatory light chain 2, ventricular/cardiac muscle isoform

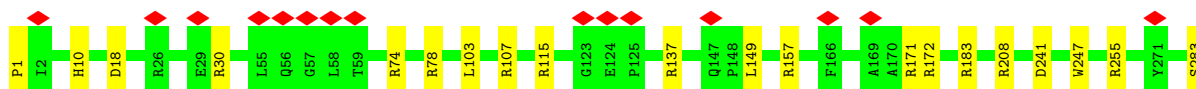




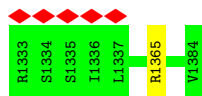
- Molecule 4: Myosin binding protein C, cardiac



- Molecule 4: Myosin binding protein C, cardiac

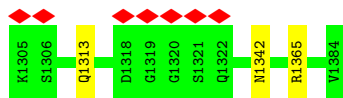


- Molecule 5: Titin



- Molecule 5: Titin





## 4 Experimental information

| Property                           | Value                                       | Source    |
|------------------------------------|---|-----------|
| EM reconstruction method           | SUBTOMOGRAM AVERAGING                       | Depositor |
| Imposed symmetry                   | HELICAL, twist=0°, rise=430 Å, axial sym=C3 | Depositor |
| Number of subtomograms used        | 1589  | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                           | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION     | Depositor |
| Microscope                         | FEI TITAN KRIOS                             | Depositor |
| Voltage (kV)                       | 300   | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 140   | Depositor |
| Minimum defocus (nm)               | 3000  | Depositor |
| Maximum defocus (nm)               | 6000  | Depositor |
| Magnification                      | 81000                                       | Depositor |
| Image detector                     | GATAN K3 BIOQUANTUM (6k x 4k)               | Depositor |
| Maximum map value                  | 13.522                                      | Depositor |
| Minimum map value                  | 0.000                                       | Depositor |
| Average map value                  | 0.028                                       | Depositor |
| Map value standard deviation       | 0.387                                       | Depositor |
| Recommended contour level          | 2.41  | Depositor |
| Map size (Å)                       | 2168.76, 2168.76, 2168.76                   | wwPDB     |
| Map dimensions                     | 372, 372, 372                               | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                            | wwPDB     |
| Pixel spacing (Å)                  | 5.83, 5.83, 5.83                            | Depositor |

## 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     | 1.24         | 13/15751 (0.1%)  | 0.95        | 66/21093 (0.3%)   |
| 1   | B     | 1.14         | 13/15751 (0.1%)  | 0.97        | 69/21093 (0.3%)   |
| 1   | H     | 1.24         | 13/15781 (0.1%)  | 0.95        | 64/21133 (0.3%)   |
| 1   | N     | 1.24         | 13/15781 (0.1%)  | 0.94        | 65/21133 (0.3%)   |
| 1   | O     | 1.14         | 12/15751 (0.1%)  | 0.97        | 81/21093 (0.4%)   |
| 1   | Q     | 1.14         | 12/15751 (0.1%)  | 0.95        | 69/21093 (0.3%)   |
| 2   | C     | 0.70         | 0/1225           | 0.97        | 5/1643 (0.3%)     |
| 2   | D     | 0.71         | 0/1225           | 0.98        | 4/1643 (0.2%)     |
| 2   | J     | 0.71         | 0/1225           | 0.93        | 2/1643 (0.1%)     |
| 2   | K     | 0.72         | 0/1225           | 0.98        | 5/1643 (0.3%)     |
| 2   | R     | 0.71         | 0/1225           | 0.94        | 4/1643 (0.2%)     |
| 2   | S     | 0.72         | 0/1225           | 0.95        | 3/1643 (0.2%)     |
| 3   | E     | 1.69         | 5/1306 (0.4%)    | 0.94        | 1/1752 (0.1%)     |
| 3   | F     | 0.74         | 0/1306           | 0.99        | 4/1752 (0.2%)     |
| 3   | L     | 1.70         | 5/1306 (0.4%)    | 0.93        | 2/1752 (0.1%)     |
| 3   | M     | 0.74         | 0/1306           | 0.95        | 3/1752 (0.2%)     |
| 3   | T     | 1.70         | 5/1306 (0.4%)    | 0.93        | 4/1752 (0.2%)     |
| 3   | U     | 0.73         | 0/1306           | 0.96        | 2/1752 (0.1%)     |
| 4   | G     | 0.72         | 0/3233           | 1.01        | 11/4398 (0.3%)    |
| 4   | V     | 0.72         | 0/3233           | 1.02        | 15/4398 (0.3%)    |
| 5   | I     | 0.70         | 0/8525           | 0.96        | 23/11602 (0.2%)   |
| 5   | P     | 0.70         | 0/8525           | 0.98        | 28/11602 (0.2%)   |
| All | All   | 1.11         | 91/133268 (0.1%) | 0.96        | 530/179008 (0.3%) |

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                   | 2                   |
| 1   | H     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | O     | 0                   | 1                   |
| 1   | Q     | 0                   | 5                   |
| 2   | S     | 0                   | 1                   |
| 3   | L     | 0                   | 1                   |
| 5   | I     | 0                   | 1                   |
| 5   | P     | 0                   | 1                   |
| All | All   | 0                   | 15                  |

All (91) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | H     | 1375 | TYR  | CD2-CE2 | 75.26 | 2.52        | 1.39     |
| 1   | O     | 1375 | TYR  | CD2-CE2 | 75.22 | 2.52        | 1.39     |
| 1   | A     | 1375 | TYR  | CD2-CE2 | 75.14 | 2.52        | 1.39     |
| 1   | B     | 1375 | TYR  | CD2-CE2 | 75.09 | 2.52        | 1.39     |
| 1   | N     | 1375 | TYR  | CD2-CE2 | 75.08 | 2.52        | 1.39     |
| 1   | Q     | 1375 | TYR  | CD1-CE1 | 75.03 | 2.52        | 1.39     |
| 1   | N     | 803  | LYS  | CD-CE   | 59.51 | 3.00        | 1.51     |
| 1   | A     | 803  | LYS  | CD-CE   | 59.47 | 3.00        | 1.51     |
| 1   | H     | 803  | LYS  | CD-CE   | 59.40 | 2.99        | 1.51     |
| 1   | A     | 1449 | PHE  | CD1-CE1 | 56.63 | 2.52        | 1.39     |
| 1   | Q     | 1449 | PHE  | CD1-CE1 | 56.56 | 2.52        | 1.39     |
| 1   | O     | 1449 | PHE  | CD1-CE1 | 56.38 | 2.52        | 1.39     |
| 1   | N     | 1449 | PHE  | CD2-CE2 | 56.33 | 2.51        | 1.39     |
| 1   | H     | 1449 | PHE  | CD2-CE2 | 56.32 | 2.51        | 1.39     |
| 1   | B     | 1449 | PHE  | CD2-CE2 | 56.24 | 2.51        | 1.39     |
| 3   | T     | 108  | PRO  | N-CD    | 33.32 | 1.94        | 1.47     |
| 3   | L     | 108  | PRO  | N-CD    | 32.17 | 1.92        | 1.47     |
| 3   | E     | 108  | PRO  | N-CD    | 32.12 | 1.92        | 1.47     |
| 3   | L     | 108  | PRO  | N-CA    | 29.00 | 1.96        | 1.47     |
| 3   | T     | 108  | PRO  | N-CA    | 28.90 | 1.96        | 1.47     |
| 3   | E     | 108  | PRO  | N-CA    | 28.77 | 1.96        | 1.47     |
| 3   | T     | 108  | PRO  | CA-CB   | 27.50 | 2.08        | 1.53     |
| 3   | E     | 108  | PRO  | CA-CB   | 27.47 | 2.08        | 1.53     |
| 3   | L     | 108  | PRO  | CA-CB   | 27.41 | 2.08        | 1.53     |
| 1   | H     | 1375 | TYR  | CE2-CZ  | 26.05 | 1.72        | 1.38     |
| 1   | A     | 1375 | TYR  | CE2-CZ  | 26.05 | 1.72        | 1.38     |
| 1   | O     | 1375 | TYR  | CE2-CZ  | 26.01 | 1.72        | 1.38     |
| 1   | Q     | 1375 | TYR  | CE1-CZ  | 25.95 | 1.72        | 1.38     |
| 1   | B     | 1375 | TYR  | CE2-CZ  | 25.94 | 1.72        | 1.38     |
| 1   | N     | 1375 | TYR  | CE2-CZ  | 25.82 | 1.72        | 1.38     |
| 1   | H     | 1375 | TYR  | CG-CD2  | 25.47 | 1.72        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1375 | TYR  | CG-CD2  | 25.46 | 1.72        | 1.39     |
| 1   | N     | 1375 | TYR  | CG-CD2  | 25.43 | 1.72        | 1.39     |
| 1   | O     | 1375 | TYR  | CG-CD2  | 25.27 | 1.72        | 1.39     |
| 1   | A     | 1375 | TYR  | CG-CD2  | 25.16 | 1.71        | 1.39     |
| 1   | Q     | 1375 | TYR  | CG-CD1  | 25.04 | 1.71        | 1.39     |
| 1   | Q     | 1375 | TYR  | CE2-CZ  | 24.58 | 1.70        | 1.38     |
| 1   | N     | 1375 | TYR  | CE1-CZ  | 24.54 | 1.70        | 1.38     |
| 1   | A     | 1375 | TYR  | CE1-CZ  | 24.34 | 1.70        | 1.38     |
| 1   | O     | 1375 | TYR  | CE1-CZ  | 24.27 | 1.70        | 1.38     |
| 1   | H     | 1375 | TYR  | CE1-CZ  | 24.25 | 1.70        | 1.38     |
| 1   | B     | 1375 | TYR  | CE1-CZ  | 24.18 | 1.70        | 1.38     |
| 1   | B     | 1375 | TYR  | CG-CD1  | 23.71 | 1.70        | 1.39     |
| 1   | N     | 1375 | TYR  | CG-CD1  | 23.69 | 1.70        | 1.39     |
| 1   | Q     | 1375 | TYR  | CG-CD2  | 23.61 | 1.69        | 1.39     |
| 1   | H     | 1375 | TYR  | CG-CD1  | 23.53 | 1.69        | 1.39     |
| 1   | A     | 1375 | TYR  | CG-CD1  | 23.40 | 1.69        | 1.39     |
| 1   | O     | 1375 | TYR  | CG-CD1  | 23.34 | 1.69        | 1.39     |
| 1   | N     | 1449 | PHE  | CG-CD2  | 22.17 | 1.72        | 1.38     |
| 1   | H     | 1449 | PHE  | CG-CD2  | 22.12 | 1.72        | 1.38     |
| 1   | A     | 1449 | PHE  | CG-CD1  | 22.04 | 1.71        | 1.38     |
| 1   | B     | 1449 | PHE  | CG-CD2  | 22.00 | 1.71        | 1.38     |
| 1   | O     | 1449 | PHE  | CG-CD1  | 21.91 | 1.71        | 1.38     |
| 1   | Q     | 1449 | PHE  | CG-CD1  | 21.89 | 1.71        | 1.38     |
| 1   | H     | 1449 | PHE  | CG-CD1  | 20.88 | 1.70        | 1.38     |
| 1   | B     | 1449 | PHE  | CG-CD1  | 20.88 | 1.70        | 1.38     |
| 1   | N     | 1449 | PHE  | CG-CD1  | 20.82 | 1.70        | 1.38     |
| 1   | A     | 1449 | PHE  | CG-CD2  | 20.82 | 1.70        | 1.38     |
| 1   | Q     | 1449 | PHE  | CG-CD2  | 20.80 | 1.70        | 1.38     |
| 1   | Q     | 1375 | TYR  | CD2-CE2 | 20.76 | 1.70        | 1.39     |
| 1   | O     | 1449 | PHE  | CG-CD2  | 20.73 | 1.69        | 1.38     |
| 1   | N     | 1375 | TYR  | CD1-CE1 | 20.65 | 1.70        | 1.39     |
| 1   | A     | 1375 | TYR  | CD1-CE1 | 20.56 | 1.70        | 1.39     |
| 1   | O     | 1375 | TYR  | CD1-CE1 | 20.50 | 1.70        | 1.39     |
| 1   | B     | 1375 | TYR  | CD1-CE1 | 20.46 | 1.70        | 1.39     |
| 1   | H     | 1375 | TYR  | CD1-CE1 | 20.37 | 1.69        | 1.39     |
| 1   | O     | 1449 | PHE  | CE1-CZ  | 18.16 | 1.71        | 1.37     |
| 1   | A     | 1449 | PHE  | CE1-CZ  | 18.11 | 1.71        | 1.37     |
| 1   | Q     | 1449 | PHE  | CE1-CZ  | 18.08 | 1.71        | 1.37     |
| 1   | N     | 1449 | PHE  | CE2-CZ  | 18.07 | 1.71        | 1.37     |
| 1   | B     | 1449 | PHE  | CE2-CZ  | 17.95 | 1.71        | 1.37     |
| 1   | H     | 1449 | PHE  | CE2-CZ  | 17.95 | 1.71        | 1.37     |
| 3   | E     | 108  | PRO  | CG-CD   | 17.59 | 2.08        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | L     | 108  | PRO  | CG-CD   | 17.50 | 2.08        | 1.50     |
| 1   | Q     | 1449 | PHE  | CE2-CZ  | 17.20 | 1.70        | 1.37     |
| 1   | N     | 1449 | PHE  | CE1-CZ  | 17.15 | 1.70        | 1.37     |
| 1   | B     | 1449 | PHE  | CE1-CZ  | 17.11 | 1.69        | 1.37     |
| 1   | A     | 1449 | PHE  | CE2-CZ  | 17.11 | 1.69        | 1.37     |
| 1   | O     | 1449 | PHE  | CE2-CZ  | 17.10 | 1.69        | 1.37     |
| 1   | H     | 1449 | PHE  | CE1-CZ  | 17.09 | 1.69        | 1.37     |
| 3   | T     | 108  | PRO  | CG-CD   | 16.76 | 2.06        | 1.50     |
| 1   | A     | 1449 | PHE  | CD2-CE2 | 15.69 | 1.70        | 1.39     |
| 1   | H     | 1449 | PHE  | CD1-CE1 | 15.69 | 1.70        | 1.39     |
| 1   | Q     | 1449 | PHE  | CD2-CE2 | 15.69 | 1.70        | 1.39     |
| 1   | B     | 1449 | PHE  | CD1-CE1 | 15.66 | 1.70        | 1.39     |
| 1   | O     | 1449 | PHE  | CD2-CE2 | 15.64 | 1.70        | 1.39     |
| 1   | N     | 1449 | PHE  | CD1-CE1 | 15.52 | 1.70        | 1.39     |
| 3   | T     | 108  | PRO  | CB-CG   | 11.37 | 2.06        | 1.50     |
| 3   | L     | 108  | PRO  | CB-CG   | 11.35 | 2.06        | 1.50     |
| 3   | E     | 108  | PRO  | CB-CG   | 11.29 | 2.06        | 1.50     |
| 1   | B     | 1855 | GLU  | CD-OE2  | -5.64 | 1.19        | 1.25     |

