



## Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 03:44 PM EST

PDB ID : 9E7M / pdb\_00009e7m  
EMDB ID : EMD-47685  
Title : In situ cryoEM structure of bacteriophage Ur-lambda tail tip complex  
Authors : Yu, H.; Liu, J.; Molineux, I.J.  
Deposited on : 2024-11-03  
Resolution : 3.37 Å(reported)

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:

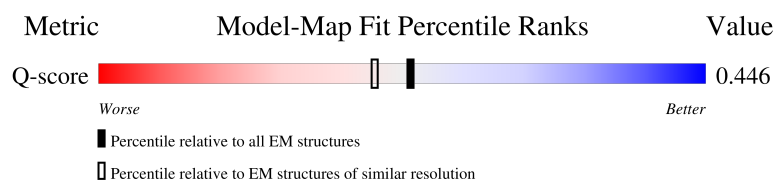
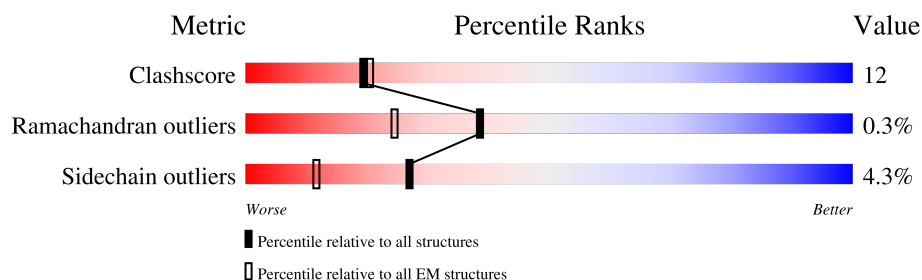
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*


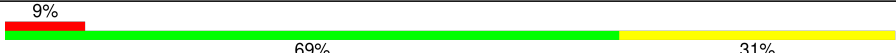
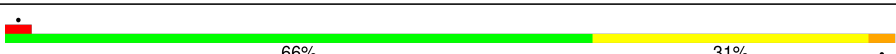
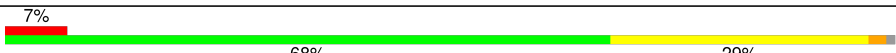
The reported resolution of this entry is 3.37 Å.

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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 210492                      | 15764                       | -  |
| Ramachandran outliers | 207382                      | 16835                       | -  |
| Sidechain outliers    | 206894                      | 16415                       | -  |
| Q-score               | -                           | 25397                       | 14287 ( 2.87 - 3.87 )                                    |

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   | Ha    | 32     |  |
| 1   | Hb    | 32     |  |
| 1   | Hc    | 32     |  |
| 2   | Ia    | 90     |  |


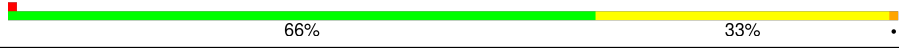

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | Ib    | 90     |                  |
| 3   | Ic    | 90     |                  |
| 4   | Ja    | 835    |                  |
| 4   | Jb    | 835    |                  |
| 4   | Jc    | 835    |                  |
| 5   | La    | 232    |                  |
| 5   | Lb    | 232    |                  |
| 5   | Lc    | 232    |                  |
| 6   | Ta    | 94     |                  |
| 6   | Tb    | 94     |                  |
| 6   | Tc    | 94     |                  |
| 6   | Td    | 94     |                  |
| 6   | Te    | 94     |                  |
| 6   | Tf    | 94     |                  |
| 6   | Tg    | 94     |                  |
| 6   | Th    | 94     |                  |
| 6   | Ti    | 94     |                  |
| 6   | Tj    | 94     |                  |
| 6   | Tk    | 94     |                  |
| 6   | Tl    | 94     |                  |
| 7   | Ma    | 109    |                  |
| 7   | Mb    | 109    |                  |
| 7   | Mc    | 109    |                  |
| 7   | Md    | 109    |                  |
| 7   | Me    | 109    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 7   | Mf    | 109    |  |
| 8   | Va    | 152    |  |
| 8   | Vb    | 152    |  |
| 8   | Vc    | 152    |  |
| 8   | Vd    | 152    |  |
| 8   | Ve    | 152    |  |
| 8   | Vf    | 152    |  |

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 48257 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 Tape measure protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | Ha    | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 237   | 146 | 44 | 45 | 2 |         |       |
| 1   | Hb    | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 149 | 45 | 45 | 2 |         |       |
| 1   | Hc    | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 149 | 45 | 45 | 2 |         |       |

- Molecule 2 is a protein called Tail tip assembly protein I.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | Ia    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 639   | 396 | 110 | 128 | 5 |         |       |
| 2   | Ib    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 640   | 396 | 111 | 129 | 4 |         |       |

- Molecule 3 is a protein called Tail tip assembly protein I.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | Ic    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 400 | 114 | 129 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Ic    | 138     | VAL      | ILE    | conflict | UNP P03730 |

- Molecule 4 is a protein called Tip attachment protein J.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | Ja    | 835      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6493  | 4070 | 1135 | 1269 | 19 |         |       |
| 4   | Jb    | 835      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6490  | 4069 | 1132 | 1269 | 20 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | Jc    | 835      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6484  | 4064 | 1132 | 1269 | 19 |         |       |

- Molecule 5 is a protein called Tail tip protein L.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | Lc    | 232      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1796  | 1115 | 309 | 363 | 9  |         |       |
| 5   | Lb    | 232      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1796  | 1115 | 309 | 363 | 9  |         |       |
| 5   | La    | 232      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1799  | 1117 | 309 | 363 | 10 |         |       |

- Molecule 6 is a protein called Tail fiber protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | Ta    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tb    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tc    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Td    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Te    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tf    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tg    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tl    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Th    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Ti    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tj    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |
| 6   | Tk    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 704   | 436 | 119 | 144 | 5 |         |       |

- Molecule 7 is a protein called Tail tip protein M.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | Ma    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 885   | 569 | 154 | 158 | 4 |         |       |
| 7   | Mb    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 870   | 558 | 150 | 158 | 4 |         |       |
| 7   | Mc    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 885   | 569 | 154 | 158 | 4 |         |       |
| 7   | Md    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 885   | 569 | 154 | 158 | 4 |         |       |
| 7   | Me    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 885   | 569 | 154 | 158 | 4 |         |       |
| 7   | Mf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 881   | 566 | 153 | 158 | 4 |         |       |

- Molecule 8 is a protein called Tail tube protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | Va    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 731 | 197 | 234 | 3 |         |       |
| 8   | Vb    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 731 | 197 | 234 | 3 |         |       |
| 8   | Vc    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 731 | 197 | 234 | 3 |         |       |
| 8   | Vd    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 731 | 197 | 234 | 3 |         |       |
| 8   | Ve    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 731 | 197 | 234 | 3 |         |       |
| 8   | Vf    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 731 | 197 | 234 | 3 |         |       |

There are 18 discrepancies between the modelled and reference sequences:

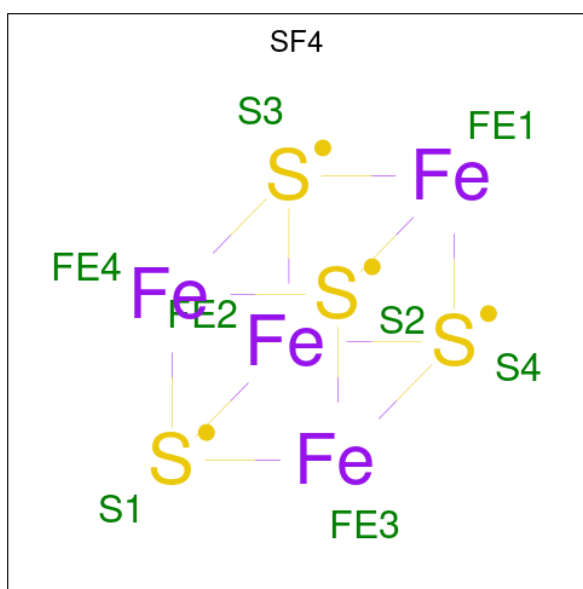
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Va    | ?       | -        | ALA    | deletion | UNP P03733 |
| Va    | ?       | -        | LYS    | deletion | UNP P03733 |
| Va    | ?       | -        | GLU    | deletion | UNP P03733 |
| Vb    | ?       | -        | ALA    | deletion | UNP P03733 |
| Vb    | ?       | -        | LYS    | deletion | UNP P03733 |
| Vb    | ?       | -        | GLU    | deletion | UNP P03733 |
| Vc    | ?       | -        | ALA    | deletion | UNP P03733 |
| Vc    | ?       | -        | LYS    | deletion | UNP P03733 |
| Vc    | ?       | -        | GLU    | deletion | UNP P03733 |
| Vd    | ?       | -        | ALA    | deletion | UNP P03733 |
| Vd    | ?       | -        | LYS    | deletion | UNP P03733 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Vd    | ?       | -        | GLU    | deletion | UNP P03733 |
| Ve    | ?       | -        | ALA    | deletion | UNP P03733 |
| Ve    | ?       | -        | LYS    | deletion | UNP P03733 |
| Ve    | ?       | -        | GLU    | deletion | UNP P03733 |
| Vf    | ?       | -        | ALA    | deletion | UNP P03733 |
| Vf    | ?       | -        | LYS    | deletion | UNP P03733 |
| Vf    | ?       | -        | GLU    | deletion | UNP P03733 |

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



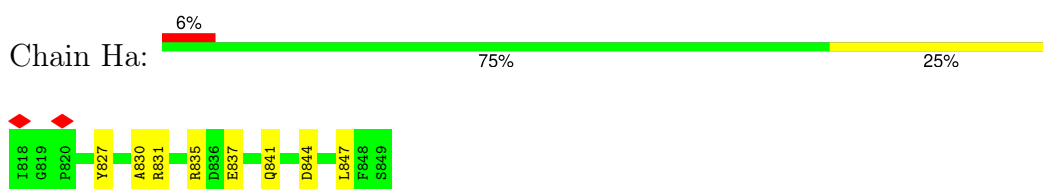
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 9   | Lc    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 9   | Lb    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 9   | La    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |



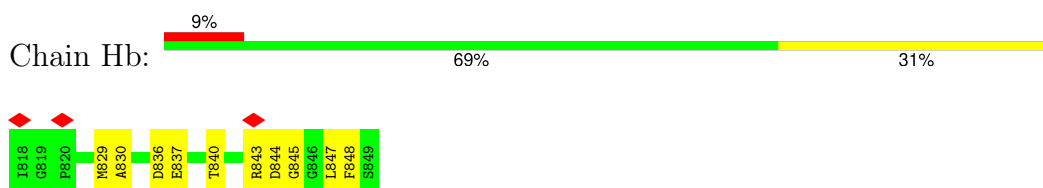
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