All (530) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | H     | 1375 | TYR  | CG-CD2-CE2 | -12.56 | 111.25      | 121.30   |
| 1   | O     | 1375 | TYR  | CG-CD2-CE2 | -12.49 | 111.31      | 121.30   |
| 1   | A     | 1375 | TYR  | CG-CD2-CE2 | -12.47 | 111.32      | 121.30   |
| 1   | B     | 1375 | TYR  | CG-CD2-CE2 | -12.47 | 111.33      | 121.30   |
| 1   | N     | 1375 | TYR  | CG-CD2-CE2 | -12.43 | 111.36      | 121.30   |
| 1   | Q     | 1375 | TYR  | CG-CD1-CE1 | -12.21 | 111.53      | 121.30   |
| 1   | O     | 712  | ARG  | NE-CZ-NH2  | 11.03  | 125.81      | 120.30   |
| 1   | O     | 1909 | ARG  | NE-CZ-NH2  | 10.59  | 125.60      | 120.30   |
| 1   | B     | 712  | ARG  | NE-CZ-NH2  | 10.54  | 125.57      | 120.30   |
| 1   | H     | 1909 | ARG  | NE-CZ-NH2  | 10.10  | 125.35      | 120.30   |
| 1   | B     | 281  | ARG  | NE-CZ-NH2  | 9.96   | 125.28      | 120.30   |
| 2   | D     | 81   | ARG  | NE-CZ-NH2  | 9.85   | 125.22      | 120.30   |
| 1   | B     | 108  | ARG  | NE-CZ-NH2  | 9.81   | 125.21      | 120.30   |
| 1   | H     | 1141 | ARG  | NE-CZ-NH2  | 9.71   | 125.15      | 120.30   |
| 1   | H     | 237  | ARG  | NE-CZ-NH2  | 9.70   | 125.15      | 120.30   |
| 1   | A     | 1375 | TYR  | CZ-CE2-CD2 | -9.66  | 111.11      | 119.80   |
| 1   | O     | 1375 | TYR  | CZ-CE2-CD2 | -9.63  | 111.13      | 119.80   |
| 1   | H     | 1375 | TYR  | CZ-CE2-CD2 | -9.62  | 111.14      | 119.80   |
| 1   | B     | 1375 | TYR  | CZ-CE2-CD2 | -9.53  | 111.22      | 119.80   |
| 1   | Q     | 1375 | TYR  | CD1-CE1-CZ | -9.49  | 111.26      | 119.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | N     | 1375 | TYR  | CZ-CE2-CD2 | -9.45 | 111.29      | 119.80   |
| 1   | Q     | 1909 | ARG  | NE-CZ-NH2  | 9.14  | 124.87      | 120.30   |
| 1   | O     | 1167 | ARG  | NE-CZ-NH2  | 8.94  | 124.77      | 120.30   |
| 1   | O     | 281  | ARG  | NE-CZ-NH2  | 8.88  | 124.74      | 120.30   |
| 1   | Q     | 952  | ARG  | NE-CZ-NH2  | 8.83  | 124.72      | 120.30   |
| 1   | A     | 1909 | ARG  | NE-CZ-NH2  | 8.73  | 124.66      | 120.30   |
| 5   | P     | 856  | ARG  | NE-CZ-NH2  | 8.71  | 124.66      | 120.30   |
| 1   | N     | 803  | LYS  | CD-CE-NZ   | 8.68  | 131.67      | 111.70   |
| 1   | O     | 237  | ARG  | NE-CZ-NH2  | 8.66  | 124.63      | 120.30   |
| 1   | A     | 1449 | PHE  | CG-CD1-CE1 | -8.64 | 111.30      | 120.80   |
| 1   | H     | 803  | LYS  | CD-CE-NZ   | 8.59  | 131.47      | 111.70   |
| 1   | Q     | 1449 | PHE  | CG-CD1-CE1 | -8.59 | 111.36      | 120.80   |
| 1   | B     | 1449 | PHE  | CG-CD2-CE2 | -8.58 | 111.36      | 120.80   |
| 1   | H     | 1449 | PHE  | CG-CD2-CE2 | -8.57 | 111.37      | 120.80   |
| 1   | N     | 1449 | PHE  | CG-CD2-CE2 | -8.57 | 111.38      | 120.80   |
| 1   | H     | 1126 | ARG  | NE-CZ-NH2  | 8.55  | 124.58      | 120.30   |
| 1   | O     | 1449 | PHE  | CG-CD1-CE1 | -8.53 | 111.41      | 120.80   |
| 1   | A     | 803  | LYS  | CD-CE-NZ   | 8.51  | 131.27      | 111.70   |
| 1   | B     | 1375 | TYR  | CD1-CE1-CZ | 8.50  | 127.45      | 119.80   |
| 1   | H     | 1375 | TYR  | CD1-CE1-CZ | 8.49  | 127.44      | 119.80   |
| 1   | O     | 1375 | TYR  | CD1-CE1-CZ | 8.47  | 127.43      | 119.80   |
| 1   | A     | 1375 | TYR  | CD1-CE1-CZ | 8.47  | 127.42      | 119.80   |
| 1   | N     | 1375 | TYR  | CD1-CE1-CZ | 8.44  | 127.40      | 119.80   |
| 1   | Q     | 1375 | TYR  | CZ-CE2-CD2 | 8.38  | 127.34      | 119.80   |
| 1   | Q     | 1167 | ARG  | NE-CZ-NH2  | 8.35  | 124.47      | 120.30   |
| 1   | H     | 1167 | ARG  | NE-CZ-NH2  | 8.30  | 124.45      | 120.30   |
| 1   | B     | 1818 | ARG  | NE-CZ-NH2  | 8.30  | 124.45      | 120.30   |
| 1   | B     | 1530 | ARG  | NE-CZ-NH2  | 8.27  | 124.44      | 120.30   |
| 1   | N     | 1167 | ARG  | NE-CZ-NH2  | 8.27  | 124.44      | 120.30   |
| 1   | B     | 798  | ARG  | NE-CZ-NH2  | 8.26  | 124.43      | 120.30   |
| 3   | U     | 58   | ARG  | NE-CZ-NH2  | 8.22  | 124.41      | 120.30   |
| 1   | B     | 652  | ARG  | NE-CZ-NH2  | 8.21  | 124.41      | 120.30   |
| 1   | N     | 870  | ARG  | NE-CZ-NH2  | 8.13  | 124.37      | 120.30   |
| 1   | A     | 1193 | ARG  | NE-CZ-NH2  | 8.12  | 124.36      | 120.30   |
| 5   | P     | 321  | ARG  | NE-CZ-NH2  | 8.10  | 124.35      | 120.30   |
| 2   | K     | 163  | ARG  | NE-CZ-NH2  | 8.08  | 124.34      | 120.30   |
| 3   | F     | 120  | ARG  | NE-CZ-NH2  | 8.06  | 124.33      | 120.30   |
| 5   | I     | 321  | ARG  | NE-CZ-NH2  | 8.05  | 124.33      | 120.30   |
| 1   | N     | 249  | ARG  | NE-CZ-NH2  | 8.03  | 124.32      | 120.30   |
| 1   | H     | 1375 | TYR  | CG-CD1-CE1 | 8.00  | 127.70      | 121.30   |
| 1   | O     | 1375 | TYR  | CG-CD1-CE1 | 7.96  | 127.67      | 121.30   |
| 1   | B     | 1375 | TYR  | CG-CD1-CE1 | 7.93  | 127.65      | 121.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | N     | 671  | ARG  | NE-CZ-NH2  | 7.91  | 124.26      | 120.30   |
| 1   | Q     | 1375 | TYR  | CG-CD2-CE2 | 7.90  | 127.62      | 121.30   |
| 1   | O     | 869  | ARG  | NE-CZ-NH2  | 7.88  | 124.24      | 120.30   |
| 1   | Q     | 712  | ARG  | NE-CZ-NH2  | 7.82  | 124.21      | 120.30   |
| 1   | H     | 1530 | ARG  | NE-CZ-NH2  | 7.81  | 124.21      | 120.30   |
| 1   | N     | 1375 | TYR  | CG-CD1-CE1 | 7.80  | 127.54      | 121.30   |
| 1   | H     | 249  | ARG  | NE-CZ-NH2  | 7.76  | 124.18      | 120.30   |
| 1   | A     | 243  | ARG  | NE-CZ-NH2  | 7.76  | 124.18      | 120.30   |
| 1   | A     | 1375 | TYR  | CG-CD1-CE1 | 7.76  | 127.51      | 121.30   |
| 1   | N     | 721  | ARG  | NE-CZ-NH2  | 7.76  | 124.18      | 120.30   |
| 1   | Q     | 652  | ARG  | NE-CZ-NH2  | 7.74  | 124.17      | 120.30   |
| 1   | A     | 1697 | ARG  | NE-CZ-NH2  | 7.73  | 124.16      | 120.30   |
| 1   | N     | 1689 | ARG  | NE-CZ-NH2  | 7.73  | 124.16      | 120.30   |
| 1   | A     | 787  | ARG  | NE-CZ-NH2  | 7.68  | 124.14      | 120.30   |
| 5   | P     | 353  | ARG  | NE-CZ-NH2  | 7.68  | 124.14      | 120.30   |
| 1   | O     | 721  | ARG  | NE-CZ-NH2  | 7.67  | 124.14      | 120.30   |
| 1   | A     | 1175 | ARG  | NE-CZ-NH2  | 7.67  | 124.13      | 120.30   |
| 5   | P     | 1145 | ARG  | NE-CZ-NH2  | 7.66  | 124.13      | 120.30   |
| 1   | A     | 1677 | ARG  | NE-CZ-NH2  | 7.60  | 124.10      | 120.30   |
| 1   | O     | 143  | ARG  | NE-CZ-NH2  | 7.58  | 124.09      | 120.30   |
| 1   | A     | 803  | LYS  | CG-CD-CE   | 7.50  | 134.40      | 111.90   |
| 1   | A     | 1372 | ARG  | NE-CZ-NH2  | 7.50  | 124.05      | 120.30   |
| 1   | Q     | 1129 | ARG  | NE-CZ-NH2  | 7.49  | 124.04      | 120.30   |
| 1   | H     | 403  | ARG  | NE-CZ-NH2  | 7.45  | 124.03      | 120.30   |
| 1   | O     | 453  | ARG  | NE-CZ-NH2  | 7.44  | 124.02      | 120.30   |
| 1   | H     | 1434 | ARG  | NE-CZ-NH2  | 7.43  | 124.02      | 120.30   |
| 1   | A     | 369  | ARG  | NE-CZ-NH2  | 7.43  | 124.02      | 120.30   |
| 1   | H     | 803  | LYS  | CG-CD-CE   | 7.42  | 134.14      | 111.90   |
| 1   | Q     | 272  | ARG  | NE-CZ-NH2  | 7.36  | 123.98      | 120.30   |
| 1   | O     | 1449 | PHE  | CD1-CE1-CZ | -7.35 | 111.28      | 120.10   |
| 1   | A     | 1449 | PHE  | CD1-CE1-CZ | -7.33 | 111.30      | 120.10   |
| 4   | V     | 137  | ARG  | NE-CZ-NH2  | 7.32  | 123.96      | 120.30   |
| 1   | N     | 1050 | ARG  | NE-CZ-NH2  | 7.32  | 123.96      | 120.30   |
| 1   | O     | 29   | ARG  | NE-CZ-NH2  | 7.31  | 123.95      | 120.30   |
| 1   | N     | 803  | LYS  | CG-CD-CE   | 7.30  | 133.81      | 111.90   |
| 1   | Q     | 1449 | PHE  | CD1-CE1-CZ | -7.30 | 111.34      | 120.10   |
| 1   | O     | 204  | ARG  | NE-CZ-NH2  | 7.30  | 123.95      | 120.30   |
| 1   | Q     | 1689 | ARG  | NE-CZ-NH2  | 7.29  | 123.95      | 120.30   |
| 1   | H     | 108  | ARG  | NE-CZ-NH2  | 7.27  | 123.94      | 120.30   |
| 1   | B     | 1845 | ARG  | NE-CZ-NH2  | 7.27  | 123.93      | 120.30   |
| 1   | N     | 1449 | PHE  | CZ-CE2-CD2 | -7.26 | 111.39      | 120.10   |
| 4   | G     | 107  | ARG  | NE-CZ-NH2  | 7.26  | 123.93      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | B     | 1175 | ARG  | NE-CZ-NH2  | 7.25  | 123.92      | 120.30   |
| 1   | B     | 1592 | ARG  | NE-CZ-NH2  | 7.25  | 123.92      | 120.30   |
| 1   | B     | 204  | ARG  | NE-CZ-NH2  | 7.23  | 123.92      | 120.30   |
| 2   | S     | 81   | ARG  | NE-CZ-NH2  | 7.22  | 123.91      | 120.30   |
| 5   | I     | 459  | ARG  | NE-CZ-NH2  | 7.21  | 123.90      | 120.30   |
| 1   | Q     | 1317 | ARG  | NE-CZ-NH2  | 7.18  | 123.89      | 120.30   |
| 1   | A     | 1317 | ARG  | NE-CZ-NH2  | 7.17  | 123.88      | 120.30   |
| 1   | B     | 1449 | PHE  | CZ-CE2-CD2 | -7.17 | 111.50      | 120.10   |
| 1   | H     | 1449 | PHE  | CZ-CE2-CD2 | -7.17 | 111.50      | 120.10   |
| 1   | H     | 281  | ARG  | NE-CZ-NH2  | 7.15  | 123.87      | 120.30   |
| 1   | Q     | 281  | ARG  | NE-CZ-NH2  | 7.14  | 123.87      | 120.30   |
| 1   | A     | 147  | ARG  | NE-CZ-NH2  | 7.11  | 123.86      | 120.30   |
| 1   | B     | 1689 | ARG  | NE-CZ-NH2  | 7.11  | 123.85      | 120.30   |
| 2   | R     | 138  | ARG  | NE-CZ-NH2  | 7.11  | 123.85      | 120.30   |
| 1   | B     | 925  | ARG  | NE-CZ-NH2  | 7.10  | 123.85      | 120.30   |
| 5   | I     | 1164 | ARG  | NE-CZ-NH2  | 7.10  | 123.85      | 120.30   |
| 1   | Q     | 1749 | ARG  | NE-CZ-NH2  | 7.09  | 123.85      | 120.30   |
| 1   | H     | 663  | ARG  | NE-CZ-NH2  | 7.09  | 123.85      | 120.30   |
| 1   | N     | 1909 | ARG  | NE-CZ-NH2  | 7.09  | 123.84      | 120.30   |
| 1   | B     | 1832 | ARG  | NE-CZ-NH2  | 7.07  | 123.83      | 120.30   |
| 1   | H     | 1375 | TYR  | CB-CG-CD1  | -7.06 | 116.76      | 121.00   |
| 5   | P     | 478  | ARG  | NE-CZ-NH2  | 7.06  | 123.83      | 120.30   |
| 1   | H     | 719  | ARG  | NE-CZ-NH2  | 7.05  | 123.82      | 120.30   |
| 1   | N     | 1317 | ARG  | NE-CZ-NH2  | 7.01  | 123.80      | 120.30   |
| 1   | Q     | 29   | ARG  | NE-CZ-NH2  | 7.01  | 123.80      | 120.30   |
| 1   | Q     | 17   | ARG  | NE-CZ-NH2  | 7.00  | 123.80      | 120.30   |
| 1   | A     | 249  | ARG  | NE-CZ-NH2  | 6.99  | 123.79      | 120.30   |
| 1   | O     | 925  | ARG  | NE-CZ-NH2  | 6.98  | 123.79      | 120.30   |
| 1   | B     | 721  | ARG  | NE-CZ-NH2  | 6.96  | 123.78      | 120.30   |
| 1   | N     | 29   | ARG  | NE-CZ-NH2  | 6.95  | 123.78      | 120.30   |
| 1   | Q     | 1699 | ARG  | NE-CZ-NH2  | 6.94  | 123.77      | 120.30   |
| 2   | C     | 81   | ARG  | NE-CZ-NH2  | 6.93  | 123.76      | 120.30   |
| 1   | Q     | 925  | ARG  | NE-CZ-NH2  | 6.92  | 123.76      | 120.30   |
| 1   | A     | 272  | ARG  | NE-CZ-NH2  | 6.91  | 123.75      | 120.30   |
| 4   | G     | 340  | ARG  | NE-CZ-NH2  | 6.91  | 123.75      | 120.30   |
| 1   | O     | 1136 | ARG  | NE-CZ-NH2  | 6.91  | 123.75      | 120.30   |
| 1   | A     | 721  | ARG  | NE-CZ-NH2  | 6.89  | 123.75      | 120.30   |
| 1   | Q     | 1093 | ARG  | NE-CZ-NH2  | 6.88  | 123.74      | 120.30   |
| 1   | O     | 1560 | ARG  | NE-CZ-NH2  | 6.87  | 123.73      | 120.30   |
| 1   | B     | 249  | ARG  | NE-CZ-NH2  | 6.85  | 123.73      | 120.30   |
| 1   | B     | 169  | ARG  | NE-CZ-NH2  | 6.85  | 123.72      | 120.30   |
| 1   | N     | 780  | ARG  | NE-CZ-NH2  | 6.84  | 123.72      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | S     | 163  | ARG  | NE-CZ-NH2 | 6.83  | 123.72      | 120.30   |
| 1   | Q     | 1344 | ARG  | NE-CZ-NH2 | 6.83  | 123.72      | 120.30   |
| 1   | N     | 1863 | ARG  | NE-CZ-NH2 | 6.83  | 123.71      | 120.30   |
| 1   | B     | 870  | ARG  | NE-CZ-NH2 | 6.82  | 123.71      | 120.30   |
| 1   | O     | 904  | ARG  | NE-CZ-NH2 | 6.80  | 123.70      | 120.30   |
| 1   | O     | 1050 | ARG  | NE-CZ-NH2 | 6.77  | 123.69      | 120.30   |
| 1   | Q     | 1303 | ARG  | NE-CZ-NH2 | 6.77  | 123.68      | 120.30   |
| 1   | B     | 1193 | ARG  | NE-CZ-NH2 | 6.76  | 123.68      | 120.30   |
| 1   | Q     | 1050 | ARG  | NE-CZ-NH2 | 6.75  | 123.68      | 120.30   |
| 1   | O     | 1141 | ARG  | NE-CZ-NH2 | 6.75  | 123.68      | 120.30   |
| 1   | N     | 1193 | ARG  | NE-CZ-NH2 | 6.75  | 123.67      | 120.30   |
| 1   | O     | 1634 | ARG  | NE-CZ-NH2 | 6.74  | 123.67      | 120.30   |
| 1   | A     | 1129 | ARG  | NE-CZ-NH2 | 6.74  | 123.67      | 120.30   |
| 1   | O     | 739  | ARG  | NE-CZ-NH2 | 6.73  | 123.67      | 120.30   |
| 1   | A     | 1699 | ARG  | NE-CZ-NH2 | 6.73  | 123.67      | 120.30   |
| 1   | N     | 703  | ARG  | NE-CZ-NH2 | 6.73  | 123.67      | 120.30   |
| 2   | D     | 63   | ARG  | NE-CZ-NH2 | 6.72  | 123.66      | 120.30   |
| 1   | H     | 870  | ARG  | NE-CZ-NH2 | 6.71  | 123.66      | 120.30   |
| 1   | N     | 108  | ARG  | NE-CZ-NH2 | 6.71  | 123.66      | 120.30   |
| 1   | Q     | 1114 | ARG  | NE-CZ-NH2 | 6.71  | 123.65      | 120.30   |
| 1   | N     | 1372 | ARG  | NE-CZ-NH2 | 6.69  | 123.65      | 120.30   |
| 1   | H     | 712  | ARG  | NE-CZ-NH2 | 6.69  | 123.64      | 120.30   |
| 4   | G     | 376  | ARG  | NE-CZ-NH2 | 6.68  | 123.64      | 120.30   |
| 1   | Q     | 1045 | ARG  | NE-CZ-NH2 | 6.67  | 123.63      | 120.30   |
| 1   | O     | 1359 | ARG  | NE-CZ-NH2 | 6.65  | 123.63      | 120.30   |
| 1   | H     | 671  | ARG  | NE-CZ-NH2 | 6.64  | 123.62      | 120.30   |
| 4   | V     | 172  | ARG  | NE-CZ-NH2 | 6.64  | 123.62      | 120.30   |
| 1   | O     | 1289 | ARG  | NE-CZ-NH2 | 6.63  | 123.62      | 120.30   |
| 1   | H     | 787  | ARG  | NE-CZ-NH2 | 6.63  | 123.61      | 120.30   |
| 5   | I     | 1232 | ARG  | NE-CZ-NH2 | 6.63  | 123.61      | 120.30   |
| 1   | H     | 1613 | ARG  | NE-CZ-NH2 | 6.62  | 123.61      | 120.30   |
| 1   | O     | 1372 | ARG  | NE-CZ-NH2 | 6.62  | 123.61      | 120.30   |
| 5   | P     | 440  | PRO  | CA-N-CD   | -6.62 | 102.23      | 111.50   |
| 1   | H     | 1699 | ARG  | NE-CZ-NH2 | 6.62  | 123.61      | 120.30   |
| 1   | Q     | 1608 | ARG  | NE-CZ-NH2 | 6.61  | 123.61      | 120.30   |
| 1   | O     | 1592 | ARG  | NE-CZ-NH2 | 6.60  | 123.60      | 120.30   |
| 1   | N     | 904  | ARG  | NE-CZ-NH2 | 6.59  | 123.59      | 120.30   |
| 1   | H     | 453  | ARG  | NE-CZ-NH2 | 6.58  | 123.59      | 120.30   |
| 1   | B     | 147  | ARG  | NE-CZ-NH2 | 6.58  | 123.59      | 120.30   |
| 2   | R     | 63   | ARG  | NE-CZ-NH2 | 6.58  | 123.59      | 120.30   |
| 1   | N     | 442  | ARG  | NE-CZ-NH2 | 6.58  | 123.59      | 120.30   |
| 1   | A     | 1141 | ARG  | NE-CZ-NH2 | 6.57  | 123.58      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 819  | ARG  | NE-CZ-NH2 | 6.54  | 123.57      | 120.30   |
| 1   | N     | 694  | ARG  | NE-CZ-NH2 | 6.54  | 123.57      | 120.30   |
| 1   | N     | 1126 | ARG  | NE-CZ-NH2 | 6.54  | 123.57      | 120.30   |
| 1   | N     | 652  | ARG  | NE-CZ-NH2 | 6.53  | 123.57      | 120.30   |
| 1   | B     | 1634 | ARG  | NE-CZ-NH2 | 6.53  | 123.56      | 120.30   |
| 1   | Q     | 108  | ARG  | NE-CZ-NH2 | 6.51  | 123.56      | 120.30   |
| 4   | G     | 137  | ARG  | NE-CZ-NH2 | 6.51  | 123.56      | 120.30   |
| 1   | B     | 369  | ARG  | NE-CZ-NH2 | 6.51  | 123.56      | 120.30   |
| 4   | G     | 26   | ARG  | NE-CZ-NH2 | 6.51  | 123.55      | 120.30   |
| 1   | O     | 1574 | ARG  | NE-CZ-NH2 | 6.50  | 123.55      | 120.30   |
| 2   | C     | 63   | ARG  | NE-CZ-NH2 | 6.48  | 123.54      | 120.30   |
| 1   | N     | 808  | ARG  | NE-CZ-NH2 | 6.48  | 123.54      | 120.30   |
| 1   | B     | 1574 | ARG  | NE-CZ-NH2 | 6.47  | 123.54      | 120.30   |
| 1   | H     | 1317 | ARG  | NE-CZ-NH2 | 6.47  | 123.54      | 120.30   |
| 1   | B     | 904  | ARG  | NE-CZ-NH2 | 6.47  | 123.53      | 120.30   |
| 1   | B     | 1129 | ARG  | NE-CZ-NH2 | 6.46  | 123.53      | 120.30   |
| 1   | H     | 1420 | ARG  | NE-CZ-NH2 | 6.46  | 123.53      | 120.30   |
| 1   | O     | 272  | ARG  | NE-CZ-NH2 | 6.46  | 123.53      | 120.30   |
| 1   | A     | 723  | ARG  | NE-CZ-NH2 | 6.46  | 123.53      | 120.30   |
| 2   | S     | 154  | ARG  | NE-CZ-NH2 | 6.45  | 123.53      | 120.30   |
| 1   | A     | 1053 | ARG  | NE-CZ-NH2 | 6.45  | 123.53      | 120.30   |
| 1   | B     | 1608 | ARG  | NE-CZ-NH2 | 6.44  | 123.52      | 120.30   |
| 4   | V     | 107  | ARG  | NE-CZ-NH2 | 6.44  | 123.52      | 120.30   |
| 1   | N     | 1289 | ARG  | NE-CZ-NH2 | 6.43  | 123.52      | 120.30   |
| 4   | G     | 361  | ARG  | NE-CZ-NH2 | 6.41  | 123.50      | 120.30   |
| 2   | K     | 154  | ARG  | NE-CZ-NH2 | 6.39  | 123.50      | 120.30   |
| 1   | N     | 237  | ARG  | NE-CZ-NH2 | 6.38  | 123.49      | 120.30   |
| 3   | T     | 58   | ARG  | NE-CZ-NH2 | 6.38  | 123.49      | 120.30   |
| 3   | M     | 40   | ARG  | NE-CZ-NH2 | 6.37  | 123.48      | 120.30   |
| 1   | N     | 1141 | ARG  | NE-CZ-NH2 | 6.37  | 123.48      | 120.30   |
| 1   | A     | 1344 | ARG  | NE-CZ-NH2 | 6.36  | 123.48      | 120.30   |
| 2   | J     | 63   | ARG  | NE-CZ-NH2 | 6.35  | 123.47      | 120.30   |
| 5   | I     | 839  | ARG  | NE-CZ-NH2 | 6.34  | 123.47      | 120.30   |
| 1   | B     | 1699 | ARG  | NE-CZ-NH2 | 6.32  | 123.46      | 120.30   |
| 1   | Q     | 808  | ARG  | NE-CZ-NH2 | 6.31  | 123.45      | 120.30   |
| 1   | O     | 1832 | ARG  | NE-CZ-NH2 | 6.31  | 123.45      | 120.30   |
| 1   | O     | 1434 | ARG  | NE-CZ-NH2 | 6.30  | 123.45      | 120.30   |
| 1   | B     | 1289 | ARG  | NE-CZ-NH2 | 6.28  | 123.44      | 120.30   |
| 4   | V     | 1    | PRO  | CA-N-CD   | -6.28 | 102.71      | 111.50   |
| 1   | B     | 1662 | ARG  | NE-CZ-NH2 | 6.28  | 123.44      | 120.30   |
| 1   | B     | 1909 | ARG  | NE-CZ-NH2 | 6.28  | 123.44      | 120.30   |
| 1   | B     | 793  | ARG  | NE-CZ-NH2 | 6.27  | 123.44      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | N     | 1608 | ARG  | NE-CZ-NH2  | 6.26  | 123.43      | 120.30   |
| 3   | T     | 50   | ARG  | NE-CZ-NH2  | 6.25  | 123.43      | 120.30   |
| 1   | O     | 808  | ARG  | NE-CZ-NH2  | 6.24  | 123.42      | 120.30   |
| 1   | A     | 777  | ARG  | NE-CZ-NH2  | 6.24  | 123.42      | 120.30   |
| 5   | I     | 806  | ARG  | NE-CZ-NH2  | 6.23  | 123.41      | 120.30   |
| 4   | V     | 363  | ARG  | NE-CZ-NH2  | 6.23  | 123.41      | 120.30   |
| 4   | G     | 1    | PRO  | CA-N-CD    | -6.21 | 102.80      | 111.50   |
| 1   | Q     | 1420 | ARG  | NE-CZ-NH2  | 6.21  | 123.40      | 120.30   |
| 1   | H     | 1449 | PHE  | CG-CD1-CE1 | 6.21  | 127.62      | 120.80   |
| 1   | O     | 1858 | ARG  | NE-CZ-NH2  | 6.21  | 123.40      | 120.30   |
| 4   | V     | 208  | ARG  | NE-CZ-NH2  | 6.21  | 123.40      | 120.30   |
| 1   | Q     | 1141 | ARG  | NE-CZ-NH2  | 6.20  | 123.40      | 120.30   |
| 1   | B     | 1277 | ARG  | NE-CZ-NH2  | 6.20  | 123.40      | 120.30   |
| 1   | A     | 1818 | ARG  | NE-CZ-NH2  | 6.20  | 123.40      | 120.30   |
| 1   | Q     | 870  | ARG  | NE-CZ-NH2  | 6.20  | 123.40      | 120.30   |
| 1   | B     | 567  | ARG  | NE-CZ-NH2  | 6.20  | 123.40      | 120.30   |
| 1   | N     | 1175 | ARG  | NE-CZ-NH2  | 6.19  | 123.39      | 120.30   |
| 1   | O     | 1093 | ARG  | NE-CZ-NH2  | 6.19  | 123.39      | 120.30   |
| 2   | R     | 81   | ARG  | NE-CZ-NH2  | 6.18  | 123.39      | 120.30   |
| 1   | N     | 1449 | PHE  | CD1-CE1-CZ | 6.18  | 127.52      | 120.10   |
| 5   | P     | 606  | ARG  | NE-CZ-NH2  | 6.17  | 123.39      | 120.30   |
| 1   | B     | 54   | ARG  | NE-CZ-NH2  | 6.17  | 123.39      | 120.30   |
| 1   | H     | 783  | ARG  | NE-CZ-NH2  | 6.17  | 123.38      | 120.30   |
| 1   | N     | 787  | ARG  | NE-CZ-NH2  | 6.17  | 123.38      | 120.30   |
| 1   | A     | 1449 | PHE  | CZ-CE2-CD2 | 6.17  | 127.50      | 120.10   |
| 1   | H     | 1880 | ARG  | NE-CZ-NH2  | 6.16  | 123.38      | 120.30   |
| 1   | N     | 1449 | PHE  | CG-CD1-CE1 | 6.16  | 127.57      | 120.80   |
| 1   | N     | 1832 | ARG  | NE-CZ-NH2  | 6.15  | 123.37      | 120.30   |
| 1   | B     | 1449 | PHE  | CD1-CE1-CZ | 6.14  | 127.47      | 120.10   |
| 1   | O     | 1317 | ARG  | NE-CZ-NH2  | 6.14  | 123.37      | 120.30   |
| 1   | H     | 1175 | ARG  | NE-CZ-NH2  | 6.14  | 123.37      | 120.30   |
| 1   | O     | 1449 | PHE  | CZ-CE2-CD2 | 6.14  | 127.47      | 120.10   |
| 5   | P     | 899  | ARG  | NE-CZ-NH2  | 6.13  | 123.37      | 120.30   |
| 1   | A     | 1574 | ARG  | NE-CZ-NH2  | 6.13  | 123.37      | 120.30   |
| 1   | O     | 54   | ARG  | NE-CZ-NH2  | 6.13  | 123.36      | 120.30   |
| 1   | Q     | 1449 | PHE  | CG-CD2-CE2 | 6.13  | 127.54      | 120.80   |
| 1   | Q     | 1796 | ARG  | NE-CZ-NH2  | 6.13  | 123.36      | 120.30   |
| 1   | B     | 1053 | ARG  | NE-CZ-NH2  | 6.13  | 123.36      | 120.30   |
| 1   | Q     | 1449 | PHE  | CZ-CE2-CD2 | 6.12  | 127.45      | 120.10   |
| 4   | V     | 183  | ARG  | NE-CZ-NH2  | 6.12  | 123.36      | 120.30   |
| 1   | O     | 1449 | PHE  | CG-CD2-CE2 | 6.10  | 127.51      | 120.80   |
| 1   | A     | 1449 | PHE  | CG-CD2-CE2 | 6.10  | 127.51      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | N     | 308  | TYR  | CB-CG-CD2  | -6.10 | 117.34      | 121.00   |
| 2   | D     | 154  | ARG  | NE-CZ-NH2  | 6.09  | 123.34      | 120.30   |
| 1   | H     | 1449 | PHE  | CD1-CE1-CZ | 6.08  | 127.40      | 120.10   |
| 1   | N     | 1420 | ARG  | NE-CZ-NH2  | 6.08  | 123.34      | 120.30   |
| 1   | B     | 1359 | ARG  | NE-CZ-NH2  | 6.08  | 123.34      | 120.30   |
| 1   | H     | 501  | TYR  | CB-CG-CD2  | -6.08 | 117.35      | 121.00   |
| 1   | N     | 798  | ARG  | NE-CZ-NH2  | 6.07  | 123.34      | 120.30   |
| 3   | F     | 9    | ARG  | NE-CZ-NH2  | 6.07  | 123.34      | 120.30   |
| 1   | B     | 237  | ARG  | NE-CZ-NH2  | 6.07  | 123.33      | 120.30   |
| 1   | H     | 925  | ARG  | NE-CZ-NH2  | 6.07  | 123.33      | 120.30   |
| 1   | O     | 777  | ARG  | NE-CZ-NH2  | 6.06  | 123.33      | 120.30   |
| 1   | B     | 1449 | PHE  | CG-CD1-CE1 | 6.06  | 127.46      | 120.80   |
| 1   | O     | 870  | ARG  | NE-CZ-NH2  | 6.04  | 123.32      | 120.30   |
| 4   | V     | 376  | ARG  | NE-CZ-NH2  | 6.03  | 123.32      | 120.30   |
| 5   | I     | 1145 | ARG  | NE-CZ-NH2  | 6.02  | 123.31      | 120.30   |
| 1   | B     | 671  | ARG  | NE-CZ-NH2  | 6.01  | 123.30      | 120.30   |
| 1   | O     | 1344 | ARG  | NE-CZ-NH2  | 6.01  | 123.31      | 120.30   |
| 1   | Q     | 1820 | ARG  | NE-CZ-NH2  | 6.01  | 123.31      | 120.30   |
| 1   | N     | 1699 | ARG  | NE-CZ-NH2  | 6.00  | 123.30      | 120.30   |
| 5   | P     | 880  | ARG  | NE-CZ-NH2  | 6.00  | 123.30      | 120.30   |
| 1   | Q     | 1175 | ARG  | NE-CZ-NH2  | 6.00  | 123.30      | 120.30   |
| 1   | Q     | 1530 | ARG  | NE-CZ-NH2  | 5.98  | 123.29      | 120.30   |
| 1   | H     | 1359 | ARG  | NE-CZ-NH2  | 5.98  | 123.29      | 120.30   |
| 1   | N     | 1093 | ARG  | NE-CZ-NH2  | 5.98  | 123.29      | 120.30   |
| 1   | O     | 369  | ARG  | NE-CZ-NH2  | 5.97  | 123.29      | 120.30   |
| 4   | V     | 115  | ARG  | NE-CZ-NH2  | 5.97  | 123.29      | 120.30   |
| 5   | I     | 913  | ARG  | NE-CZ-NH2  | 5.96  | 123.28      | 120.30   |
| 1   | B     | 941  | ARG  | NE-CZ-NH2  | 5.96  | 123.28      | 120.30   |
| 5   | P     | 1081 | ARG  | NE-CZ-NH2  | 5.96  | 123.28      | 120.30   |
| 1   | O     | 108  | ARG  | NE-CZ-NH2  | 5.95  | 123.28      | 120.30   |
| 1   | N     | 1574 | ARG  | NE-CZ-NH2  | 5.95  | 123.27      | 120.30   |
| 1   | O     | 706  | ARG  | NE-CZ-NH2  | 5.94  | 123.27      | 120.30   |
| 1   | H     | 1372 | ARG  | NE-CZ-NH2  | 5.92  | 123.26      | 120.30   |
| 1   | A     | 1880 | ARG  | NE-CZ-NH2  | 5.91  | 123.26      | 120.30   |
| 5   | P     | 547  | ARG  | NE-CZ-NH2  | 5.89  | 123.25      | 120.30   |
| 1   | B     | 1260 | ARG  | NE-CZ-NH2  | 5.88  | 123.24      | 120.30   |
| 5   | I     | 1192 | ARG  | NE-CZ-NH2  | 5.88  | 123.24      | 120.30   |
| 5   | P     | 680  | ARG  | NE-CZ-NH2  | 5.88  | 123.24      | 120.30   |
| 1   | H     | 904  | ARG  | NE-CZ-NH2  | 5.88  | 123.24      | 120.30   |
| 1   | N     | 1749 | ARG  | NE-CZ-NH2  | 5.86  | 123.23      | 120.30   |
| 1   | Q     | 1337 | ARG  | NE-CZ-NH2  | 5.86  | 123.23      | 120.30   |
| 2   | K     | 81   | ARG  | NE-CZ-NH2  | 5.85  | 123.22      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | Q     | 1149 | ARG  | NE-CZ-NH2 | 5.84  | 123.22      | 120.30   |
| 3   | E     | 40   | ARG  | NE-CZ-NH2 | 5.83  | 123.22      | 120.30   |
| 1   | Q     | 1475 | ARG  | NE-CZ-NH2 | 5.82  | 123.21      | 120.30   |
| 2   | C     | 154  | ARG  | NE-CZ-NH2 | 5.81  | 123.20      | 120.30   |
| 1   | B     | 1136 | ARG  | NE-CZ-NH2 | 5.80  | 123.20      | 120.30   |
| 1   | Q     | 869  | ARG  | NE-CZ-NH2 | 5.80  | 123.20      | 120.30   |
| 5   | P     | 700  | ARG  | NE-CZ-NH2 | 5.80  | 123.20      | 120.30   |
| 1   | B     | 952  | ARG  | NE-CZ-NH2 | 5.79  | 123.19      | 120.30   |
| 1   | N     | 712  | ARG  | NE-CZ-NH2 | 5.78  | 123.19      | 120.30   |
| 1   | B     | 1337 | ARG  | NE-CZ-NH2 | 5.78  | 123.19      | 120.30   |
| 1   | O     | 1126 | ARG  | NE-CZ-NH2 | 5.77  | 123.19      | 120.30   |
| 1   | A     | 1303 | ARG  | NE-CZ-NH2 | 5.76  | 123.18      | 120.30   |
| 1   | B     | 1925 | ARG  | NE-CZ-NH2 | 5.76  | 123.18      | 120.30   |
| 1   | H     | 204  | ARG  | NE-CZ-NH2 | 5.76  | 123.18      | 120.30   |
| 1   | H     | 952  | ARG  | NE-CZ-NH2 | 5.76  | 123.18      | 120.30   |
| 1   | Q     | 721  | ARG  | NE-CZ-NH2 | 5.76  | 123.18      | 120.30   |
| 5   | I     | 404  | ARG  | NE-CZ-NH2 | 5.75  | 123.17      | 120.30   |
| 1   | Q     | 204  | ARG  | NE-CZ-NH2 | 5.74  | 123.17      | 120.30   |
| 5   | I     | 1265 | ARG  | NE-CZ-NH2 | 5.74  | 123.17      | 120.30   |
| 5   | P     | 721  | ARG  | NE-CZ-NH2 | 5.72  | 123.16      | 120.30   |
| 1   | Q     | 1250 | ARG  | NE-CZ-NH2 | 5.72  | 123.16      | 120.30   |
| 1   | B     | 1045 | ARG  | NE-CZ-NH2 | 5.72  | 123.16      | 120.30   |
| 1   | Q     | 249  | ARG  | NE-CZ-NH2 | 5.72  | 123.16      | 120.30   |
| 1   | O     | 249  | ARG  | NE-CZ-NH2 | 5.71  | 123.16      | 120.30   |
| 1   | N     | 308  | TYR  | CA-CB-CG  | 5.71  | 124.25      | 113.40   |
| 1   | O     | 703  | ARG  | NE-CZ-NH2 | 5.71  | 123.16      | 120.30   |
| 1   | B     | 712  | ARG  | NE-CZ-NH1 | -5.70 | 117.45      | 120.30   |
| 1   | A     | 1608 | ARG  | NE-CZ-NH2 | 5.70  | 123.15      | 120.30   |
| 3   | M     | 129  | ARG  | NE-CZ-NH2 | 5.69  | 123.15      | 120.30   |
| 1   | Q     | 1677 | ARG  | NE-CZ-NH2 | 5.69  | 123.15      | 120.30   |
| 1   | N     | 1846 | ARG  | NE-CZ-NH2 | 5.69  | 123.14      | 120.30   |
| 1   | B     | 1588 | ARG  | NE-CZ-NH2 | 5.69  | 123.14      | 120.30   |
| 3   | T     | 129  | ARG  | NE-CZ-NH2 | 5.69  | 123.14      | 120.30   |
| 4   | G     | 363  | ARG  | NE-CZ-NH2 | 5.68  | 123.14      | 120.30   |
| 5   | P     | 875  | ARG  | NE-CZ-NH2 | 5.67  | 123.14      | 120.30   |
| 1   | A     | 793  | ARG  | NE-CZ-NH2 | 5.67  | 123.14      | 120.30   |
| 1   | H     | 1114 | ARG  | NE-CZ-NH2 | 5.67  | 123.13      | 120.30   |
| 1   | Q     | 442  | ARG  | NE-CZ-NH2 | 5.66  | 123.13      | 120.30   |
| 1   | A     | 1277 | ARG  | NE-CZ-NH2 | 5.66  | 123.13      | 120.30   |
| 1   | A     | 1420 | ARG  | NE-CZ-NH2 | 5.66  | 123.13      | 120.30   |
| 1   | B     | 243  | ARG  | NE-CZ-NH2 | 5.66  | 123.13      | 120.30   |
| 2   | D     | 163  | ARG  | NE-CZ-NH2 | 5.66  | 123.13      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | H     | 780  | ARG  | NE-CZ-NH2  | 5.65  | 123.12      | 120.30   |
| 5   | P     | 1232 | ARG  | NE-CZ-NH2  | 5.63  | 123.12      | 120.30   |
| 5   | I     | 1365 | ARG  | NE-CZ-NH2  | 5.62  | 123.11      | 120.30   |
| 1   | Q     | 807  | ARG  | NE-CZ-NH2  | 5.62  | 123.11      | 120.30   |
| 1   | A     | 1858 | ARG  | NE-CZ-NH2  | 5.62  | 123.11      | 120.30   |
| 1   | B     | 1093 | ARG  | NE-CZ-NH2  | 5.62  | 123.11      | 120.30   |
| 1   | O     | 793  | ARG  | NE-CZ-NH2  | 5.61  | 123.11      | 120.30   |
| 3   | T     | 40   | ARG  | NE-CZ-NH2  | 5.61  | 123.11      | 120.30   |
| 3   | F     | 40   | ARG  | NE-CZ-NH2  | 5.61  | 123.11      | 120.30   |
| 1   | Q     | 1634 | ARG  | NE-CZ-NH2  | 5.61  | 123.10      | 120.30   |
| 1   | Q     | 1289 | ARG  | NE-CZ-NH2  | 5.61  | 123.10      | 120.30   |
| 5   | I     | 580  | ARG  | NE-CZ-NH2  | 5.60  | 123.10      | 120.30   |
| 2   | J     | 154  | ARG  | NE-CZ-NH2  | 5.58  | 123.09      | 120.30   |
| 1   | Q     | 719  | ARG  | NE-CZ-NH2  | 5.58  | 123.09      | 120.30   |
| 2   | C     | 138  | ARG  | NE-CZ-NH2  | 5.57  | 123.09      | 120.30   |
| 1   | A     | 739  | ARG  | NE-CZ-NH2  | 5.57  | 123.08      | 120.30   |
| 1   | A     | 1382 | ARG  | NE-CZ-NH2  | 5.57  | 123.08      | 120.30   |
| 1   | N     | 54   | ARG  | NE-CZ-NH2  | 5.57  | 123.08      | 120.30   |
| 1   | O     | 23   | ARG  | NE-CZ-NH2  | 5.56  | 123.08      | 120.30   |
| 1   | Q     | 787  | ARG  | NE-CZ-NH2  | 5.54  | 123.07      | 120.30   |
| 2   | K     | 63   | ARG  | NE-CZ-NH2  | 5.54  | 123.07      | 120.30   |
| 1   | N     | 941  | ARG  | NE-CZ-NH2  | 5.54  | 123.07      | 120.30   |
| 1   | O     | 1126 | ARG  | NE-CZ-NH1  | -5.53 | 117.53      | 120.30   |
| 5   | P     | 976  | ARG  | NE-CZ-NH2  | 5.52  | 123.06      | 120.30   |
| 1   | Q     | 706  | ARG  | NE-CZ-NH2  | 5.52  | 123.06      | 120.30   |
| 1   | Q     | 1447 | ARG  | NE-CZ-NH2  | 5.52  | 123.06      | 120.30   |
| 5   | P     | 1265 | ARG  | NE-CZ-NH2  | 5.51  | 123.06      | 120.30   |
| 1   | O     | 1045 | ARG  | NE-CZ-NH2  | 5.50  | 123.05      | 120.30   |
| 1   | O     | 1588 | ARG  | NE-CZ-NH2  | 5.50  | 123.05      | 120.30   |
| 1   | N     | 819  | ARG  | NE-CZ-NH2  | 5.50  | 123.05      | 120.30   |
| 1   | A     | 1268 | ARG  | NE-CZ-NH2  | 5.50  | 123.05      | 120.30   |
| 1   | H     | 1277 | ARG  | NE-CZ-NH2  | 5.50  | 123.05      | 120.30   |
| 3   | L     | 120  | ARG  | NE-CZ-NH2  | 5.49  | 123.05      | 120.30   |
| 1   | O     | 403  | ARG  | NE-CZ-NH2  | 5.49  | 123.05      | 120.30   |
| 1   | N     | 308  | TYR  | CB-CG-CD1  | 5.49  | 124.29      | 121.00   |
| 1   | A     | 243  | ARG  | NH1-CZ-NH2 | -5.49 | 113.36      | 119.40   |
| 4   | V     | 255  | ARG  | NE-CZ-NH2  | 5.48  | 123.04      | 120.30   |
| 1   | A     | 1167 | ARG  | NE-CZ-NH2  | 5.48  | 123.04      | 120.30   |
| 5   | P     | 819  | ARG  | NE-CZ-NH2  | 5.46  | 123.03      | 120.30   |
| 2   | K     | 94   | ARG  | NE-CZ-NH2  | 5.46  | 123.03      | 120.30   |
| 1   | H     | 567  | ARG  | NE-CZ-NH2  | 5.45  | 123.03      | 120.30   |
| 1   | N     | 952  | ARG  | NE-CZ-NH2  | 5.45  | 123.03      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 17   | ARG  | NE-CZ-NH2 | 5.45  | 123.02      | 120.30   |
| 1   | H     | 142  | TYR  | CB-CG-CD2 | -5.45 | 117.73      | 121.00   |
| 1   | Q     | 54   | ARG  | NE-CZ-NH2 | 5.45  | 123.02      | 120.30   |
| 1   | A     | 1289 | ARG  | NE-CZ-NH2 | 5.43  | 123.02      | 120.30   |
| 5   | P     | 580  | ARG  | NE-CZ-NH2 | 5.43  | 123.02      | 120.30   |
| 1   | H     | 1136 | ARG  | NE-CZ-NH2 | 5.42  | 123.01      | 120.30   |
| 1   | H     | 1608 | ARG  | NE-CZ-NH2 | 5.42  | 123.01      | 120.30   |
| 5   | I     | 782  | ARG  | NE-CZ-NH2 | 5.42  | 123.01      | 120.30   |
| 1   | O     | 190  | ARG  | NE-CZ-NH2 | 5.42  | 123.01      | 120.30   |
| 5   | P     | 1365 | ARG  | NE-CZ-NH2 | 5.42  | 123.01      | 120.30   |
| 1   | B     | 1846 | ARG  | NE-CZ-NH2 | 5.41  | 123.01      | 120.30   |
| 1   | H     | 1832 | ARG  | NE-CZ-NH2 | 5.41  | 123.01      | 120.30   |
| 1   | O     | 1268 | ARG  | NE-CZ-NH2 | 5.41  | 123.00      | 120.30   |
| 1   | O     | 281  | ARG  | NE-CZ-NH1 | -5.41 | 117.60      | 120.30   |
| 5   | I     | 646  | ARG  | NE-CZ-NH2 | 5.40  | 123.00      | 120.30   |
| 1   | O     | 1846 | ARG  | NE-CZ-NH2 | 5.40  | 123.00      | 120.30   |
| 1   | A     | 501  | TYR  | CB-CG-CD2 | -5.39 | 117.76      | 121.00   |
| 1   | N     | 719  | ARG  | NE-CZ-NH2 | 5.39  | 123.00      | 120.30   |
| 1   | O     | 798  | ARG  | NE-CZ-NH2 | 5.39  | 123.00      | 120.30   |
| 1   | O     | 780  | ARG  | NE-CZ-NH2 | 5.39  | 122.99      | 120.30   |
| 1   | A     | 1375 | TYR  | CB-CG-CD1 | -5.38 | 117.77      | 121.00   |
| 1   | A     | 780  | ARG  | NE-CZ-NH2 | 5.38  | 122.99      | 120.30   |
| 1   | O     | 819  | ARG  | NE-CZ-NH2 | 5.38  | 122.99      | 120.30   |
| 1   | Q     | 281  | ARG  | CD-NE-CZ  | 5.37  | 131.12      | 123.60   |
| 1   | B     | 1176 | ARG  | NE-CZ-NH2 | 5.36  | 122.98      | 120.30   |
| 1   | A     | 1530 | ARG  | NE-CZ-NH2 | 5.36  | 122.98      | 120.30   |
| 1   | A     | 671  | ARG  | NE-CZ-NH2 | 5.36  | 122.98      | 120.30   |
| 1   | H     | 1820 | ARG  | NE-CZ-NH2 | 5.36  | 122.98      | 120.30   |
| 1   | Q     | 715  | TYR  | CB-CG-CD2 | -5.35 | 117.79      | 121.00   |
| 1   | Q     | 703  | ARG  | NE-CZ-NH2 | 5.35  | 122.98      | 120.30   |
| 1   | H     | 1841 | ARG  | NE-CZ-NH2 | 5.35  | 122.97      | 120.30   |
| 1   | A     | 1250 | ARG  | NE-CZ-NH2 | 5.34  | 122.97      | 120.30   |
| 1   | A     | 952  | ARG  | NE-CZ-NH2 | 5.34  | 122.97      | 120.30   |
| 1   | N     | 272  | ARG  | NE-CZ-NH2 | 5.34  | 122.97      | 120.30   |
| 1   | O     | 1818 | ARG  | NE-CZ-NH2 | 5.33  | 122.96      | 120.30   |
| 1   | A     | 281  | ARG  | NE-CZ-NH2 | 5.33  | 122.96      | 120.30   |
| 5   | P     | 551  | ARG  | NE-CZ-NH2 | 5.32  | 122.96      | 120.30   |
| 1   | Q     | 1818 | ARG  | NE-CZ-NH2 | 5.32  | 122.96      | 120.30   |
| 1   | O     | 719  | ARG  | NE-CZ-NH2 | 5.32  | 122.96      | 120.30   |
| 1   | Q     | 147  | ARG  | NE-CZ-NH2 | 5.31  | 122.96      | 120.30   |
| 1   | A     | 1114 | ARG  | NE-CZ-NH2 | 5.31  | 122.96      | 120.30   |
| 5   | I     | 976  | ARG  | NE-CZ-NH2 | 5.30  | 122.95      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5   | P     | 459  | ARG  | NE-CZ-NH2 | 5.30  | 122.95      | 120.30   |
| 1   | Q     | 858  | ARG  | NE-CZ-NH2 | 5.30  | 122.95      | 120.30   |
| 1   | B     | 1820 | ARG  | NE-CZ-NH2 | 5.30  | 122.95      | 120.30   |
| 1   | N     | 1447 | ARG  | NE-CZ-NH2 | 5.30  | 122.95      | 120.30   |
| 1   | H     | 1053 | ARG  | NE-CZ-NH2 | 5.29  | 122.95      | 120.30   |
| 1   | O     | 1880 | ARG  | NE-CZ-NH2 | 5.29  | 122.94      | 120.30   |
| 5   | I     | 353  | ARG  | NE-CZ-NH2 | 5.29  | 122.94      | 120.30   |
| 3   | U     | 40   | ARG  | NE-CZ-NH2 | 5.28  | 122.94      | 120.30   |
| 1   | N     | 1344 | ARG  | NE-CZ-NH2 | 5.27  | 122.94      | 120.30   |
| 1   | N     | 29   | ARG  | CD-NE-CZ  | 5.27  | 130.98      | 123.60   |
| 1   | O     | 1475 | ARG  | NE-CZ-NH2 | 5.27  | 122.94      | 120.30   |
| 1   | H     | 1337 | ARG  | NE-CZ-NH2 | 5.27  | 122.94      | 120.30   |
| 1   | A     | 706  | ARG  | NE-CZ-NH2 | 5.27  | 122.93      | 120.30   |
| 1   | O     | 1841 | ARG  | NE-CZ-NH2 | 5.26  | 122.93      | 120.30   |
| 1   | Q     | 1845 | ARG  | NE-CZ-NH2 | 5.24  | 122.92      | 120.30   |
| 4   | V     | 171  | ARG  | NE-CZ-NH2 | 5.24  | 122.92      | 120.30   |
| 1   | N     | 1129 | ARG  | NE-CZ-NH2 | 5.24  | 122.92      | 120.30   |
| 5   | I     | 381  | ARG  | NE-CZ-NH2 | 5.23  | 122.91      | 120.30   |
| 1   | O     | 1530 | ARG  | NE-CZ-NH2 | 5.22  | 122.91      | 120.30   |
| 1   | Q     | 1375 | TYR  | CB-CG-CD2 | -5.21 | 117.88      | 121.00   |
| 1   | B     | 1447 | ARG  | NE-CZ-NH2 | 5.20  | 122.90      | 120.30   |
| 1   | H     | 29   | ARG  | NE-CZ-NH2 | 5.20  | 122.90      | 120.30   |
| 1   | O     | 1114 | ARG  | NE-CZ-NH2 | 5.20  | 122.90      | 120.30   |
| 1   | Q     | 453  | ARG  | NE-CZ-NH2 | 5.19  | 122.89      | 120.30   |
| 5   | I     | 547  | ARG  | NE-CZ-NH2 | 5.18  | 122.89      | 120.30   |
| 4   | G     | 105  | ARG  | NE-CZ-NH2 | 5.18  | 122.89      | 120.30   |
| 1   | H     | 1289 | ARG  | NE-CZ-NH2 | 5.18  | 122.89      | 120.30   |
| 5   | P     | 1072 | ARG  | NE-CZ-NH2 | 5.18  | 122.89      | 120.30   |
| 1   | O     | 1277 | ARG  | NE-CZ-NH2 | 5.17  | 122.89      | 120.30   |
| 1   | Q     | 1500 | ARG  | NE-CZ-NH2 | 5.17  | 122.89      | 120.30   |
| 1   | O     | 588  | TYR  | CB-CG-CD2 | -5.17 | 117.90      | 121.00   |
| 1   | O     | 147  | ARG  | NE-CZ-NH2 | 5.17  | 122.88      | 120.30   |
| 1   | A     | 1841 | ARG  | NE-CZ-NH2 | 5.16  | 122.88      | 120.30   |
| 1   | B     | 1434 | ARG  | NE-CZ-NH2 | 5.16  | 122.88      | 120.30   |
| 2   | C     | 94   | ARG  | NE-CZ-NH2 | 5.16  | 122.88      | 120.30   |
| 1   | O     | 1337 | ARG  | NE-CZ-NH2 | 5.16  | 122.88      | 120.30   |
| 3   | L     | 50   | ARG  | NE-CZ-NH2 | 5.16  | 122.88      | 120.30   |
| 5   | P     | 353  | ARG  | NE-CZ-NH1 | -5.15 | 117.72      | 120.30   |
| 1   | H     | 23   | ARG  | NE-CZ-NH2 | 5.15  | 122.88      | 120.30   |
| 1   | O     | 1608 | ARG  | NE-CZ-NH2 | 5.14  | 122.87      | 120.30   |
| 1   | A     | 1662 | ARG  | NE-CZ-NH2 | 5.14  | 122.87      | 120.30   |
| 5   | P     | 652  | ARG  | NE-CZ-NH2 | 5.14  | 122.87      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 1050 | ARG  | NE-CZ-NH2 | 5.14  | 122.87      | 120.30   |
| 1   | H     | 793  | ARG  | NE-CZ-NH2 | 5.14  | 122.87      | 120.30   |
| 1   | B     | 1126 | ARG  | NE-CZ-NH2 | 5.12  | 122.86      | 120.30   |
| 4   | G     | 172  | ARG  | NE-CZ-NH2 | 5.12  | 122.86      | 120.30   |
| 1   | A     | 1699 | ARG  | NE-CZ-NH1 | -5.12 | 117.74      | 120.30   |
| 5   | I     | 1072 | ARG  | NE-CZ-NH2 | 5.11  | 122.86      | 120.30   |
| 1   | Q     | 694  | ARG  | NE-CZ-NH2 | 5.11  | 122.86      | 120.30   |
| 1   | O     | 1500 | ARG  | NE-CZ-NH2 | 5.11  | 122.86      | 120.30   |
| 1   | N     | 1818 | ARG  | NE-CZ-NH2 | 5.11  | 122.85      | 120.30   |
| 1   | O     | 1093 | ARG  | NE-CZ-NH1 | -5.10 | 117.75      | 120.30   |
| 1   | N     | 1382 | ARG  | NE-CZ-NH2 | 5.10  | 122.85      | 120.30   |
| 3   | F     | 50   | ARG  | NE-CZ-NH2 | 5.10  | 122.85      | 120.30   |
| 5   | P     | 404  | ARG  | NE-CZ-NH2 | 5.10  | 122.85      | 120.30   |
| 1   | O     | 1250 | ARG  | NE-CZ-NH2 | 5.09  | 122.85      | 120.30   |
| 1   | A     | 143  | ARG  | NE-CZ-NH2 | 5.09  | 122.84      | 120.30   |
| 1   | O     | 787  | ARG  | NE-CZ-NH2 | 5.09  | 122.84      | 120.30   |
| 5   | P     | 1200 | ARG  | NE-CZ-NH2 | 5.09  | 122.84      | 120.30   |
| 1   | N     | 453  | ARG  | NE-CZ-NH2 | 5.08  | 122.84      | 120.30   |
| 1   | N     | 777  | ARG  | NE-CZ-NH2 | 5.08  | 122.84      | 120.30   |
| 4   | V     | 78   | ARG  | NE-CZ-NH2 | 5.08  | 122.84      | 120.30   |
| 1   | O     | 1689 | ARG  | NE-CZ-NH2 | 5.08  | 122.84      | 120.30   |
| 4   | G     | 78   | ARG  | NE-CZ-NH2 | 5.08  | 122.84      | 120.30   |
| 5   | I     | 478  | ARG  | NE-CZ-NH2 | 5.08  | 122.84      | 120.30   |
| 1   | B     | 1841 | ARG  | NE-CZ-NH2 | 5.07  | 122.84      | 120.30   |
| 1   | O     | 1375 | TYR  | CB-CG-CD1 | -5.07 | 117.95      | 121.00   |
| 4   | V     | 325  | ARG  | NE-CZ-NH2 | 5.07  | 122.84      | 120.30   |
| 1   | A     | 1846 | ARG  | NE-CZ-NH2 | 5.07  | 122.83      | 120.30   |
| 1   | H     | 1560 | ARG  | NE-CZ-NH2 | 5.07  | 122.83      | 120.30   |
| 2   | R     | 163  | ARG  | NE-CZ-NH2 | 5.06  | 122.83      | 120.30   |
| 5   | I     | 880  | ARG  | NE-CZ-NH2 | 5.05  | 122.83      | 120.30   |
| 1   | A     | 798  | ARG  | NE-CZ-NH2 | 5.05  | 122.82      | 120.30   |
| 1   | A     | 29   | ARG  | NE-CZ-NH2 | 5.04  | 122.82      | 120.30   |
| 1   | H     | 1863 | ARG  | NE-CZ-NH2 | 5.03  | 122.82      | 120.30   |
| 1   | O     | 108  | ARG  | NE-CZ-NH1 | -5.03 | 117.78      | 120.30   |
| 1   | B     | 780  | ARG  | NE-CZ-NH2 | 5.03  | 122.81      | 120.30   |
| 1   | B     | 1613 | ARG  | NE-CZ-NH2 | 5.03  | 122.81      | 120.30   |
| 1   | B     | 1858 | ARG  | NE-CZ-NH2 | 5.02  | 122.81      | 120.30   |
| 1   | H     | 1845 | ARG  | NE-CZ-NH2 | 5.02  | 122.81      | 120.30   |
| 5   | I     | 943  | ARG  | NE-CZ-NH2 | 5.02  | 122.81      | 120.30   |
| 1   | N     | 1277 | ARG  | NE-CZ-NH2 | 5.02  | 122.81      | 120.30   |
| 1   | B     | 1560 | ARG  | NE-CZ-NH2 | 5.01  | 122.81      | 120.30   |
| 1   | H     | 858  | ARG  | NE-CZ-NH2 | 5.01  | 122.81      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|------|-------------|----------|
| 3   | M     | 58   | ARG  | NE-CZ-NH2 | 5.01 | 122.81      | 120.30   |
| 4   | V     | 157  | ARG  | NE-CZ-NH2 | 5.01 | 122.81      | 120.30   |
| 4   | V     | 74   | ARG  | NE-CZ-NH2 | 5.01 | 122.81      | 120.30   |
| 1   | Q     | 1863 | ARG  | NE-CZ-NH2 | 5.01 | 122.80      | 120.30   |
| 1   | H     | 1846 | ARG  | NE-CZ-NH2 | 5.01 | 122.80      | 120.30   |
| 1   | A     | 1749 | ARG  | NE-CZ-NH2 | 5.00 | 122.80      | 120.30   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1375 | TYR  | Sidechain |
| 1   | B     | 194  | TYR  | Sidechain |
| 1   | B     | 925  | ARG  | Sidechain |
| 1   | H     | 1375 | TYR  | Sidechain |
| 1   | H     | 1608 | ARG  | Sidechain |
| 5   | I     | 1192 | ARG  | Sidechain |
| 3   | L     | 40   | ARG  | Sidechain |
| 1   | O     | 103  | TYR  | Sidechain |
| 5   | P     | 378  | TYR  | Sidechain |
| 1   | Q     | 1375 | TYR  | Sidechain |
| 1   | Q     | 272  | ARG  | Sidechain |
| 1   | Q     | 432  | TYR  | Sidechain |
| 1   | Q     | 442  | ARG  | Sidechain |
| 1   | Q     | 833  | TYR  | Sidechain |
| 2   | S     | 63   | ARG  | Sidechain |