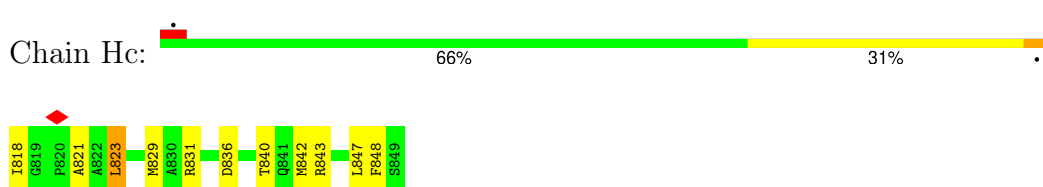
- Molecule 1: Tape measure protein



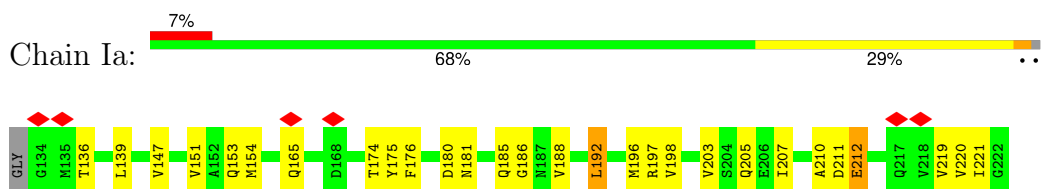
- Molecule 1: Tape measure protein



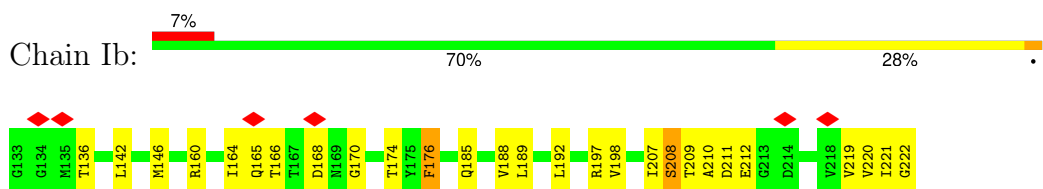
- Molecule 1: Tape measure protein



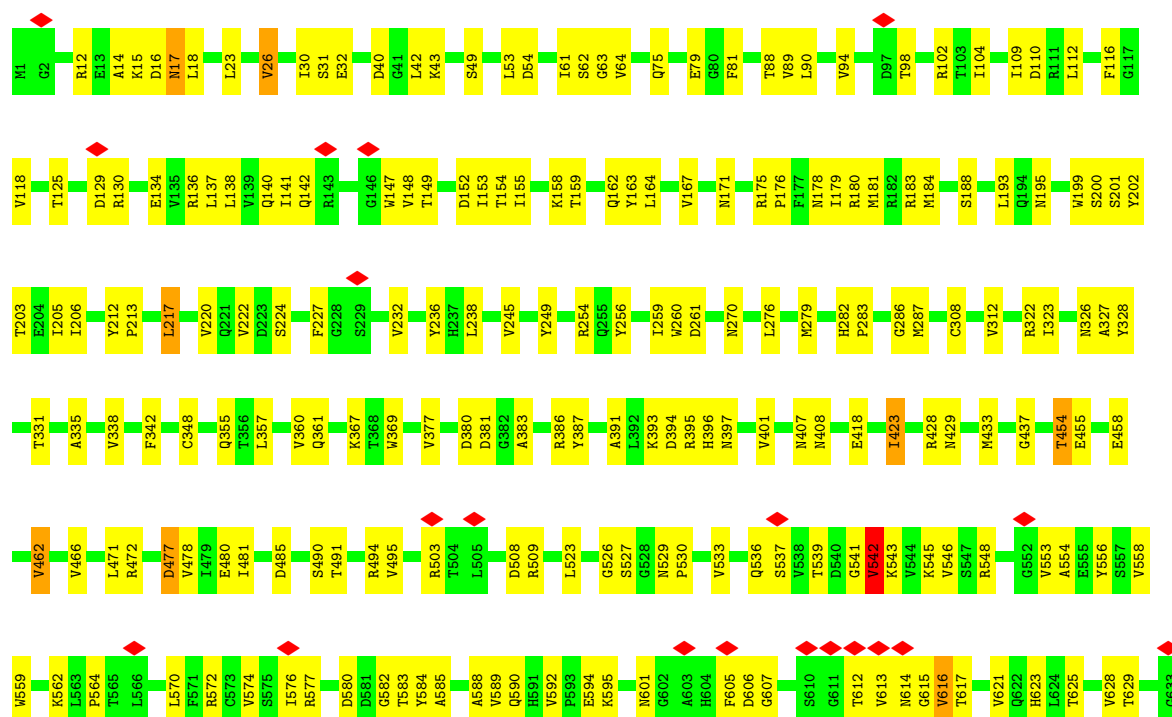
- Molecule 2: Tail tip assembly protein I

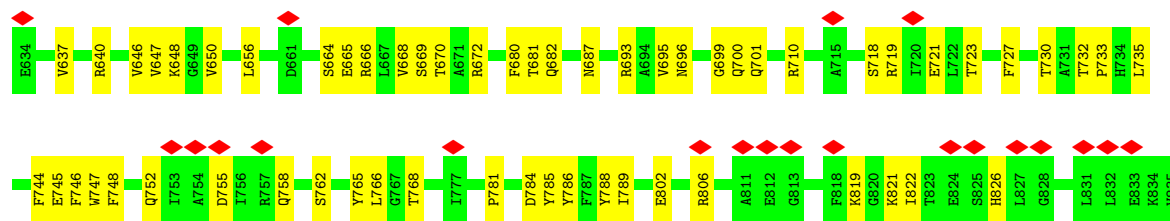


- Molecule 2: Tail tip assembly protein I

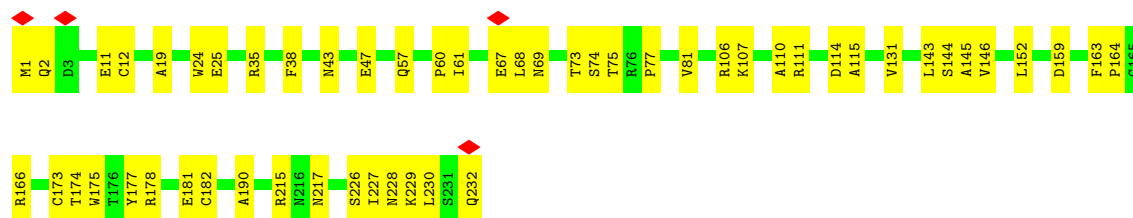
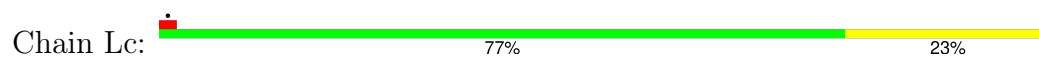




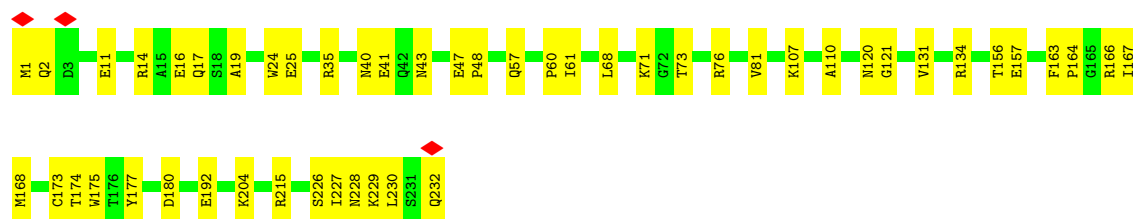
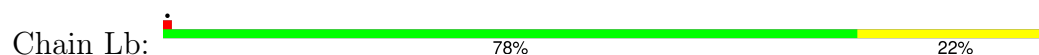




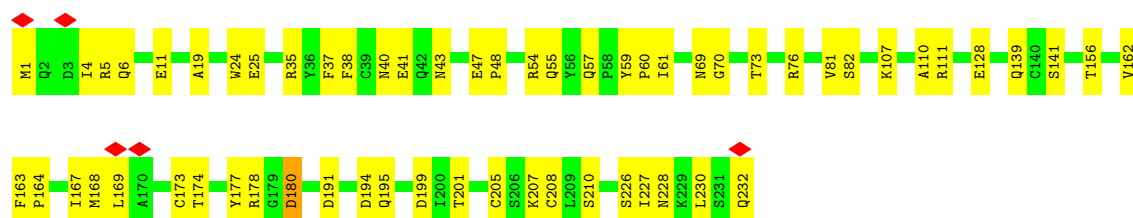
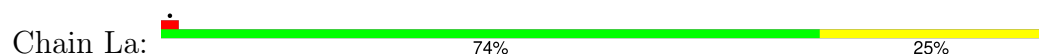
• Molecule 5: Tail tip protein L



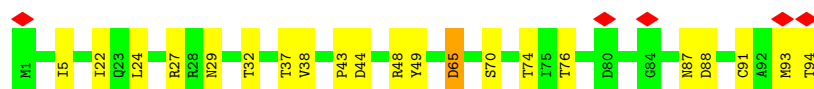
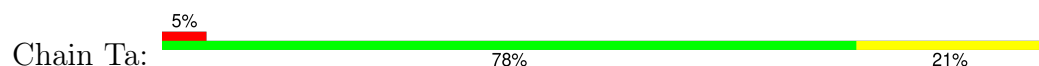
• Molecule 5: Tail tip protein L



• Molecule 5: Tail tip protein L



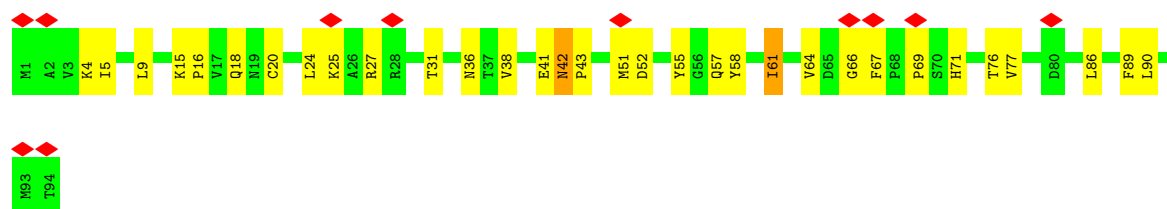
• Molecule 6: Tail fiber protein



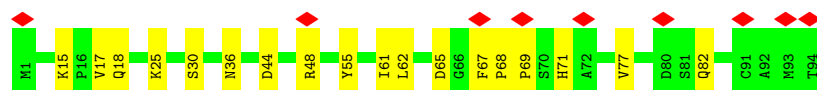
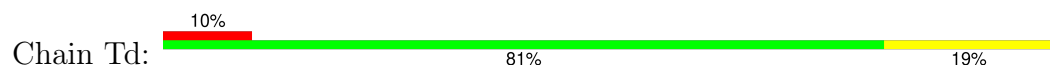
• Molecule 6: Tail fiber protein



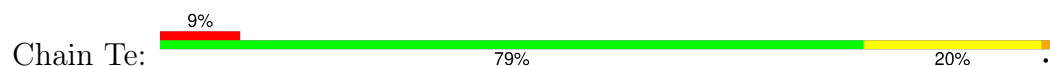
- Molecule 6: Tail fiber protein



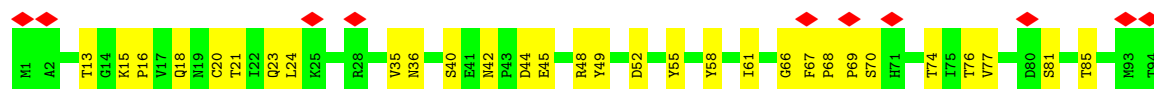
- Molecule 6: Tail fiber protein



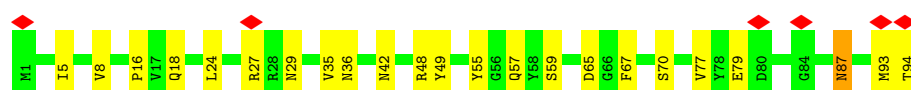
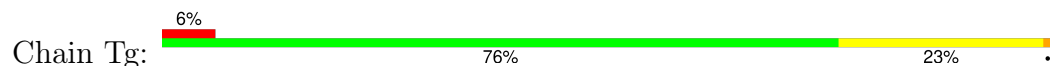
- Molecule 6: Tail fiber protein



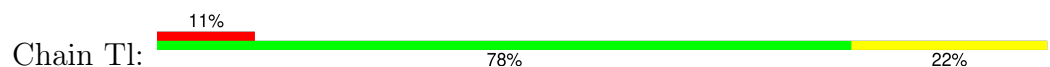
- Molecule 6: Tail fiber protein



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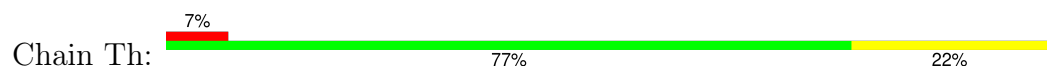


- Molecule 6: Tail fiber protein

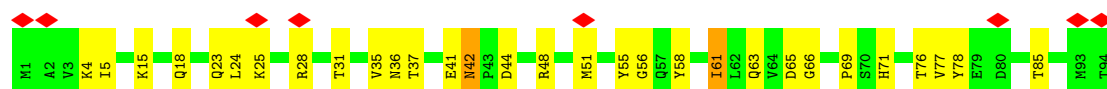




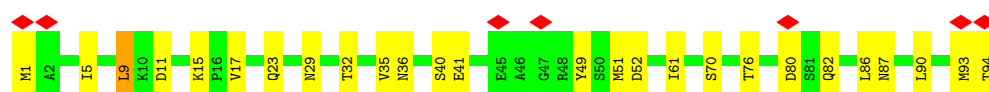
- Molecule 6: Tail fiber protein



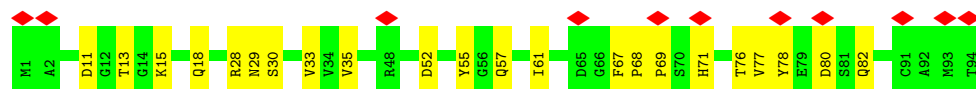
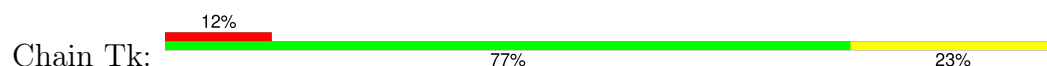
- Molecule 6: Tail fiber protein