## 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     | 15571 | 0        | 15684    | 85      | 0            |
| 1   | B     | 15571 | 0        | 15684    | 52      | 0            |
| 1   | H     | 15600 | 0        | 15711    | 83      | 0            |
| 1   | N     | 15600 | 0        | 15712    | 87      | 0            |
| 1   | O     | 15571 | 0        | 15683    | 57      | 0            |
| 1   | Q     | 15571 | 0        | 15684    | 54      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | C     | 1206   | 0        | 1182     | 0       | 0            |
| 2   | D     | 1206   | 0        | 1182     | 0       | 0            |
| 2   | J     | 1206   | 0        | 1182     | 0       | 0            |
| 2   | K     | 1206   | 0        | 1182     | 0       | 0            |
| 2   | R     | 1206   | 0        | 1182     | 0       | 0            |
| 2   | S     | 1206   | 0        | 1182     | 0       | 0            |
| 3   | E     | 1283   | 0        | 1245     | 37      | 0            |
| 3   | F     | 1283   | 0        | 1245     | 0       | 0            |
| 3   | L     | 1283   | 0        | 1245     | 35      | 0            |
| 3   | M     | 1283   | 0        | 1245     | 0       | 0            |
| 3   | T     | 1283   | 0        | 1245     | 38      | 0            |
| 3   | U     | 1283   | 0        | 1245     | 0       | 0            |
| 4   | G     | 3151   | 0        | 3155     | 0       | 0            |
| 4   | V     | 3151   | 0        | 3155     | 0       | 0            |
| 5   | I     | 8349   | 0        | 8362     | 0       | 0            |
| 5   | P     | 8349   | 0        | 8362     | 0       | 0            |
| All | All   | 131418 | 0        | 131754   | 282     | 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 1.

All (282) 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:1375:TYR:CE2 | 1:B:1375:TYR:CE2 | 2.12                     | 1.38              |
| 1:A:1375:TYR:CD2 | 1:B:1375:TYR:CE2 | 2.12                     | 1.38              |
| 1:A:1449:PHE:CD1 | 1:B:1449:PHE:CD2 | 2.12                     | 1.38              |
| 1:A:1375:TYR:CE2 | 1:B:1375:TYR:CD2 | 2.12                     | 1.38              |
| 1:A:1375:TYR:CD2 | 1:B:1375:TYR:CD2 | 2.12                     | 1.38              |
| 1:A:1449:PHE:CE1 | 1:B:1449:PHE:CD2 | 2.12                     | 1.38              |
| 1:A:1449:PHE:CE1 | 1:B:1449:PHE:CE2 | 2.12                     | 1.37              |
| 1:H:1449:PHE:CD2 | 1:O:1449:PHE:CD1 | 2.12                     | 1.37              |
| 1:H:1449:PHE:CE2 | 1:O:1449:PHE:CE1 | 2.12                     | 1.37              |
| 1:N:1375:TYR:CE2 | 1:Q:1375:TYR:CD1 | 2.12                     | 1.37              |
| 1:N:1449:PHE:CE2 | 1:Q:1449:PHE:CD1 | 2.12                     | 1.37              |
| 1:H:1375:TYR:CE2 | 1:O:1375:TYR:CD2 | 2.12                     | 1.37              |
| 1:H:1375:TYR:CE2 | 1:O:1375:TYR:CE2 | 2.12                     | 1.37              |
| 1:N:1375:TYR:CD2 | 1:Q:1375:TYR:CD1 | 2.12                     | 1.37              |
| 1:N:1449:PHE:CD2 | 1:Q:1449:PHE:CD1 | 2.12                     | 1.37              |
| 1:H:1449:PHE:CD2 | 1:O:1449:PHE:CE1 | 2.12                     | 1.36              |
| 1:H:1375:TYR:CD2 | 1:O:1375:TYR:CD2 | 2.12                     | 1.36              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1449:PHE:CE2 | 1:O:1449:PHE:CD1 | 2.12                     | 1.36              |
| 1:N:1449:PHE:CE2 | 1:Q:1449:PHE:CE1 | 2.12                     | 1.36              |
| 1:H:1375:TYR:CD2 | 1:O:1375:TYR:CE2 | 2.12                     | 1.36              |
| 1:A:1449:PHE:CD1 | 1:B:1449:PHE:CE2 | 2.12                     | 1.35              |
| 1:N:1375:TYR:CD2 | 1:Q:1375:TYR:CE1 | 2.12                     | 1.35              |
| 1:N:1375:TYR:CE2 | 1:Q:1375:TYR:CE1 | 2.12                     | 1.35              |
| 1:N:1449:PHE:CD2 | 1:Q:1449:PHE:CE1 | 2.12                     | 1.34              |
| 3:T:108:PRO:CD   | 3:T:108:PRO:CG   | 2.06                     | 1.34              |
| 3:L:108:PRO:CB   | 3:L:108:PRO:CG   | 2.06                     | 1.32              |
| 3:L:108:PRO:CG   | 3:L:108:PRO:CD   | 2.08                     | 1.32              |
| 3:E:108:PRO:CA   | 3:E:108:PRO:CB   | 2.08                     | 1.31              |
| 3:T:108:PRO:CB   | 3:T:108:PRO:CA   | 2.08                     | 1.31              |
| 3:T:108:PRO:CG   | 3:T:108:PRO:CB   | 2.06                     | 1.31              |
| 3:L:108:PRO:CB   | 3:L:108:PRO:CA   | 2.08                     | 1.31              |
| 3:E:108:PRO:CB   | 3:E:108:PRO:CG   | 2.06                     | 1.30              |
| 3:E:108:PRO:N    | 3:E:108:PRO:CD   | 1.92                     | 1.30              |
| 3:E:108:PRO:CG   | 3:E:108:PRO:CD   | 2.08                     | 1.30              |
| 3:L:108:PRO:CD   | 3:L:108:PRO:N    | 1.92                     | 1.30              |
| 3:E:108:PRO:CA   | 3:E:108:PRO:N    | 1.96                     | 1.29              |
| 3:T:108:PRO:CD   | 3:T:108:PRO:N    | 1.94                     | 1.29              |
| 3:T:108:PRO:CA   | 3:T:108:PRO:N    | 1.96                     | 1.29              |
| 3:L:108:PRO:CA   | 3:L:108:PRO:N    | 1.96                     | 1.28              |
| 1:A:1375:TYR:CG  | 1:B:1375:TYR:CE2 | 2.30                     | 1.20              |
| 1:A:1449:PHE:CE1 | 1:B:1449:PHE:CG  | 2.30                     | 1.20              |
| 1:H:1375:TYR:CG  | 1:O:1375:TYR:CE2 | 2.30                     | 1.20              |
| 1:A:1449:PHE:CG  | 1:B:1449:PHE:CE2 | 2.30                     | 1.19              |
| 1:H:1375:TYR:CZ  | 1:O:1375:TYR:CE2 | 2.31                     | 1.19              |
| 1:N:1449:PHE:CE2 | 1:Q:1449:PHE:CG  | 2.30                     | 1.19              |
| 1:N:1449:PHE:CG  | 1:Q:1449:PHE:CE1 | 2.30                     | 1.19              |
| 1:A:1449:PHE:CE1 | 1:B:1449:PHE:CZ  | 2.31                     | 1.19              |
| 1:H:1449:PHE:CZ  | 1:O:1449:PHE:CD1 | 2.31                     | 1.19              |
| 1:N:1375:TYR:CZ  | 1:Q:1375:TYR:CE1 | 2.31                     | 1.19              |
| 1:A:1375:TYR:CD2 | 1:B:1375:TYR:CZ  | 2.31                     | 1.19              |
| 1:H:1375:TYR:CD2 | 1:O:1375:TYR:CG  | 2.31                     | 1.19              |
| 1:H:1449:PHE:CG  | 1:O:1449:PHE:CD1 | 2.31                     | 1.19              |
| 1:N:1375:TYR:CD2 | 1:Q:1375:TYR:CZ  | 2.31                     | 1.19              |
| 1:A:1375:TYR:CE2 | 1:B:1375:TYR:CZ  | 2.31                     | 1.19              |
| 1:A:1449:PHE:CZ  | 1:B:1449:PHE:CE2 | 2.31                     | 1.19              |
| 1:H:1449:PHE:CG  | 1:O:1449:PHE:CE1 | 2.31                     | 1.19              |
| 1:N:1449:PHE:CE2 | 1:Q:1449:PHE:CZ  | 2.31                     | 1.19              |
| 1:A:1375:TYR:CD2 | 1:B:1375:TYR:CG  | 2.31                     | 1.19              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1375:TYR:CD2 | 1:O:1375:TYR:CZ  | 2.31                     | 1.19              |
| 1:H:1375:TYR:CZ  | 1:O:1375:TYR:CD2 | 2.31                     | 1.19              |
| 1:H:1375:TYR:CE2 | 1:O:1375:TYR:CG  | 2.30                     | 1.18              |
| 1:H:1449:PHE:CE2 | 1:O:1449:PHE:CZ  | 2.31                     | 1.18              |
| 1:N:1375:TYR:CE2 | 1:Q:1375:TYR:CG  | 2.30                     | 1.18              |
| 1:N:1375:TYR:CD2 | 1:Q:1375:TYR:CG  | 2.31                     | 1.18              |
| 1:H:1449:PHE:CD2 | 1:O:1449:PHE:CG  | 2.31                     | 1.18              |
| 1:H:1449:PHE:CD2 | 1:O:1449:PHE:CZ  | 2.31                     | 1.18              |
| 1:H:1449:PHE:CE2 | 1:O:1449:PHE:CG  | 2.30                     | 1.18              |
| 1:N:1375:TYR:CZ  | 1:Q:1375:TYR:CD1 | 2.30                     | 1.18              |
| 1:N:1375:TYR:CG  | 1:Q:1375:TYR:CD1 | 2.31                     | 1.18              |
| 1:H:1375:TYR:CE2 | 1:O:1375:TYR:CZ  | 2.31                     | 1.18              |
| 1:A:1375:TYR:CZ  | 1:B:1375:TYR:CD2 | 2.31                     | 1.18              |
| 1:A:1449:PHE:CD1 | 1:B:1449:PHE:CG  | 2.31                     | 1.18              |
| 1:A:1449:PHE:CZ  | 1:B:1449:PHE:CD2 | 2.31                     | 1.18              |
| 1:N:1449:PHE:CD2 | 1:Q:1449:PHE:CG  | 2.31                     | 1.18              |
| 1:A:1375:TYR:CG  | 1:B:1375:TYR:CD2 | 2.31                     | 1.17              |
| 1:A:1375:TYR:CZ  | 1:B:1375:TYR:CE2 | 2.30                     | 1.17              |
| 1:N:1375:TYR:CG  | 1:Q:1375:TYR:CE1 | 2.31                     | 1.17              |
| 1:N:1375:TYR:CE2 | 1:Q:1375:TYR:CZ  | 2.31                     | 1.17              |
| 1:N:1449:PHE:CD2 | 1:Q:1449:PHE:CZ  | 2.31                     | 1.17              |
| 1:N:1449:PHE:CZ  | 1:Q:1449:PHE:CD1 | 2.31                     | 1.17              |
| 1:A:1375:TYR:CE2 | 1:B:1375:TYR:CG  | 2.31                     | 1.17              |
| 1:A:1449:PHE:CD1 | 1:B:1449:PHE:CZ  | 2.31                     | 1.17              |
| 1:H:1375:TYR:CG  | 1:O:1375:TYR:CD2 | 2.31                     | 1.17              |
| 1:N:1449:PHE:CG  | 1:Q:1449:PHE:CD1 | 2.31                     | 1.17              |
| 1:N:1449:PHE:CZ  | 1:Q:1449:PHE:CE1 | 2.31                     | 1.17              |
| 1:A:1449:PHE:CG  | 1:B:1449:PHE:CD2 | 2.31                     | 1.17              |
| 1:H:1449:PHE:CZ  | 1:O:1449:PHE:CE1 | 2.31                     | 1.16              |
| 1:N:1449:PHE:CE2 | 1:Q:1449:PHE:CD2 | 2.35                     | 1.15              |
| 1:A:1449:PHE:CD2 | 1:B:1449:PHE:CD2 | 2.35                     | 1.15              |
| 1:A:1375:TYR:CE2 | 1:B:1375:TYR:CD1 | 2.35                     | 1.15              |
| 1:A:1375:TYR:CD2 | 1:B:1375:TYR:CE1 | 2.35                     | 1.15              |
| 1:A:1375:TYR:CD1 | 1:B:1375:TYR:CD2 | 2.35                     | 1.15              |
| 1:A:1449:PHE:CE1 | 1:B:1449:PHE:CE1 | 2.35                     | 1.15              |
| 1:A:1449:PHE:CD2 | 1:B:1449:PHE:CE2 | 2.35                     | 1.15              |
| 1:H:1449:PHE:CD2 | 1:O:1449:PHE:CE2 | 2.35                     | 1.15              |
| 1:N:1375:TYR:CD1 | 1:Q:1375:TYR:CD1 | 2.35                     | 1.15              |
| 1:N:1449:PHE:CE2 | 1:Q:1449:PHE:CE2 | 2.35                     | 1.15              |
| 1:N:1449:PHE:CD1 | 1:Q:1449:PHE:CD1 | 2.35                     | 1.15              |
| 1:H:1449:PHE:CE1 | 1:O:1449:PHE:CE1 | 2.35                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:1375:TYR:CD1 | 1:Q:1375:TYR:CE1 | 2.35                     | 1.15              |
| 1:N:1449:PHE:CD2 | 1:Q:1449:PHE:CD2 | 2.35                     | 1.15              |
| 1:N:1449:PHE:CD1 | 1:Q:1449:PHE:CE1 | 2.35                     | 1.15              |
| 1:H:1375:TYR:CD1 | 1:O:1375:TYR:CD2 | 2.35                     | 1.15              |
| 1:H:1449:PHE:CE1 | 1:O:1449:PHE:CD1 | 2.35                     | 1.15              |
| 1:A:1375:TYR:CE1 | 1:B:1375:TYR:CD2 | 2.35                     | 1.14              |
| 1:N:1375:TYR:CE1 | 1:Q:1375:TYR:CE1 | 2.35                     | 1.14              |
| 1:A:803:LYS:CE   | 3:E:108:PRO:CA   | 2.25                     | 1.14              |
| 1:A:1375:TYR:CE2 | 1:B:1375:TYR:CE1 | 2.35                     | 1.14              |
| 1:A:1375:TYR:CD1 | 1:B:1375:TYR:CE2 | 2.35                     | 1.14              |
| 1:A:1449:PHE:CD1 | 1:B:1449:PHE:CE1 | 2.35                     | 1.14              |
| 1:H:1375:TYR:CE2 | 1:O:1375:TYR:CD1 | 2.35                     | 1.14              |
| 1:H:1375:TYR:CD2 | 1:O:1375:TYR:CE1 | 2.35                     | 1.14              |
| 1:H:1375:TYR:CE1 | 1:O:1375:TYR:CE2 | 2.35                     | 1.14              |
| 1:H:1449:PHE:CD1 | 1:O:1449:PHE:CD1 | 2.34                     | 1.14              |
| 1:N:1449:PHE:CD2 | 1:Q:1449:PHE:CE2 | 2.35                     | 1.14              |
| 1:A:1449:PHE:CE2 | 1:B:1449:PHE:CE2 | 2.35                     | 1.14              |
| 1:H:1375:TYR:CD2 | 1:O:1375:TYR:CD1 | 2.35                     | 1.14              |
| 1:N:1375:TYR:CE1 | 1:Q:1375:TYR:CD1 | 2.35                     | 1.14              |
| 1:N:1449:PHE:CE1 | 1:Q:1449:PHE:CE1 | 2.35                     | 1.14              |
| 1:A:1449:PHE:CD1 | 1:B:1449:PHE:CD1 | 2.35                     | 1.14              |
| 1:H:803:LYS:CD   | 3:L:108:PRO:CA   | 2.26                     | 1.14              |
| 1:N:1375:TYR:CE2 | 1:Q:1375:TYR:CD2 | 2.35                     | 1.14              |
| 1:N:1449:PHE:CE1 | 1:Q:1449:PHE:CD1 | 2.35                     | 1.14              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:CA   | 2.26                     | 1.14              |
| 1:H:1449:PHE:CD2 | 1:O:1449:PHE:CD2 | 2.35                     | 1.14              |
| 1:N:803:LYS:CE   | 3:T:108:PRO:CA   | 2.26                     | 1.14              |
| 1:N:1375:TYR:CE2 | 1:Q:1375:TYR:CE2 | 2.35                     | 1.14              |
| 1:A:1375:TYR:CD2 | 1:B:1375:TYR:CD1 | 2.35                     | 1.13              |
| 1:A:1449:PHE:CE2 | 1:B:1449:PHE:CD2 | 2.35                     | 1.13              |
| 1:H:803:LYS:CE   | 3:L:108:PRO:CB   | 2.26                     | 1.13              |
| 1:H:1375:TYR:CE1 | 1:O:1375:TYR:CD2 | 2.35                     | 1.13              |
| 1:H:1449:PHE:CE2 | 1:O:1449:PHE:CD2 | 2.35                     | 1.13              |
| 1:H:1449:PHE:CD1 | 1:O:1449:PHE:CE1 | 2.35                     | 1.13              |
| 1:N:803:LYS:CD   | 3:T:108:PRO:CA   | 2.26                     | 1.13              |
| 1:A:803:LYS:CE   | 3:E:108:PRO:CB   | 2.26                     | 1.13              |
| 1:H:803:LYS:CE   | 3:L:108:PRO:CA   | 2.25                     | 1.13              |
| 1:N:1375:TYR:CD2 | 1:Q:1375:TYR:CE2 | 2.35                     | 1.13              |
| 1:H:1375:TYR:CD1 | 1:O:1375:TYR:CE2 | 2.35                     | 1.13              |
| 1:N:1375:TYR:CD2 | 1:Q:1375:TYR:CD2 | 2.35                     | 1.13              |
| 1:A:1449:PHE:CE1 | 1:B:1449:PHE:CD1 | 2.35                     | 1.13              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1449:PHE:CE2 | 1:O:1449:PHE:CE2 | 2.35                     | 1.13              |
| 1:A:1375:TYR:CE1 | 1:B:1375:TYR:CE2 | 2.35                     | 1.12              |
| 1:H:1375:TYR:CE2 | 1:O:1375:TYR:CE1 | 2.35                     | 1.12              |
| 1:H:803:LYS:CD   | 3:L:108:PRO:CG   | 2.27                     | 1.12              |
| 1:N:803:LYS:CE   | 3:T:108:PRO:CB   | 2.28                     | 1.11              |
| 1:N:803:LYS:CE   | 3:T:108:PRO:CG   | 2.28                     | 1.11              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:CG   | 2.27                     | 1.11              |
| 1:N:803:LYS:CD   | 3:T:108:PRO:CB   | 2.28                     | 1.10              |
| 1:A:803:LYS:CE   | 3:E:108:PRO:CD   | 2.28                     | 1.10              |
| 1:N:803:LYS:CE   | 3:T:108:PRO:CD   | 2.29                     | 1.10              |
| 1:N:803:LYS:CD   | 3:T:108:PRO:CD   | 2.29                     | 1.10              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:CB   | 2.30                     | 1.09              |
| 1:H:803:LYS:CE   | 3:L:108:PRO:CD   | 2.28                     | 1.09              |
| 1:H:803:LYS:CD   | 3:L:108:PRO:CB   | 2.29                     | 1.09              |
| 1:N:803:LYS:CD   | 3:T:108:PRO:CG   | 2.30                     | 1.09              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:CD   | 2.31                     | 1.08              |
| 1:H:803:LYS:CD   | 3:L:108:PRO:CD   | 2.31                     | 1.08              |
| 1:H:803:LYS:CE   | 3:L:108:PRO:CG   | 2.30                     | 1.08              |
| 1:A:803:LYS:CE   | 3:E:108:PRO:CG   | 2.30                     | 1.08              |
| 1:N:803:LYS:CE   | 3:T:108:PRO:N    | 2.26                     | 0.99              |
| 1:B:1375:TYR:CE2 | 1:B:1375:TYR:CD2 | 2.52                     | 0.98              |
| 1:O:1375:TYR:CD2 | 1:O:1375:TYR:CE2 | 2.52                     | 0.98              |
| 1:A:1375:TYR:CE2 | 1:A:1375:TYR:CD2 | 2.52                     | 0.98              |
| 1:H:1375:TYR:CE2 | 1:H:1375:TYR:CD2 | 2.52                     | 0.98              |
| 1:A:1449:PHE:CD1 | 1:A:1449:PHE:CE1 | 2.52                     | 0.98              |
| 1:Q:1449:PHE:CD1 | 1:Q:1449:PHE:CE1 | 2.52                     | 0.98              |
| 1:O:1449:PHE:CD1 | 1:O:1449:PHE:CE1 | 2.52                     | 0.98              |
| 1:H:1449:PHE:CD2 | 1:H:1449:PHE:CE2 | 2.51                     | 0.97              |
| 1:A:803:LYS:CE   | 3:E:108:PRO:N    | 2.27                     | 0.97              |
| 1:N:1375:TYR:CE2 | 1:N:1375:TYR:CD2 | 2.52                     | 0.97              |
| 1:Q:1375:TYR:CD1 | 1:Q:1375:TYR:CE1 | 2.51                     | 0.97              |
| 1:B:1449:PHE:CD2 | 1:B:1449:PHE:CE2 | 2.51                     | 0.97              |
| 1:N:803:LYS:HE2  | 3:T:108:PRO:CD   | 1.92                     | 0.97              |
| 1:N:803:LYS:HE3  | 3:T:108:PRO:CA   | 1.93                     | 0.97              |
| 1:N:803:LYS:HD3  | 3:T:108:PRO:CG   | 1.94                     | 0.97              |
| 1:N:1449:PHE:CE2 | 1:N:1449:PHE:CD2 | 2.51                     | 0.97              |
| 1:H:803:LYS:CE   | 3:L:108:PRO:N    | 2.28                     | 0.96              |
| 1:H:803:LYS:CD   | 3:L:108:PRO:N    | 2.29                     | 0.96              |
| 1:N:803:LYS:CD   | 3:T:108:PRO:N    | 2.29                     | 0.96              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:N    | 2.29                     | 0.95              |
| 1:A:803:LYS:HD2  | 3:E:108:PRO:CD   | 1.97                     | 0.95              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:803:LYS:HD2 | 3:L:108:PRO:CD  | 1.95                     | 0.94              |
| 1:N:803:LYS:HD2 | 3:T:108:PRO:CB  | 1.96                     | 0.93              |
| 1:A:803:LYS:HE3 | 3:E:108:PRO:CB  | 1.96                     | 0.93              |
| 1:H:803:LYS:HE3 | 3:L:108:PRO:CB  | 1.98                     | 0.91              |
| 1:A:803:LYS:HE2 | 3:E:108:PRO:N   | 1.90                     | 0.86              |
| 1:H:803:LYS:HE2 | 3:L:108:PRO:N   | 1.90                     | 0.83              |
| 1:H:803:LYS:HD3 | 3:L:108:PRO:CA  | 2.09                     | 0.83              |
| 1:A:803:LYS:HD3 | 3:E:108:PRO:N   | 1.97                     | 0.79              |
| 1:H:803:LYS:HE3 | 3:L:108:PRO:CA  | 2.13                     | 0.78              |
| 1:A:803:LYS:HD3 | 3:E:108:PRO:CA  | 2.13                     | 0.78              |
| 1:H:803:LYS:HD3 | 3:L:108:PRO:N   | 1.99                     | 0.78              |
| 1:N:803:LYS:HD2 | 3:T:108:PRO:CA  | 2.17                     | 0.74              |
| 1:A:803:LYS:HE3 | 3:E:108:PRO:CA  | 2.16                     | 0.74              |
| 1:N:803:LYS:HE2 | 3:T:108:PRO:HD2 | 1.71                     | 0.73              |
| 1:N:803:LYS:HD3 | 3:T:108:PRO:HG3 | 1.72                     | 0.71              |
| 1:A:803:LYS:CG  | 3:E:108:PRO:HB3 | 2.21                     | 0.70              |
| 1:A:803:LYS:HD2 | 3:E:108:PRO:CG  | 2.20                     | 0.70              |
| 1:H:803:LYS:CG  | 3:L:108:PRO:HB3 | 2.21                     | 0.70              |
| 1:H:803:LYS:CG  | 3:L:108:PRO:CB  | 2.69                     | 0.70              |
| 1:A:803:LYS:CG  | 3:E:108:PRO:CB  | 2.70                     | 0.69              |
| 1:H:803:LYS:HD2 | 3:L:108:PRO:HD3 | 1.75                     | 0.67              |
| 1:N:803:LYS:HE3 | 3:T:108:PRO:C   | 2.14                     | 0.67              |
| 1:A:803:LYS:HE3 | 3:E:108:PRO:HB2 | 1.75                     | 0.67              |
| 1:A:803:LYS:HD2 | 3:E:108:PRO:HD3 | 1.77                     | 0.67              |
| 1:H:803:LYS:HE3 | 3:L:108:PRO:HB2 | 1.77                     | 0.64              |
| 1:N:803:LYS:HD2 | 3:T:108:PRO:HB3 | 1.76                     | 0.63              |
| 1:H:803:LYS:HD2 | 3:L:108:PRO:CG  | 2.24                     | 0.63              |
| 1:A:803:LYS:HE2 | 3:E:108:PRO:CA  | 2.30                     | 0.61              |
| 1:N:803:LYS:CD  | 3:T:108:PRO:HA  | 2.30                     | 0.60              |
| 1:H:803:LYS:NZ  | 3:L:108:PRO:CG  | 2.65                     | 0.59              |
| 1:N:803:LYS:HD3 | 3:T:108:PRO:CD  | 2.27                     | 0.58              |
| 1:A:803:LYS:NZ  | 3:E:108:PRO:CG  | 2.66                     | 0.58              |
| 1:O:96:LEU:HD13 | 1:O:96:LEU:H    | 1.68                     | 0.58              |
| 1:H:803:LYS:HE2 | 3:L:108:PRO:CA  | 2.32                     | 0.57              |
| 1:N:803:LYS:NZ  | 3:T:108:PRO:CB  | 2.69                     | 0.55              |
| 1:N:803:LYS:CG  | 3:T:108:PRO:N   | 2.69                     | 0.55              |
| 1:H:803:LYS:HD3 | 3:L:108:PRO:HA  | 1.86                     | 0.55              |
| 1:N:803:LYS:HZ2 | 3:T:108:PRO:HB2 | 1.71                     | 0.55              |
| 1:N:803:LYS:HE3 | 3:T:108:PRO:N   | 2.19                     | 0.55              |
| 1:H:803:LYS:CD  | 3:L:108:PRO:HA  | 2.31                     | 0.54              |
| 1:H:803:LYS:NZ  | 3:L:108:PRO:HG2 | 2.22                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:803:LYS:NZ   | 3:E:108:PRO:HG2  | 2.23                     | 0.53              |
| 1:A:803:LYS:HG3  | 3:E:108:PRO:HB3  | 1.91                     | 0.53              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:HA   | 2.31                     | 0.51              |
| 1:A:1449:PHE:CD2 | 1:B:1449:PHE:HE2 | 2.22                     | 0.50              |
| 1:A:1449:PHE:HD1 | 1:B:1449:PHE:CD1 | 2.22                     | 0.49              |
| 1:H:1375:TYR:CE1 | 1:O:1375:TYR:HD2 | 2.22                     | 0.49              |
| 1:N:803:LYS:NZ   | 3:T:108:PRO:HB2  | 2.27                     | 0.49              |
| 1:H:1449:PHE:HD2 | 1:O:1449:PHE:CD2 | 2.22                     | 0.49              |
| 1:H:1449:PHE:HE2 | 1:O:1449:PHE:CD2 | 2.22                     | 0.48              |
| 1:H:1375:TYR:HE2 | 1:O:1375:TYR:CD1 | 2.22                     | 0.47              |
| 1:N:803:LYS:NZ   | 3:T:108:PRO:CG   | 2.76                     | 0.47              |
| 1:A:1449:PHE:CE2 | 1:B:1449:PHE:HD2 | 2.23                     | 0.47              |
| 1:N:1449:PHE:CD1 | 1:Q:1449:PHE:HD1 | 2.22                     | 0.47              |
| 1:H:803:LYS:HE3  | 3:L:108:PRO:C    | 2.34                     | 0.47              |
| 1:N:1449:PHE:HD2 | 1:Q:1449:PHE:CE2 | 2.22                     | 0.47              |
| 1:H:1375:TYR:HE2 | 1:O:1375:TYR:CE1 | 2.23                     | 0.47              |
| 1:H:803:LYS:CD   | 3:L:108:PRO:HG3  | 2.38                     | 0.47              |
| 1:A:245:GLY:HA3  | 1:A:266:TYR:CD2  | 2.49                     | 0.47              |
| 1:B:801:PHE:CE2  | 1:B:803:LYS:HE2  | 2.50                     | 0.47              |
| 1:A:1375:TYR:CD1 | 1:B:1375:TYR:HD2 | 2.23                     | 0.46              |
| 1:N:803:LYS:HZ3  | 3:T:108:PRO:HG2  | 1.80                     | 0.46              |
| 1:H:1449:PHE:CE1 | 1:O:1449:PHE:HD1 | 2.22                     | 0.46              |
| 1:A:803:LYS:HD3  | 3:E:108:PRO:HA   | 1.90                     | 0.46              |
| 1:H:803:LYS:CE   | 3:L:108:PRO:C    | 2.84                     | 0.46              |
| 1:H:1449:PHE:HE2 | 1:O:1449:PHE:CE2 | 2.22                     | 0.46              |
| 1:H:1449:PHE:HD2 | 1:O:1449:PHE:CE2 | 2.22                     | 0.45              |
| 1:H:1449:PHE:CD1 | 1:O:1449:PHE:HD1 | 2.22                     | 0.45              |
| 1:N:1449:PHE:CE1 | 1:Q:1449:PHE:HD1 | 2.22                     | 0.45              |
| 1:N:1375:TYR:HD2 | 1:Q:1375:TYR:CE2 | 2.22                     | 0.45              |
| 1:N:1375:TYR:HE2 | 1:Q:1375:TYR:CE2 | 2.22                     | 0.45              |
| 1:N:1449:PHE:CE1 | 1:Q:1449:PHE:HE1 | 2.23                     | 0.44              |
| 1:A:1449:PHE:CD2 | 1:B:1449:PHE:HD2 | 2.22                     | 0.44              |
| 1:N:1375:TYR:HE2 | 1:Q:1375:TYR:CD2 | 2.23                     | 0.44              |
| 1:O:281:ARG:HH12 | 1:O:284:HIS:CE1  | 2.36                     | 0.44              |
| 1:A:803:LYS:HE3  | 3:E:108:PRO:C    | 2.38                     | 0.44              |
| 1:N:803:LYS:HE2  | 3:T:108:PRO:N    | 2.25                     | 0.44              |
| 1:N:803:LYS:HG2  | 3:T:108:PRO:N    | 2.33                     | 0.44              |
| 1:A:1449:PHE:CE2 | 1:B:1449:PHE:HE2 | 2.22                     | 0.43              |
| 1:A:1375:TYR:HD2 | 1:B:1375:TYR:CD1 | 2.22                     | 0.43              |
| 1:A:803:LYS:NZ   | 3:E:108:PRO:CD   | 2.82                     | 0.43              |
| 1:H:803:LYS:HG3  | 3:L:108:PRO:HB3  | 1.97                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1375:TYR:CD1 | 1:O:1375:TYR:HD2 | 2.22                     | 0.43              |
| 1:A:803:LYS:CE   | 3:E:108:PRO:C    | 2.85                     | 0.43              |
| 1:N:1375:TYR:CE1 | 1:Q:1375:TYR:HD1 | 2.22                     | 0.43              |
| 1:A:1449:PHE:HE1 | 1:B:1449:PHE:CE1 | 2.23                     | 0.43              |
| 3:T:10:ILE:HG22  | 3:T:11:GLU:H     | 1.85                     | 0.42              |
| 1:O:706:ARG:HG3  | 1:O:707:LYS:H    | 1.84                     | 0.42              |
| 1:N:1449:PHE:HE2 | 1:Q:1449:PHE:CE2 | 2.22                     | 0.42              |
| 1:N:1449:PHE:CD1 | 1:Q:1449:PHE:HE1 | 2.22                     | 0.41              |
| 1:O:1644:LYS:HE2 | 1:O:1644:LYS:HA  | 2.01                     | 0.41              |
| 1:A:1449:PHE:HD1 | 1:B:1449:PHE:CE1 | 2.22                     | 0.41              |
| 1:N:1375:TYR:CE1 | 1:Q:1375:TYR:HE1 | 2.23                     | 0.41              |
| 1:N:803:LYS:CD   | 3:T:108:PRO:HD3  | 2.40                     | 0.41              |
| 1:N:1375:TYR:CD1 | 1:Q:1375:TYR:HD1 | 2.22                     | 0.41              |
| 1:H:1375:TYR:HD2 | 1:O:1375:TYR:CE1 | 2.23                     | 0.41              |
| 1:A:803:LYS:CD   | 3:E:108:PRO:HG3  | 2.38                     | 0.41              |
| 1:A:803:LYS:HZ3  | 3:E:108:PRO:HD2  | 1.87                     | 0.40              |
| 1:N:803:LYS:CE   | 1:N:803:LYS:CD   | 3.00                     | 0.40              |
| 1:A:803:LYS:CE   | 1:A:803:LYS:CD   | 2.99                     | 0.40              |
| 1:N:803:LYS:CE   | 3:T:108:PRO:HG2  | 2.41                     | 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 PDB entries followed by that with respect to all EM entries.