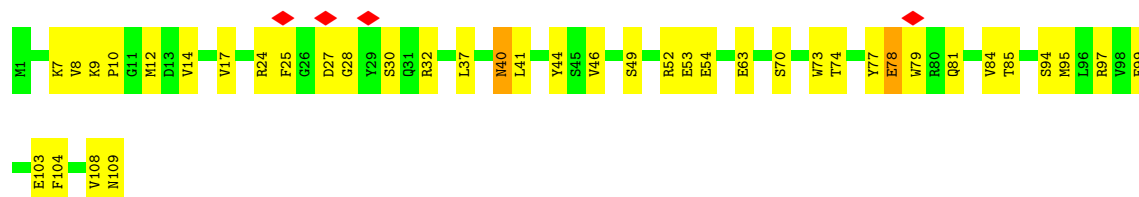
- Molecule 6: Tail fiber protein



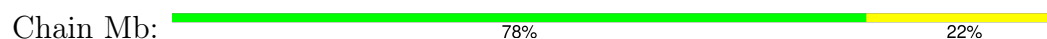
- Molecule 6: Tail fiber protein

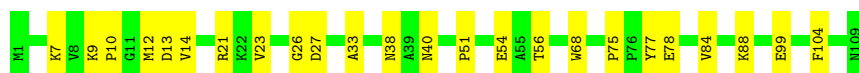


- Molecule 7: Tail tip protein M

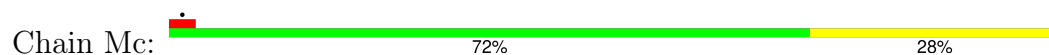


- Molecule 7: Tail tip protein M





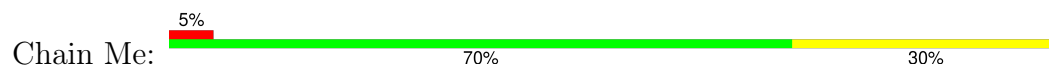
- Molecule 7: Tail tip protein M



- Molecule 7: Tail tip protein M



- Molecule 7: Tail tip protein M



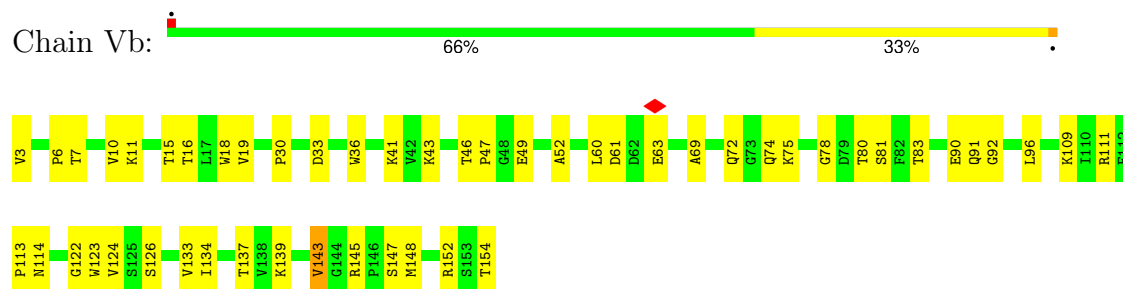
- Molecule 7: Tail tip protein M



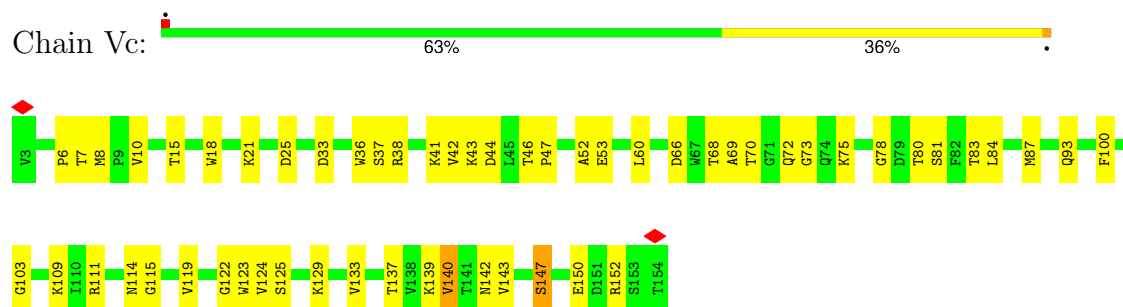
- Molecule 8: Tail tube protein



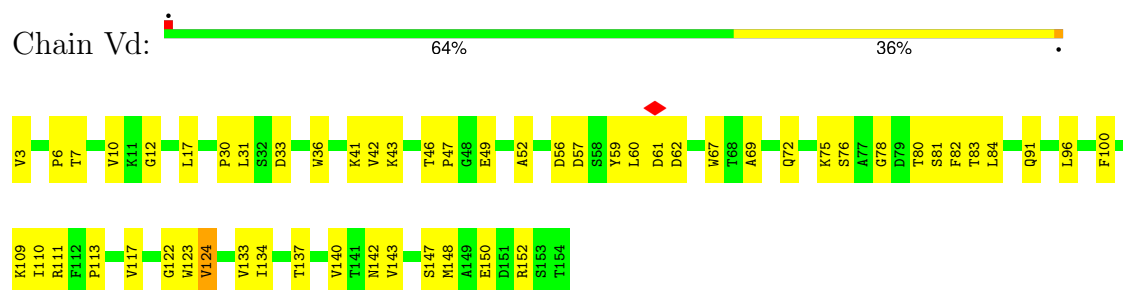
- Molecule 8: Tail tube protein



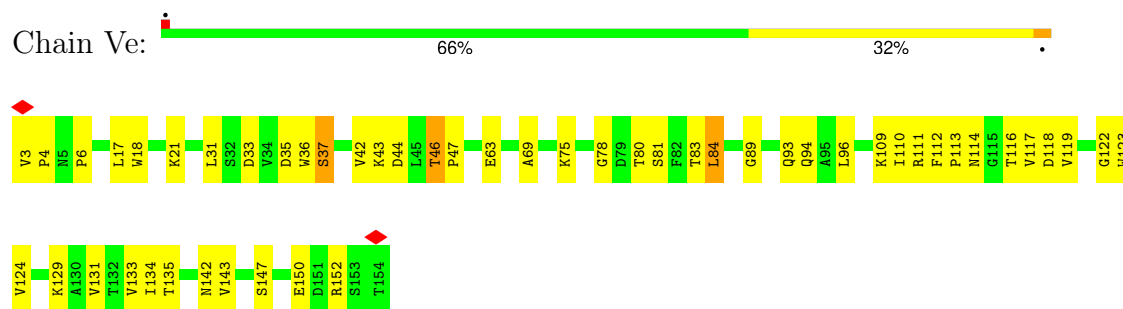
- Molecule 8: Tail tube protein



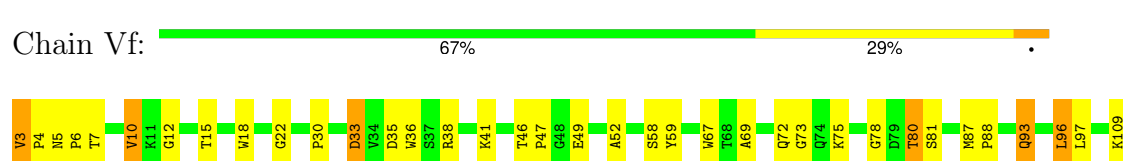
- Molecule 8: Tail tube protein



- Molecule 8: Tail tube protein



- Molecule 8: Tail tube protein





|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| I110 | R111 | F112 | P113 | V117 | D118 | V119 | G122 | W123 | V124 | K129 | I134 | V143 | S147 | M148 | A149 | E150 | D151 | R152 | S153 | T154 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 6517                            | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | TFS KRIOS                       | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                              | Depositor |
| Minimum defocus (nm)                 | 600                             | Depositor |
| Maximum defocus (nm)                 | 1200                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K3 (6k x 4k)              | Depositor |
| Maximum map value                    | 1.106                           | Depositor |
| Minimum map value                    | -0.328                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.023                           | Depositor |
| Recommended contour level            | 0.12                            | Depositor |
| Map size ( $\text{\AA}$ )            | 491.90402, 491.90402, 491.90402 | wwPDB     |
| Map dimensions                       | 448, 448, 448                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.098, 1.098, 1.098             | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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   | Ha    | 0.14         | 0/239   | 0.36        | 0/319   |
| 1   | Hb    | 0.13         | 0/243   | 0.37        | 0/323   |
| 1   | Hc    | 0.15         | 0/243   | 0.34        | 0/323   |
| 2   | Ia    | 0.23         | 0/645   | 0.55        | 0/872   |
| 2   | Ib    | 0.17         | 0/646   | 0.42        | 0/874   |
| 3   | Ic    | 0.19         | 0/654   | 0.46        | 0/883   |
| 4   | Ja    | 0.16         | 0/6633  | 0.37        | 0/9035  |
| 4   | Jb    | 0.16         | 0/6630  | 0.37        | 0/9031  |
| 4   | Jc    | 0.15         | 0/6624  | 0.35        | 0/9024  |
| 5   | La    | 0.16         | 0/1834  | 0.36        | 0/2484  |
| 5   | Lb    | 0.16         | 0/1831  | 0.35        | 0/2481  |
| 5   | Lc    | 0.16         | 0/1831  | 0.36        | 0/2481  |
| 6   | Ta    | 0.12         | 0/715   | 0.29        | 0/972   |
| 6   | Tb    | 0.18         | 0/715   | 0.47        | 0/972   |
| 6   | Tc    | 0.16         | 0/715   | 0.40        | 0/972   |
| 6   | Td    | 0.14         | 0/715   | 0.37        | 0/972   |
| 6   | Te    | 0.15         | 0/715   | 0.37        | 0/972   |
| 6   | Tf    | 0.16         | 0/715   | 0.41        | 0/972   |
| 6   | Tg    | 0.24         | 0/715   | 0.43        | 0/972   |
| 6   | Th    | 0.15         | 0/715   | 0.42        | 0/972   |
| 6   | Ti    | 0.15         | 0/715   | 0.39        | 0/972   |
| 6   | Tj    | 0.15         | 0/715   | 0.42        | 0/972   |
| 6   | Tk    | 0.14         | 0/715   | 0.38        | 0/972   |
| 6   | Tl    | 0.13         | 0/715   | 0.39        | 0/972   |
| 7   | Ma    | 0.19         | 0/910   | 0.45        | 0/1231  |
| 7   | Mb    | 0.17         | 0/893   | 0.38        | 0/1208  |
| 7   | Mc    | 0.16         | 0/910   | 0.38        | 0/1231  |
| 7   | Md    | 0.18         | 0/910   | 0.41        | 0/1231  |
| 7   | Me    | 0.18         | 0/910   | 0.41        | 0/1231  |
| 7   | Mf    | 0.16         | 0/906   | 0.34        | 0/1227  |
| 8   | Va    | 0.14         | 0/1194  | 0.36        | 0/1630  |
| 8   | Vb    | 0.15         | 0/1194  | 0.37        | 0/1630  |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 8   | Vc    | 0.16         | 0/1194  | 0.40        | 0/1630         |
| 8   | Vd    | 0.15         | 0/1194  | 0.36        | 0/1630         |
| 8   | Ve    | 0.22         | 0/1194  | 0.46        | 1/1630 (0.1%)  |
| 8   | Vf    | 0.16         | 0/1194  | 0.36        | 0/1630         |
| All | All   | 0.16         | 0/49236 | 0.38        | 1/66933 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | Ve    | 113 | PRO  | N-CA-C | -5.99 | 106.05      | 113.84   |

There are no chirality outliers.

There are no planarity outliers.

## 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   | Ha    | 237   | 0        | 232      | 10      | 0            |
| 1   | Hb    | 241   | 0        | 243      | 9       | 0            |
| 1   | Hc    | 241   | 0        | 243      | 8       | 0            |
| 2   | Ia    | 639   | 0        | 640      | 26      | 0            |
| 2   | Ib    | 640   | 0        | 636      | 28      | 0            |
| 3   | Ic    | 648   | 0        | 652      | 22      | 0            |
| 4   | Ja    | 6493  | 0        | 6350     | 201     | 0            |
| 4   | Jb    | 6490  | 0        | 6346     | 181     | 0            |
| 4   | Jc    | 6484  | 0        | 6330     | 200     | 0            |
| 5   | La    | 1799  | 0        | 1706     | 43      | 0            |
| 5   | Lb    | 1796  | 0        | 1699     | 43      | 0            |
| 5   | Lc    | 1796  | 0        | 1699     | 45      | 0            |
| 6   | Ta    | 704   | 0        | 692      | 11      | 0            |
| 6   | Tb    | 704   | 0        | 692      | 19      | 0            |
| 6   | Tc    | 704   | 0        | 692      | 22      | 0            |
| 6   | Td    | 704   | 0        | 692      | 14      | 0            |
| 6   | Te    | 704   | 0        | 692      | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | Tf    | 704   | 0        | 692      | 16      | 0            |
| 6   | Tg    | 704   | 0        | 692      | 13      | 0            |
| 6   | Th    | 704   | 0        | 692      | 15      | 0            |
| 6   | Ti    | 704   | 0        | 692      | 21      | 0            |
| 6   | Tj    | 704   | 0        | 692      | 13      | 0            |
| 6   | Tk    | 704   | 0        | 692      | 15      | 0            |
| 6   | Tl    | 704   | 0        | 692      | 13      | 0            |
| 7   | Ma    | 885   | 0        | 881      | 39      | 0            |
| 7   | Mb    | 870   | 0        | 862      | 15      | 0            |
| 7   | Mc    | 885   | 0        | 881      | 30      | 0            |
| 7   | Md    | 885   | 0        | 881      | 32      | 0            |
| 7   | Me    | 885   | 0        | 881      | 27      | 0            |
| 7   | Mf    | 881   | 0        | 870      | 27      | 0            |
| 8   | Va    | 1165  | 0        | 1113     | 37      | 0            |
| 8   | Vb    | 1165  | 0        | 1113     | 36      | 0            |
| 8   | Vc    | 1165  | 0        | 1113     | 42      | 0            |
| 8   | Vd    | 1165  | 0        | 1113     | 42      | 0            |
| 8   | Ve    | 1165  | 0        | 1113     | 31      | 0            |
| 8   | Vf    | 1165  | 0        | 1113     | 38      | 0            |
| 9   | La    | 8     | 0        | 0        | 0       | 0            |
| 9   | Lb    | 8     | 0        | 0        | 0       | 0            |
| 9   | Lc    | 8     | 0        | 0        | 0       | 0            |
| All | All   | 48257 | 0        | 47014    | 1183    | 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 12.