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     | 1924/1935 (99%)  | 1836 (95%) | 75 (4%) | 13 (1%)  | 22 63       |
| 1   | B     | 1924/1935 (99%)  | 1810 (94%) | 98 (5%) | 16 (1%)  | 19 60       |
| 1   | H     | 1928/1935 (100%) | 1834 (95%) | 78 (4%) | 16 (1%)  | 19 60       |
| 1   | N     | 1928/1935 (100%) | 1854 (96%) | 62 (3%) | 12 (1%)  | 25 66       |
| 1   | O     | 1924/1935 (99%)  | 1825 (95%) | 86 (4%) | 13 (1%)  | 22 63       |

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| Mol | Chain | Analysed           | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|--------------------|-------------|----------|----------|-------------|-----|
| 1   | Q     | 1924/1935 (99%)    | 1827 (95%)  | 81 (4%)  | 16 (1%)  | 19          | 60  |
| 2   | C     | 150/152 (99%)      | 140 (93%)   | 6 (4%)   | 4 (3%)   | 5           | 31  |
| 2   | D     | 150/152 (99%)      | 138 (92%)   | 8 (5%)   | 4 (3%)   | 5           | 31  |
| 2   | J     | 150/152 (99%)      | 138 (92%)   | 10 (7%)  | 2 (1%)   | 12          | 48  |
| 2   | K     | 150/152 (99%)      | 138 (92%)   | 12 (8%)  | 0        | 100         | 100 |
| 2   | R     | 150/152 (99%)      | 133 (89%)   | 16 (11%) | 1 (1%)   | 22          | 63  |
| 2   | S     | 150/152 (99%)      | 136 (91%)   | 11 (7%)  | 3 (2%)   | 7           | 38  |
| 3   | E     | 158/160 (99%)      | 139 (88%)   | 14 (9%)  | 5 (3%)   | 4           | 26  |
| 3   | F     | 158/160 (99%)      | 134 (85%)   | 19 (12%) | 5 (3%)   | 4           | 26  |
| 3   | L     | 158/160 (99%)      | 141 (89%)   | 14 (9%)  | 3 (2%)   | 8           | 38  |
| 3   | M     | 158/160 (99%)      | 137 (87%)   | 19 (12%) | 2 (1%)   | 12          | 48  |
| 3   | T     | 158/160 (99%)      | 138 (87%)   | 17 (11%) | 3 (2%)   | 8           | 38  |
| 3   | U     | 158/160 (99%)      | 139 (88%)   | 13 (8%)  | 6 (4%)   | 3           | 24  |
| 4   | G     | 398/400 (100%)     | 371 (93%)   | 25 (6%)  | 2 (0%)   | 29          | 69  |
| 4   | V     | 398/400 (100%)     | 376 (94%)   | 15 (4%)  | 7 (2%)   | 8           | 40  |
| 5   | I     | 1077/1079 (100%)   | 1036 (96%)  | 35 (3%)  | 6 (1%)   | 25          | 66  |
| 5   | P     | 1077/1079 (100%)   | 1035 (96%)  | 40 (4%)  | 2 (0%)   | 47          | 81  |
| All | All   | 16350/16440 (100%) | 15455 (94%) | 754 (5%) | 141 (1%) | 21          | 57  |

All (141) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 605 | VAL  |
| 1   | B     | 451 | GLN  |
| 3   | E     | 163 | GLU  |
| 3   | F     | 92  | GLY  |
| 1   | N     | 575 | ALA  |
| 1   | O     | 210 | THR  |
| 5   | P     | 440 | PRO  |
| 1   | Q     | 211 | PRO  |
| 4   | V     | 18  | ASP  |
| 1   | A     | 238 | ASN  |
| 1   | A     | 455 | TYR  |
| 1   | A     | 785 | ILE  |
| 1   | B     | 15  | PHE  |
| 1   | B     | 128 | TYR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 566        | PRO         |
| 2          | D            | 176        | GLN         |
| 3          | E            | 59         | VAL         |
| 3          | E            | 147        | THR         |
| 1          | H            | 274        | ILE         |
| 1          | H            | 642        | SER         |
| 3          | L            | 59         | VAL         |
| 1          | N            | 603        | GLU         |
| 1          | O            | 624        | TYR         |
| 1          | O            | 640        | LYS         |
| 1          | O            | 803        | LYS         |
| 1          | Q            | 86         | LYS         |
| 1          | Q            | 1476       | SER         |
| 2          | R            | 95         | VAL         |
| 2          | S            | 67         | GLY         |
| 3          | T            | 108        | PRO         |
| 3          | T            | 146        | VAL         |
| 3          | U            | 16         | ASN         |
| 4          | V            | 10         | HIS         |
| 4          | V            | 247        | TRP         |
| 1          | A            | 322        | SER         |
| 1          | B            | 273        | VAL         |
| 1          | B            | 639        | LYS         |
| 2          | C            | 100        | LYS         |
| 1          | H            | 455        | TYR         |
| 1          | H            | 738        | SER         |
| 1          | H            | 750        | ASP         |
| 1          | H            | 829        | TRP         |
| 5          | I            | 901        | LEU         |
| 5          | I            | 1286       | GLU         |
| 5          | I            | 1305       | LYS         |
| 5          | I            | 1306       | SER         |
| 2          | J            | 163        | ARG         |
| 1          | N            | 45         | GLU         |
| 1          | N            | 232        | ASN         |
| 1          | N            | 367        | LYS         |
| 1          | N            | 679        | LYS         |
| 1          | O            | 532        | SER         |
| 1          | O            | 614        | LEU         |
| 1          | O            | 713        | ILE         |
| 1          | Q            | 614        | LEU         |
| 2          | S            | 163        | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 3          | T            | 145        | ASP         |
| 3          | U            | 23         | GLN         |
| 3          | U            | 96         | GLU         |
| 4          | V            | 103        | LEU         |
| 4          | V            | 149        | LEU         |
| 4          | V            | 300        | ILE         |
| 4          | V            | 332        | ASN         |
| 1          | A            | 114        | ILE         |
| 1          | A            | 277        | LEU         |
| 1          | A            | 282        | ASP         |
| 1          | A            | 364        | PHE         |
| 1          | A            | 396        | LEU         |
| 1          | A            | 558        | GLY         |
| 1          | A            | 1476       | SER         |
| 1          | B            | 86         | LYS         |
| 1          | B            | 643        | SER         |
| 2          | C            | 101        | GLN         |
| 2          | C            | 163        | ARG         |
| 2          | D            | 106        | SER         |
| 2          | D            | 172        | LEU         |
| 3          | F            | 57         | GLY         |
| 4          | G            | 10         | HIS         |
| 1          | H            | 45         | GLU         |
| 1          | H            | 378        | THR         |
| 1          | H            | 603        | GLU         |
| 1          | H            | 729        | ALA         |
| 5          | I            | 321        | ARG         |
| 2          | J            | 107        | LYS         |
| 3          | L            | 33         | PHE         |
| 3          | M            | 20         | MET         |
| 1          | N            | 644        | PHE         |
| 1          | O            | 315        | GLN         |
| 5          | P            | 704        | ALA         |
| 1          | Q            | 315        | GLN         |
| 1          | Q            | 560        | SER         |
| 1          | Q            | 640        | LYS         |
| 1          | Q            | 644        | PHE         |
| 1          | B            | 32         | ASP         |
| 1          | B            | 34         | LYS         |
| 1          | B            | 293        | LYS         |
| 1          | B            | 371        | GLU         |
| 1          | B            | 603        | GLU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 751        | ILE         |
| 1          | H            | 28         | THR         |
| 1          | H            | 83         | LYS         |
| 1          | H            | 316        | GLY         |
| 1          | H            | 379        | GLU         |
| 3          | M            | 58         | ARG         |
| 1          | N            | 637        | LYS         |
| 1          | O            | 96         | LEU         |
| 1          | Q            | 256        | GLY         |
| 1          | Q            | 723        | ARG         |
| 1          | Q            | 803        | LYS         |
| 1          | A            | 207        | LYS         |
| 1          | B            | 599        | ASP         |
| 2          | D            | 175        | GLY         |
| 3          | E            | 19         | SER         |
| 3          | E            | 108        | PRO         |
| 1          | H            | 10         | GLY         |
| 1          | H            | 372        | GLN         |
| 3          | L            | 108        | PRO         |
| 1          | N            | 57         | GLY         |
| 1          | N            | 835        | LYS         |
| 1          | O            | 726        | ASN         |
| 1          | Q            | 768        | GLY         |
| 3          | U            | 143        | PRO         |
| 2          | C            | 98         | LYS         |
| 3          | F            | 156        | VAL         |
| 4          | G            | 102        | ILE         |
| 1          | Q            | 452        | PRO         |
| 1          | Q            | 824        | VAL         |
| 3          | U            | 94         | ASP         |
| 3          | F            | 94         | ASP         |
| 3          | F            | 146        | VAL         |
| 5          | I            | 999        | GLU         |
| 2          | S            | 86         | ASN         |
| 1          | N            | 785        | ILE         |
| 1          | O            | 629        | ALA         |
| 1          | O            | 641        | GLY         |
| 1          | Q            | 569        | VAL         |
| 3          | U            | 95         | PRO         |
| 1          | B            | 127        | PRO         |
| 1          | N            | 634        | GLY         |
| 1          | O            | 751        | ILE         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 828 | PRO  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 1688/1693 (100%)   | 1665 (99%)  | 23 (1%)  | 67          | 80 |
| 1   | B     | 1688/1693 (100%)   | 1659 (98%)  | 29 (2%)  | 60          | 78 |
| 1   | H     | 1690/1693 (100%)   | 1656 (98%)  | 34 (2%)  | 55          | 74 |
| 1   | N     | 1690/1693 (100%)   | 1660 (98%)  | 30 (2%)  | 59          | 77 |
| 1   | O     | 1688/1693 (100%)   | 1670 (99%)  | 18 (1%)  | 73          | 84 |
| 1   | Q     | 1688/1693 (100%)   | 1661 (98%)  | 27 (2%)  | 62          | 79 |
| 2   | C     | 131/131 (100%)     | 128 (98%)   | 3 (2%)   | 50          | 70 |
| 2   | D     | 131/131 (100%)     | 127 (97%)   | 4 (3%)   | 40          | 62 |
| 2   | J     | 131/131 (100%)     | 126 (96%)   | 5 (4%)   | 33          | 57 |
| 2   | K     | 131/131 (100%)     | 125 (95%)   | 6 (5%)   | 27          | 52 |
| 2   | R     | 131/131 (100%)     | 127 (97%)   | 4 (3%)   | 40          | 62 |
| 2   | S     | 131/131 (100%)     | 128 (98%)   | 3 (2%)   | 50          | 70 |
| 3   | E     | 139/139 (100%)     | 136 (98%)   | 3 (2%)   | 52          | 71 |
| 3   | F     | 139/139 (100%)     | 138 (99%)   | 1 (1%)   | 84          | 90 |
| 3   | L     | 139/139 (100%)     | 133 (96%)   | 6 (4%)   | 29          | 53 |
| 3   | M     | 139/139 (100%)     | 135 (97%)   | 4 (3%)   | 42          | 64 |
| 3   | T     | 139/139 (100%)     | 137 (99%)   | 2 (1%)   | 67          | 80 |
| 3   | U     | 139/139 (100%)     | 134 (96%)   | 5 (4%)   | 35          | 59 |
| 4   | G     | 344/344 (100%)     | 341 (99%)   | 3 (1%)   | 78          | 87 |
| 4   | V     | 344/344 (100%)     | 339 (98%)   | 5 (2%)   | 65          | 80 |
| 5   | I     | 928/928 (100%)     | 918 (99%)   | 10 (1%)  | 73          | 84 |
| 5   | P     | 928/928 (100%)     | 907 (98%)   | 21 (2%)  | 50          | 70 |
| All | All   | 14296/14322 (100%) | 14050 (98%) | 246 (2%) | 62          | 78 |