All (1183) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Jc:16:ASP:HB2   | 4:Jc:666:ARG:HB3  | 1.50                     | 0.92              |
| 4:Ja:535:VAL:H    | 4:Ja:548:ARG:HH21 | 1.20                     | 0.90              |
| 4:Jb:43:LYS:HB3   | 4:Jb:53:LEU:HB2   | 1.56                     | 0.87              |
| 4:Jb:378:MET:HE1  | 7:Mb:26:GLY:HA2   | 1.57                     | 0.87              |
| 4:Ja:616:VAL:HG12 | 5:La:232:GLN:HB2  | 1.59                     | 0.85              |
| 4:Jc:43:LYS:HB3   | 4:Jc:53:LEU:HB2   | 1.56                     | 0.84              |
| 6:Tf:61:ILE:HG23  | 6:Tf:69:PRO:HB3   | 1.61                     | 0.81              |
| 4:Jb:16:ASP:HB2   | 4:Jb:666:ARG:HB3  | 1.62                     | 0.81              |
| 8:Ve:21:LYS:HD2   | 8:Ve:37:SER:HB3   | 1.64                     | 0.80              |
| 8:Vb:15:THR:HA    | 8:Vb:111:ARG:O    | 1.82                     | 0.80              |
| 4:Jc:213:PRO:HG3  | 5:Lb:175:TRP:HH2  | 1.47                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:472:ARG:HH12 | 4:Ja:579:ASN:HD21 | 1.30                     | 0.79              |
| 4:Jb:526:GLY:H    | 4:Jb:530:PRO:HD2  | 1.47                     | 0.78              |
| 4:Ja:353:ASN:HD21 | 4:Ja:475:PRO:HB2  | 1.50                     | 0.76              |
| 4:Jb:698:TRP:HE1  | 5:Lb:232:GLN:HA   | 1.49                     | 0.76              |
| 4:Ja:141:ILE:HG22 | 4:Ja:179:ILE:HG22 | 1.67                     | 0.76              |
| 4:Jb:241:ARG:NH1  | 4:Jb:285:TYR:OH   | 2.19                     | 0.76              |
| 4:Ja:14:ALA:H     | 4:Ja:15:LYS:HZ3   | 1.32                     | 0.75              |
| 4:Jc:357:LEU:HD22 | 5:Lb:156:THR:HG21 | 1.69                     | 0.74              |
| 8:Vc:21:LYS:HD3   | 8:Vc:37:SER:HB3   | 1.68                     | 0.74              |
| 4:Jb:616:VAL:HG12 | 5:Lb:232:GLN:HB2  | 1.70                     | 0.74              |
| 4:Ja:140:GLN:HG2  | 4:Ja:149:THR:HA   | 1.69                     | 0.73              |
| 5:Lc:75:THR:HG22  | 5:Lc:77:PRO:HD3   | 1.70                     | 0.72              |
| 8:Vb:46:THR:HG1   | 8:Vb:81:SER:HG    | 1.35                     | 0.72              |
| 4:Jb:471:LEU:HB3  | 4:Jb:472:ARG:HH21 | 1.53                     | 0.72              |
| 4:Jb:140:GLN:HG2  | 4:Jb:149:THR:HA   | 1.71                     | 0.72              |
| 6:Tc:66:GLY:HA3   | 7:Ma:79:TRP:HA    | 1.71                     | 0.72              |
| 6:Tb:41:GLU:HB3   | 6:Tb:51:MET:HE1   | 1.72                     | 0.72              |
| 4:Jc:276:LEU:HD12 | 4:Jc:342:PHE:HB3  | 1.72                     | 0.71              |
| 5:Lb:43:ASN:HD21  | 5:Lb:47:GLU:HB2   | 1.55                     | 0.71              |
| 4:Jc:153:ILE:HD11 | 4:Jc:167:VAL:HG21 | 1.72                     | 0.71              |
| 4:Jc:615:GLY:O    | 4:Jc:617:THR:N    | 2.23                     | 0.71              |
| 7:Mf:53:GLU:OE2   | 7:Mf:53:GLU:N     | 2.23                     | 0.71              |
| 4:Ja:578:GLU:HB2  | 4:Ja:586:ILE:HB   | 1.72                     | 0.71              |
| 5:Lc:177:TYR:OH   | 5:Lc:215:ARG:NE   | 2.24                     | 0.71              |
| 5:Lb:177:TYR:OH   | 5:Lb:215:ARG:NE   | 2.24                     | 0.70              |
| 8:Ve:147:SER:OG   | 8:Ve:152:ARG:NH2  | 2.23                     | 0.70              |
| 4:Ja:43:LYS:HB3   | 4:Ja:53:LEU:HB2   | 1.73                     | 0.70              |
| 4:Jc:747:TRP:HB2  | 4:Jc:788:TYR:HB2  | 1.74                     | 0.70              |
| 8:Va:147:SER:OG   | 8:Va:152:ARG:NH2  | 2.24                     | 0.70              |
| 4:Jc:755:ASP:HB3  | 4:Jc:758:GLN:HG2  | 1.75                     | 0.69              |
| 4:Jc:141:ILE:HG22 | 4:Jc:179:ILE:HG22 | 1.72                     | 0.69              |
| 4:Jc:175:ARG:NH1  | 4:Jc:176:PRO:O    | 2.26                     | 0.69              |
| 4:Jc:213:PRO:HG3  | 5:Lb:175:TRP:CH2  | 2.25                     | 0.69              |
| 6:Ta:87:ASN:ND2   | 6:Td:30:SER:O     | 2.21                     | 0.69              |
| 7:Ma:63:GLU:OE1   | 7:Mf:40:ASN:ND2   | 2.25                     | 0.69              |
| 4:Jc:75:GLN:NE2   | 4:Jc:212:TYR:O    | 2.23                     | 0.69              |
| 7:Ma:84:VAL:HG11  | 7:Ma:104:PHE:HB3  | 1.75                     | 0.69              |
| 8:Vf:15:THR:HA    | 8:Vf:111:ARG:O    | 1.93                     | 0.69              |
| 6:Ta:27:ARG:HH21  | 6:Ta:74:THR:HG21  | 1.58                     | 0.69              |
| 7:Me:49:SER:OG    | 7:Me:97:ARG:NH1   | 2.26                     | 0.68              |
| 4:Ja:577:ARG:HH21 | 5:Lc:68:LEU:H     | 1.41                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:695:VAL:HB   | 4:Ja:699:GLY:HA2  | 1.74                     | 0.68              |
| 6:Tc:64:VAL:H     | 6:Tc:67:PHE:HB2   | 1.58                     | 0.68              |
| 8:Vf:30:PRO:O     | 8:Vf:109:LYS:NZ   | 2.27                     | 0.68              |
| 6:Tj:5:ILE:HG22   | 6:Tj:49:TYR:HE1   | 1.57                     | 0.68              |
| 4:Jc:733:PRO:HG2  | 4:Jc:744:PHE:HD2  | 1.58                     | 0.68              |
| 8:Vd:148:MET:HE3  | 8:Vd:148:MET:HA   | 1.75                     | 0.68              |
| 4:Jc:140:GLN:HG2  | 4:Jc:149:THR:HA   | 1.76                     | 0.68              |
| 4:Jc:526:GLY:H    | 4:Jc:530:PRO:HD2  | 1.58                     | 0.67              |
| 7:Md:84:VAL:HG21  | 7:Md:104:PHE:HB3  | 1.76                     | 0.67              |
| 8:Ve:122:GLY:HA2  | 8:Ve:143:VAL:HG12 | 1.76                     | 0.67              |
| 4:Ja:624:LEU:HD22 | 4:Ja:705:ALA:HB1  | 1.76                     | 0.67              |
| 2:Ia:192:LEU:HD13 | 4:Jc:328:TYR:HD1  | 1.60                     | 0.67              |
| 4:Jb:143:ARG:NH2  | 4:Jb:148:VAL:O    | 2.28                     | 0.67              |
| 4:Jb:753:ILE:HD11 | 4:Jb:759:VAL:HG12 | 1.77                     | 0.67              |
| 4:Ja:576:ILE:HB   | 4:Ja:588:ALA:HB3  | 1.77                     | 0.67              |