All (246) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 34   | LYS  |
| 1   | A     | 67   | LYS  |
| 1   | A     | 239  | ASP  |
| 1   | A     | 315  | GLN  |
| 1   | A     | 363  | LYS  |
| 1   | A     | 504  | GLU  |
| 1   | A     | 518  | GLN  |
| 1   | A     | 588  | TYR  |
| 1   | A     | 706  | ARG  |
| 1   | A     | 715  | TYR  |
| 1   | A     | 732  | GLU  |
| 1   | A     | 791  | GLN  |
| 1   | A     | 808  | ARG  |
| 1   | A     | 814  | ILE  |
| 1   | A     | 826  | ASN  |
| 1   | A     | 870  | ARG  |
| 1   | A     | 952  | ARG  |
| 1   | A     | 1408 | ASN  |
| 1   | A     | 1446 | GLN  |
| 1   | A     | 1473 | GLU  |
| 1   | A     | 1574 | ARG  |
| 1   | A     | 1715 | LEU  |
| 1   | A     | 1842 | LYS  |
| 1   | B     | 54   | ARG  |
| 1   | B     | 113  | MET  |
| 1   | B     | 194  | TYR  |
| 1   | B     | 210  | THR  |
| 1   | B     | 276  | GLN  |
| 1   | B     | 346  | LYS  |
| 1   | B     | 368  | GLN  |
| 1   | B     | 403  | ARG  |
| 1   | B     | 418  | GLN  |
| 1   | B     | 559  | LYS  |
| 1   | B     | 572  | LYS  |
| 1   | B     | 615  | LYS  |
| 1   | B     | 616  | LEU  |
| 1   | B     | 645  | GLN  |
| 1   | B     | 723  | ARG  |
| 1   | B     | 762  | LYS  |
| 1   | B     | 829  | TRP  |
| 1   | B     | 837  | LYS  |
| 1   | B     | 869  | ARG  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 906        | ASP         |
| 1          | B            | 932        | MET         |
| 1          | B            | 952        | ARG         |
| 1          | B            | 1001       | GLU         |
| 1          | B            | 1048       | LEU         |
| 1          | B            | 1098       | GLN         |
| 1          | B            | 1300       | GLN         |
| 1          | B            | 1411       | CYS         |
| 1          | B            | 1444       | LYS         |
| 1          | B            | 1842       | LYS         |
| 2          | C            | 63         | ARG         |
| 2          | C            | 171        | LYS         |
| 2          | C            | 185        | TYR         |
| 2          | D            | 55         | LYS         |
| 2          | D            | 63         | ARG         |
| 2          | D            | 129        | THR         |
| 2          | D            | 154        | ARG         |
| 3          | E            | 58         | ARG         |
| 3          | E            | 164        | GLU         |
| 3          | E            | 165        | LYS         |
| 3          | F            | 50         | ARG         |
| 4          | G            | 30         | ARG         |
| 4          | G            | 159        | SER         |
| 4          | G            | 325        | ARG         |
| 1          | H            | 6          | MET         |
| 1          | H            | 43         | LYS         |
| 1          | H            | 87         | ILE         |
| 1          | H            | 171        | ASN         |
| 1          | H            | 172        | GLN         |
| 1          | H            | 193        | GLN         |
| 1          | H            | 206        | LYS         |
| 1          | H            | 208        | ASP         |
| 1          | H            | 213        | LYS         |
| 1          | H            | 224        | ASN         |
| 1          | H            | 232        | ASN         |
| 1          | H            | 276        | GLN         |
| 1          | H            | 325        | ASP         |
| 1          | H            | 397        | LYS         |
| 1          | H            | 408        | ASN         |
| 1          | H            | 424        | ILE         |
| 1          | H            | 448        | GLU         |
| 1          | H            | 450        | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | H            | 468        | PHE         |
| 1          | H            | 546        | MET         |
| 1          | H            | 603        | GLU         |
| 1          | H            | 726        | ASN         |
| 1          | H            | 777        | ARG         |
| 1          | H            | 786        | THR         |
| 1          | H            | 845        | THR         |
| 1          | H            | 870        | ARG         |
| 1          | H            | 922        | MET         |
| 1          | H            | 968        | LYS         |
| 1          | H            | 1050       | ARG         |
| 1          | H            | 1052       | LYS         |
| 1          | H            | 1242       | LYS         |
| 1          | H            | 1569       | LYS         |
| 1          | H            | 1720       | ASN         |
| 1          | H            | 1833       | ASN         |
| 5          | I            | 478        | ARG         |
| 5          | I            | 485        | THR         |
| 5          | I            | 665        | ARG         |
| 5          | I            | 715        | LYS         |
| 5          | I            | 862        | THR         |
| 5          | I            | 874        | THR         |
| 5          | I            | 934        | LYS         |
| 5          | I            | 1031       | LYS         |
| 5          | I            | 1304       | THR         |
| 5          | I            | 1305       | LYS         |
| 2          | J            | 63         | ARG         |
| 2          | J            | 114        | PHE         |
| 2          | J            | 129        | THR         |
| 2          | J            | 137        | LEU         |
| 2          | J            | 185        | TYR         |
| 2          | K            | 51         | ILE         |
| 2          | K            | 63         | ARG         |
| 2          | K            | 119        | GLN         |
| 2          | K            | 125        | LYS         |
| 2          | K            | 129        | THR         |
| 2          | K            | 167        | ASP         |
| 3          | L            | 7          | LYS         |
| 3          | L            | 58         | ARG         |
| 3          | L            | 91         | LYS         |
| 3          | L            | 106        | PHE         |
| 3          | L            | 142        | PHE         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 3          | L            | 151        | ASP         |
| 3          | M            | 10         | ILE         |
| 3          | M            | 40         | ARG         |
| 3          | M            | 47         | ASN         |
| 3          | M            | 94         | ASP         |
| 1          | N            | 28         | THR         |
| 1          | N            | 79         | GLN         |
| 1          | N            | 87         | ILE         |
| 1          | N            | 172        | GLN         |
| 1          | N            | 204        | ARG         |
| 1          | N            | 213        | LYS         |
| 1          | N            | 240        | ASN         |
| 1          | N            | 308        | TYR         |
| 1          | N            | 309        | ASP         |
| 1          | N            | 315        | GLN         |
| 1          | N            | 369        | ARG         |
| 1          | N            | 380        | GLU         |
| 1          | N            | 419        | GLN         |
| 1          | N            | 424        | ILE         |
| 1          | N            | 453        | ARG         |
| 1          | N            | 476        | LEU         |
| 1          | N            | 603        | GLU         |
| 1          | N            | 611        | LYS         |
| 1          | N            | 684        | MET         |
| 1          | N            | 726        | ASN         |
| 1          | N            | 775        | GLU         |
| 1          | N            | 784        | ILE         |
| 1          | N            | 845        | THR         |
| 1          | N            | 870        | ARG         |
| 1          | N            | 1277       | ARG         |
| 1          | N            | 1420       | ARG         |
| 1          | N            | 1575       | LYS         |
| 1          | N            | 1646       | LEU         |
| 1          | N            | 1809       | LYS         |
| 1          | N            | 1930       | LYS         |
| 1          | O            | 83         | LYS         |
| 1          | O            | 96         | LEU         |
| 1          | O            | 160        | ASN         |
| 1          | O            | 164        | TYR         |
| 1          | O            | 244        | PHE         |
| 1          | O            | 394        | ASP         |
| 1          | O            | 498        | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | O            | 542        | LYS         |
| 1          | O            | 628        | ASP         |
| 1          | O            | 803        | LYS         |
| 1          | O            | 847        | LYS         |
| 1          | O            | 871        | LYS         |
| 1          | O            | 911        | ASN         |
| 1          | O            | 1040       | GLN         |
| 1          | O            | 1136       | ARG         |
| 1          | O            | 1390       | LYS         |
| 1          | O            | 1706       | LEU         |
| 1          | O            | 1749       | ARG         |
| 5          | P            | 320        | THR         |
| 5          | P            | 440        | PRO         |
| 5          | P            | 523        | LYS         |
| 5          | P            | 532        | LEU         |
| 5          | P            | 664        | LEU         |
| 5          | P            | 676        | SER         |
| 5          | P            | 715        | LYS         |
| 5          | P            | 874        | THR         |
| 5          | P            | 917        | LYS         |
| 5          | P            | 937        | ASN         |
| 5          | P            | 948        | LYS         |
| 5          | P            | 960        | ASN         |
| 5          | P            | 1040       | GLN         |
| 5          | P            | 1054       | LYS         |
| 5          | P            | 1094       | LYS         |
| 5          | P            | 1126       | ARG         |
| 5          | P            | 1128       | GLN         |
| 5          | P            | 1160       | LYS         |
| 5          | P            | 1287       | TYR         |
| 5          | P            | 1313       | GLN         |
| 5          | P            | 1342       | ASN         |
| 1          | Q            | 20         | GLU         |
| 1          | Q            | 80         | ASN         |
| 1          | Q            | 146        | LYS         |
| 1          | Q            | 203        | ASP         |
| 1          | Q            | 207        | LYS         |
| 1          | Q            | 211        | PRO         |
| 1          | Q            | 278        | LYS         |
| 1          | Q            | 362        | MET         |
| 1          | Q            | 380        | GLU         |
| 1          | Q            | 433        | GLU         |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | Q     | 504  | GLU  |
| 1   | Q     | 515  | MET  |
| 1   | Q     | 524  | ILE  |
| 1   | Q     | 635  | LYS  |
| 1   | Q     | 653  | GLU  |
| 1   | Q     | 715  | TYR  |
| 1   | Q     | 734  | GLN  |
| 1   | Q     | 853  | LYS  |
| 1   | Q     | 968  | LYS  |
| 1   | Q     | 1024 | LYS  |
| 1   | Q     | 1043 | LYS  |
| 1   | Q     | 1262 | LYS  |
| 1   | Q     | 1279 | LYS  |
| 1   | Q     | 1390 | LYS  |
| 1   | Q     | 1537 | LYS  |
| 1   | Q     | 1694 | GLN  |
| 1   | Q     | 1727 | LYS  |
| 2   | R     | 102  | GLU  |
| 2   | R     | 149  | MET  |
| 2   | R     | 172  | LEU  |
| 2   | R     | 191  | HIS  |
| 2   | S     | 63   | ARG  |
| 2   | S     | 66   | LYS  |
| 2   | S     | 101  | GLN  |
| 3   | T     | 23   | GLN  |
| 3   | T     | 46   | LYS  |
| 3   | U     | 33   | PHE  |
| 3   | U     | 41   | ASP  |
| 3   | U     | 46   | LYS  |
| 3   | U     | 58   | ARG  |
| 3   | U     | 165  | LYS  |
| 4   | V     | 30   | ARG  |
| 4   | V     | 241  | ASP  |
| 4   | V     | 283  | SER  |
| 4   | V     | 290  | LYS  |
| 4   | V     | 325  | ARG  |

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 104  | ASN  |
| 1   | H     | 1720 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 1833 | ASN  |
| 1   | O     | 1486 | 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 monosaccharides 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.

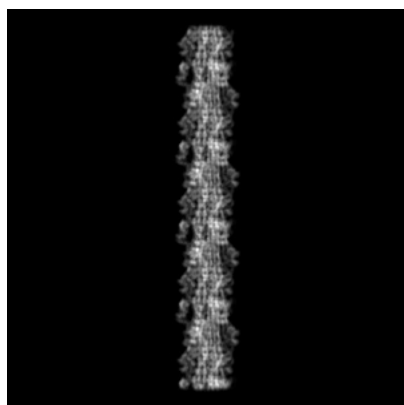
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18198. These allow visual inspection of the internal detail of the map and identification of artifacts.

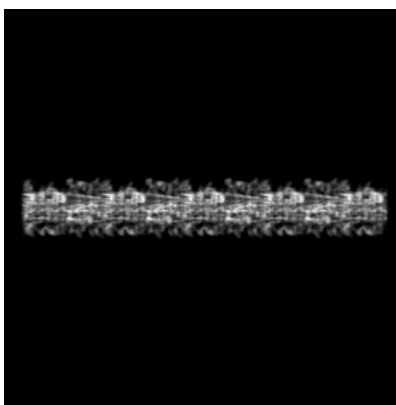
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

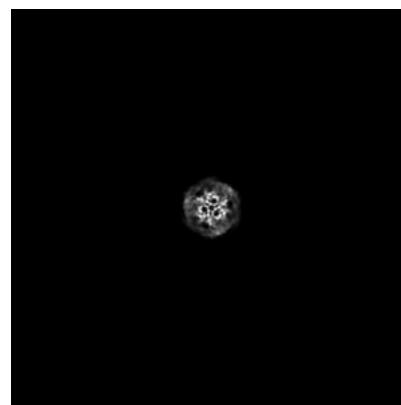
#### 6.1.1 Primary map



X



Y

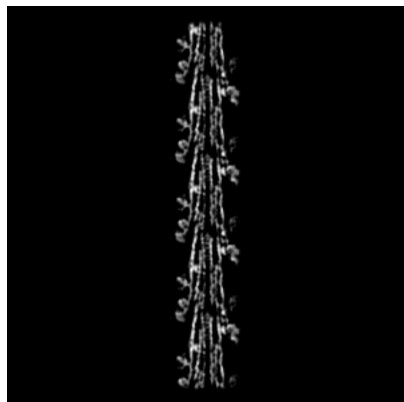


Z

The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

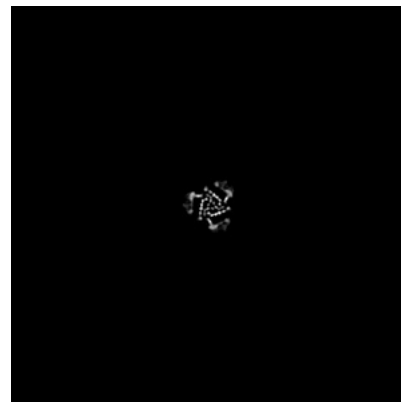
#### 6.2.1 Primary map



X Index: 186



Y Index: 186



Z Index: 186

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 183



Y Index: 193

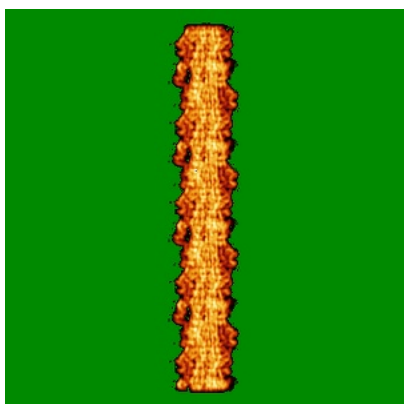


Z Index: 172

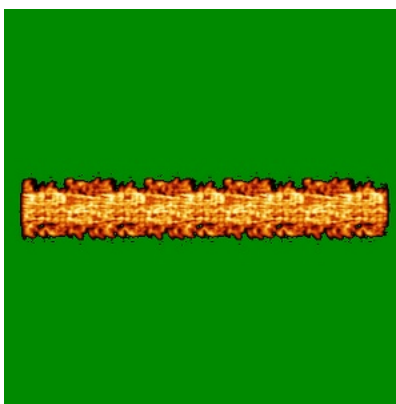
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

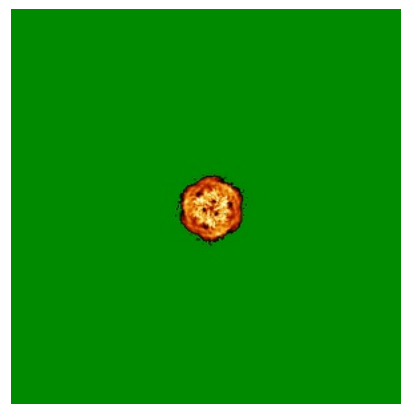
### 6.4.1 Primary map



X



Y

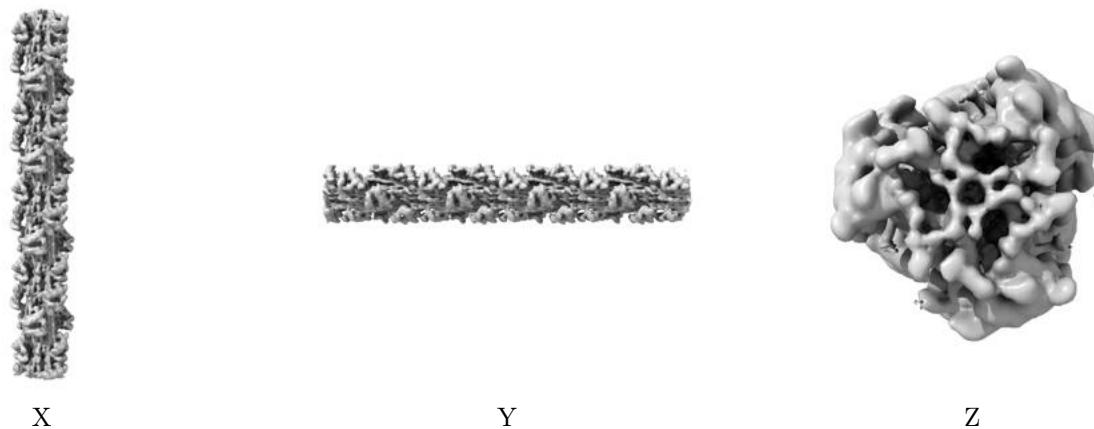


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

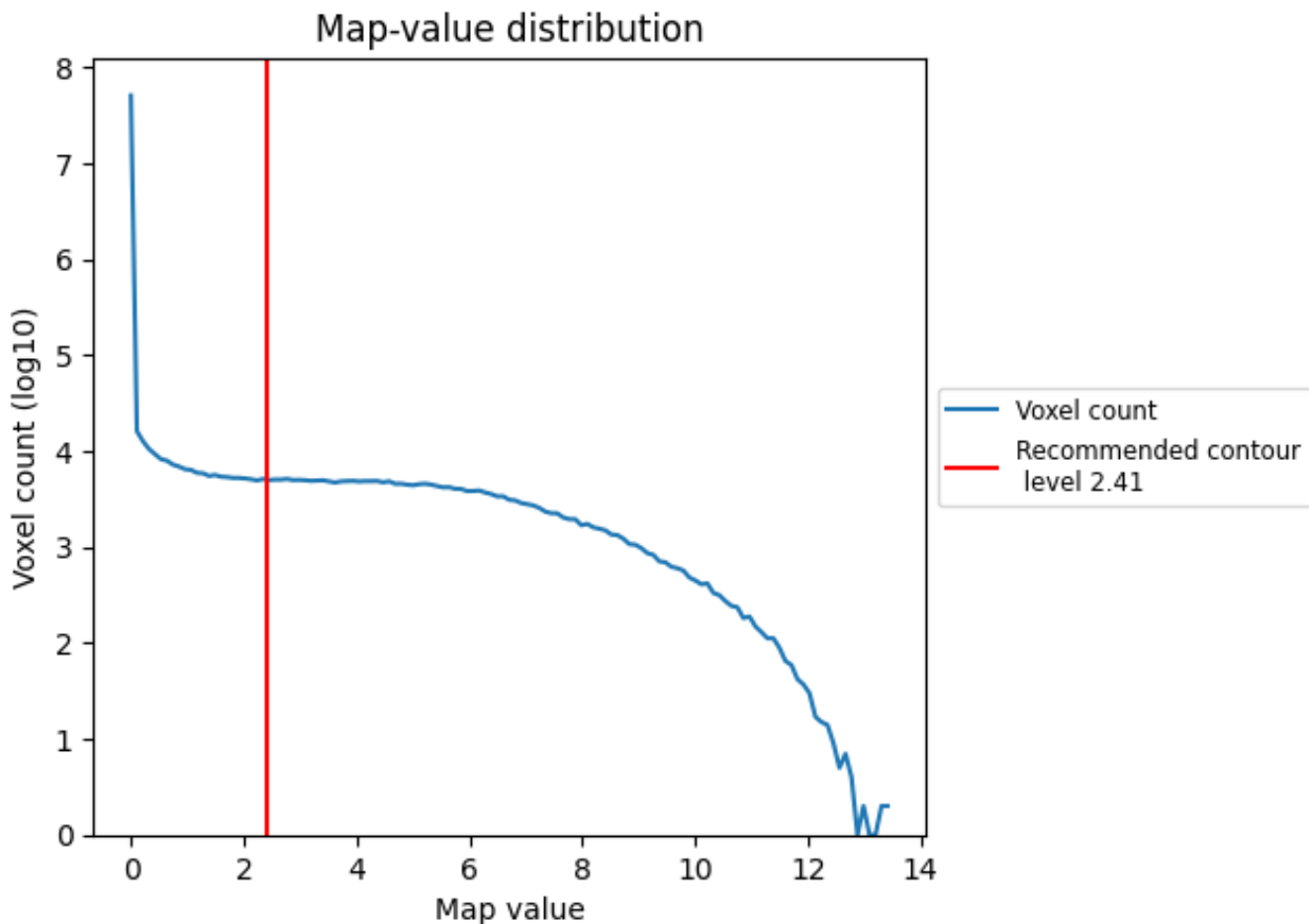
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

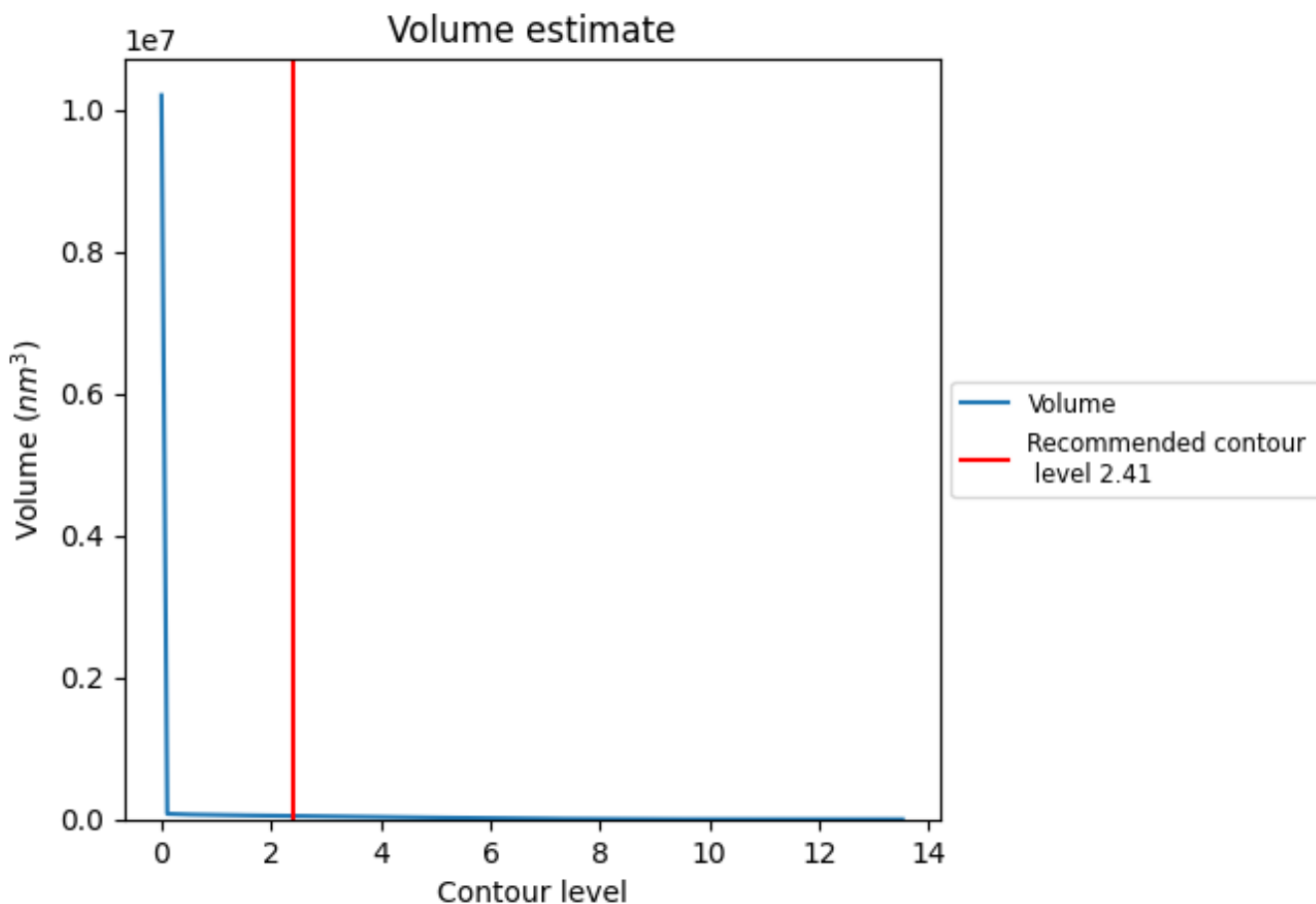
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

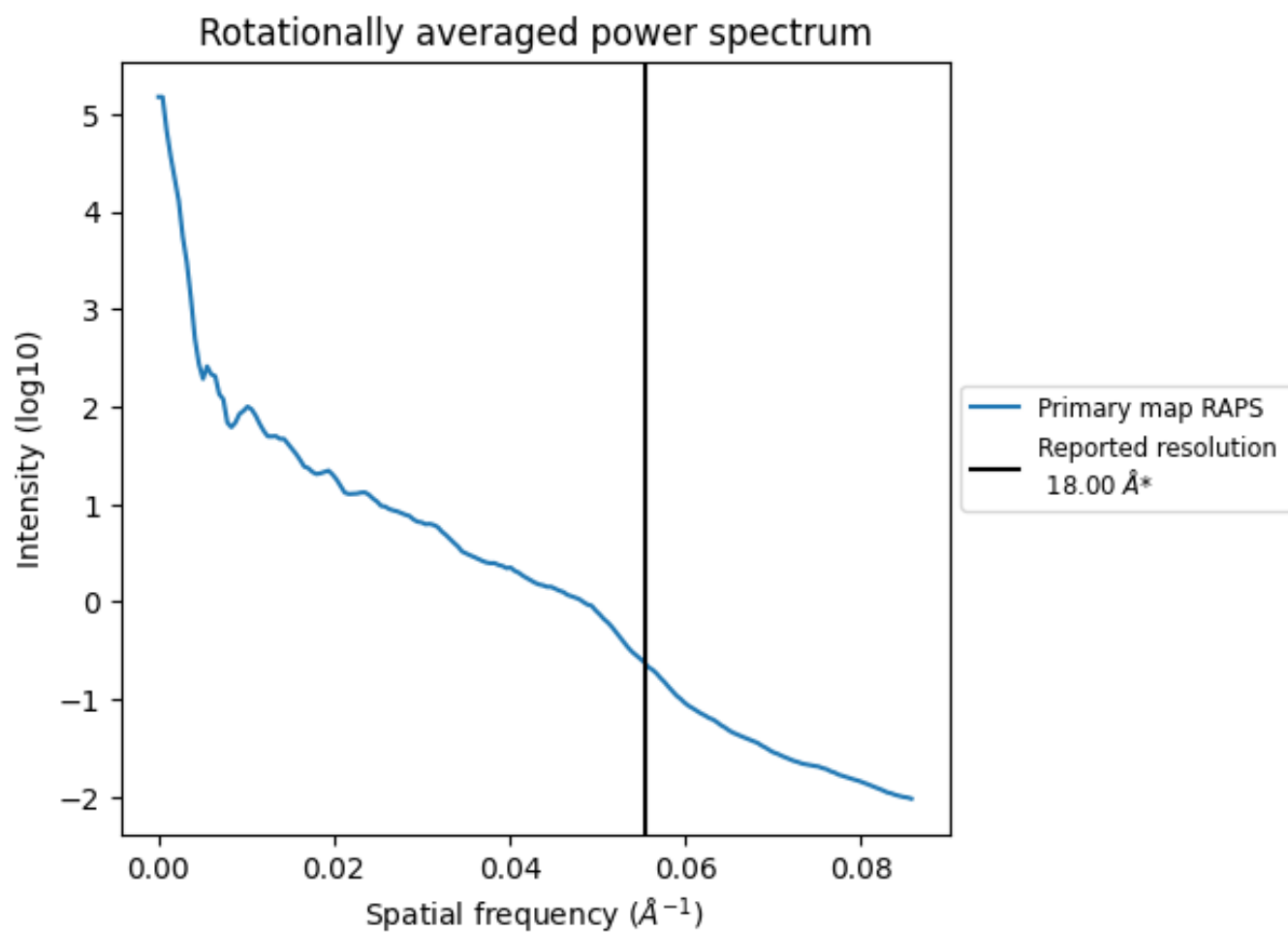


The volume at the recommended contour level is  $47100 \text{ nm}^3$ ; this corresponds to an approximate mass of 42547 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.056 Å<sup>-1</sup>

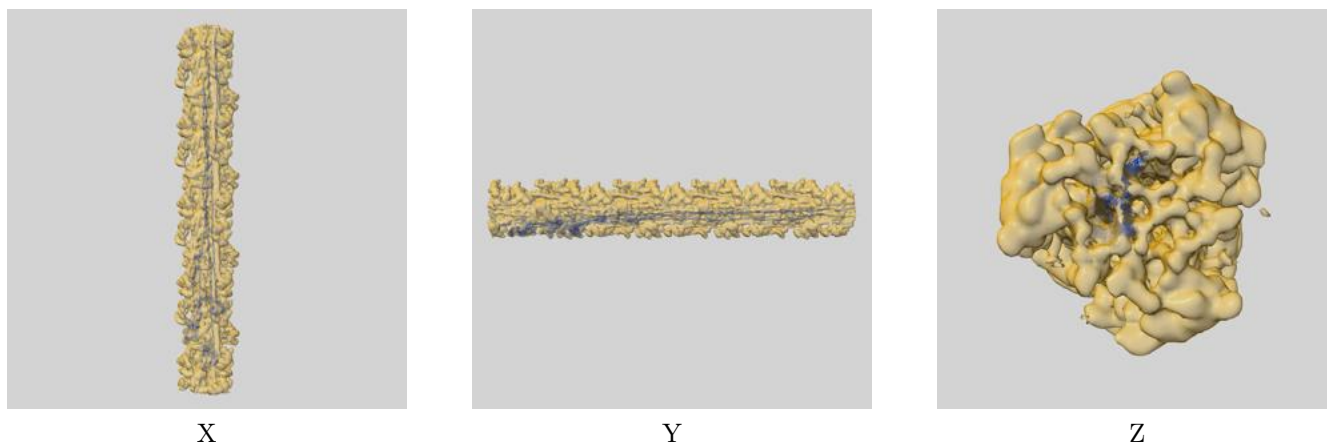
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18198 and PDB model 8Q6T. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



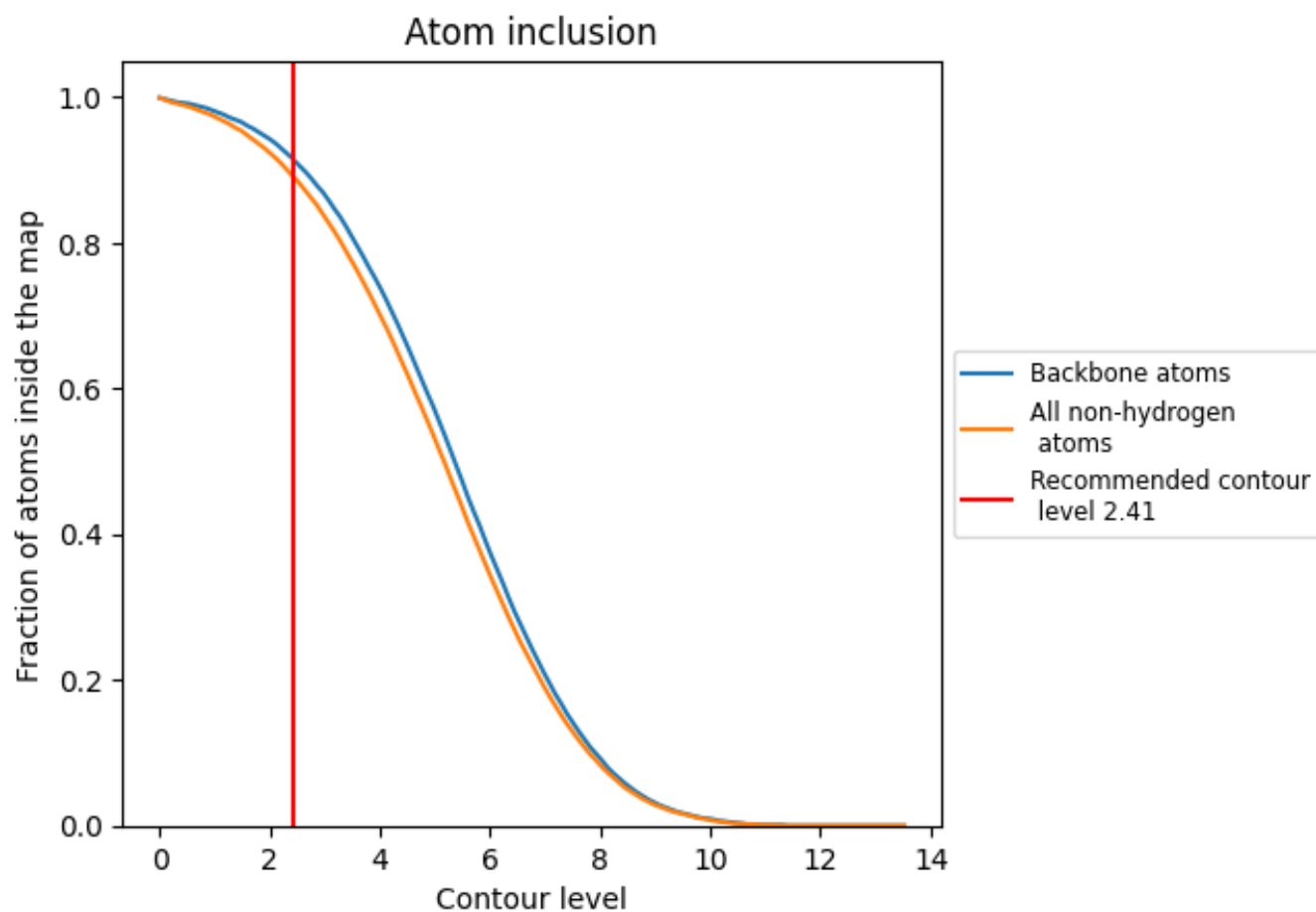
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.41).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.41) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8920   |  0.0560   |
| A     |  0.8380   |  0.0430   |
| B     |  0.8820   |  0.0610   |
| C     |  0.5730   |  0.0040   |
| D     |  0.8670   |  0.0470   |
| E     |  0.8080   |  0.0530   |
| F     |  0.8500   |  0.0420   |
| G     |  0.9600   |  0.0610   |
| H     |  0.8710   |  0.0520   |
| I     |  0.9420   |  0.0690   |
| J     |  0.9500   |  0.0670   |
| K     |  0.9330   |  0.0530   |
| L     |  0.8900   |  0.0650   |
| M     |  0.9450   |  0.0550   |
| N     |  0.9010  |  0.0600  |
| O     |  0.8910 |  0.0610 |
| P     |  0.9560 |  0.0590 |
| Q     |  0.9050 |  0.0550 |
| R     |  0.9400 |  0.0650 |
| S     |  0.8980 |  0.0550 |
| T     |  0.8570 |  0.0360 |
| U     |  0.9690 |  0.0660 |
| V     |  0.9470 |  0.0550 |