| 2:Ib:188:VAL:HG21 | 4:Jb:332:GLN:HB2  | 1.75                     | 0.66              |
| 7:Mb:40:ASN:ND2   | 7:Mc:63:GLU:OE2   | 2.28                     | 0.66              |
| 3:Ic:197:ARG:HH21 | 4:Ja:235:ASN:HD22 | 1.44                     | 0.66              |
| 2:Ia:205:GLN:H    | 5:Lb:229:LYS:HZ2  | 1.44                     | 0.66              |
| 6:Ti:18:GLN:CD    | 6:Ti:18:GLN:H     | 2.04                     | 0.66              |
| 4:Jb:721:GLU:HB3  | 4:Jb:732:THR:HG23 | 1.76                     | 0.66              |
| 4:Ja:812:GLU:HA   | 4:Ja:815:LEU:HD23 | 1.76                     | 0.66              |
| 4:Jb:175:ARG:NH1  | 4:Jb:176:PRO:O    | 2.28                     | 0.66              |
| 7:Mb:84:VAL:HG21  | 7:Mb:104:PHE:HB3  | 1.78                     | 0.66              |
| 8:Vd:122:GLY:HA2  | 8:Vd:143:VAL:HG12 | 1.78                     | 0.66              |
| 7:Ma:9:LYS:HE3    | 7:Ma:49:SER:HB3   | 1.79                     | 0.66              |
| 7:Ma:99:GLU:N     | 7:Ma:99:GLU:OE1   | 2.29                     | 0.66              |
| 8:Vc:15:THR:HA    | 8:Vc:111:ARG:O    | 1.96                     | 0.66              |
| 8:Vd:150:GLU:OE2  | 8:Vd:150:GLU:N    | 2.29                     | 0.65              |
| 8:Vb:134:ILE:HD12 | 8:Vb:134:ILE:H    | 1.61                     | 0.65              |
| 6:Tb:45:GLU:OE2   | 6:Tb:45:GLU:N     | 2.29                     | 0.65              |
| 4:Jc:594:GLU:HG2  | 4:Jc:595:LYS:HD3  | 1.79                     | 0.65              |
| 6:Th:45:GLU:N     | 6:Th:45:GLU:OE2   | 2.30                     | 0.65              |
| 7:Ma:74:THR:OG1   | 7:Ma:81:GLN:OE1   | 2.12                     | 0.65              |
| 4:Jc:746:PHE:HD1  | 4:Jc:789:ILE:HD12 | 1.62                     | 0.64              |
| 8:Vc:122:GLY:HA2  | 8:Vc:143:VAL:HG12 | 1.77                     | 0.64              |
| 8:Vd:134:ILE:H    | 8:Vd:134:ILE:HD12 | 1.62                     | 0.64              |
| 7:Me:40:ASN:ND2   | 7:Mf:63:GLU:OE1   | 2.30                     | 0.64              |
| 4:Jc:746:PHE:HB2  | 4:Jc:766:LEU:HD11 | 1.79                     | 0.64              |
| 6:Te:45:GLU:OE2   | 6:Te:45:GLU:N     | 2.30                     | 0.64              |
| 8:Va:21:LYS:HD2   | 8:Va:37:SER:HB3   | 1.79                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:Vd:82:PHE:HD2  | 8:Vd:84:LEU:HD21  | 1.62                     | 0.64              |
| 4:Jc:79:GLU:OE1  | 4:Jc:79:GLU:N     | 2.31                     | 0.64              |
| 1:Ha:835:ARG:NH1 | 1:Hb:837:GLU:OE1  | 2.30                     | 0.64              |
| 4:Jc:381:ASP:OD2 | 4:Jc:386:ARG:NH2  | 2.31                     | 0.64              |
| 4:Jb:118:VAL:O   | 4:Jb:162:GLN:HA   | 1.97                     | 0.64              |
| 4:Jb:395:ARG:O   | 4:Jb:429:ASN:ND2  | 2.31                     | 0.64              |
| 6:Tl:61:ILE:HG23 | 6:Tl:69:PRO:HB3   | 1.80                     | 0.64              |
| 4:Ja:373:ARG:HG3 | 4:Ja:486:TYR:HE2  | 1.63                     | 0.63              |
| 4:Jb:471:LEU:HG  | 4:Jb:585:ALA:HB2  | 1.78                     | 0.63              |
| 4:Jb:494:ARG:NH1 | 7:Mb:27:ASP:OD2   | 2.30                     | 0.63              |
| 4:Ja:606:ASP:OD2 | 5:La:210:SER:OG   | 2.16                     | 0.63              |
| 4:Jc:18:LEU:H    | 4:Jc:18:LEU:HD23  | 1.63                     | 0.63              |
| 5:La:41:GLU:HB2  | 7:Ma:27:ASP:HB2   | 1.78                     | 0.63              |
| 8:Vb:122:GLY:HA2 | 8:Vb:143:VAL:HG12 | 1.79                     | 0.63              |
| 8:Vf:150:GLU:N   | 8:Vf:150:GLU:OE2  | 2.29                     | 0.63              |
| 4:Jc:147:TRP:CD1 | 4:Jc:180:ARG:HE   | 2.16                     | 0.63              |
| 5:Lc:60:PRO:HG3  | 7:Me:25:PHE:CE1   | 2.33                     | 0.63              |
| 2:Ib:208:SER:OG  | 2:Ib:209:THR:N    | 2.32                     | 0.63              |
| 4:Jb:147:TRP:HB3 | 4:Jb:180:ARG:HH22 | 1.62                     | 0.63              |
| 4:Ja:784:ASP:OD1 | 4:Ja:806:ARG:NE   | 2.30                     | 0.63              |
| 4:Jb:79:GLU:OE2  | 4:Jb:79:GLU:N     | 2.32                     | 0.63              |
| 8:Va:122:GLY:HA2 | 8:Va:143:VAL:HG12 | 1.80                     | 0.63              |
| 4:Jb:393:LYS:HE2 | 5:Lb:157:GLU:HG2  | 1.79                     | 0.63              |
| 8:Vd:52:ALA:HA   | 8:Vd:75:LYS:HA    | 1.81                     | 0.63              |
| 4:Ja:575:SER:HB2 | 4:Ja:590:GLN:HE22 | 1.64                     | 0.63              |
| 4:Ja:18:LEU:HD23 | 4:Ja:18:LEU:H     | 1.64                     | 0.62              |
| 4:Ja:143:ARG:NH2 | 4:Ja:148:VAL:O    | 2.29                     | 0.62              |
| 8:Vf:52:ALA:HA   | 8:Vf:75:LYS:HA    | 1.80                     | 0.62              |
| 6:Tb:86:LEU:HA   | 6:Tb:89:PHE:HD2   | 1.63                     | 0.62              |
| 6:Tj:80:ASP:O    | 6:Tj:82:GLN:NE2   | 2.33                     | 0.62              |
| 7:Me:84:VAL:HG21 | 7:Me:104:PHE:HB3  | 1.81                     | 0.62              |
| 4:Ja:746:PHE:HB2 | 4:Ja:766:LEU:HD11 | 1.81                     | 0.62              |
| 4:Jc:695:VAL:HB  | 4:Jc:699:GLY:HA2  | 1.81                     | 0.62              |
| 6:Tc:24:LEU:HB3  | 6:Tc:58:TYR:HD2   | 1.64                     | 0.62              |
| 8:Vb:41:LYS:HG3  | 8:Vb:43:LYS:HZ2   | 1.63                     | 0.62              |
| 6:Tg:55:TYR:HA   | 6:Tg:77:VAL:HG13  | 1.80                     | 0.62              |
| 7:Ma:27:ASP:OD1  | 7:Mb:38:ASN:N     | 2.32                     | 0.62              |
| 7:Md:40:ASN:ND2  | 7:Me:63:GLU:OE2   | 2.32                     | 0.62              |
| 4:Ja:183:ARG:NH2 | 4:Ja:195:ASN:O    | 2.33                     | 0.62              |
| 6:Tf:15:LYS:NZ   | 6:Tf:16:PRO:O     | 2.32                     | 0.62              |
| 4:Jc:554:ALA:HB1 | 4:Jc:558:VAL:HG11 | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:105:THR:HG23 | 4:Ja:176:PRO:HG3  | 1.80                     | 0.62              |
| 4:Ja:604:HIS:CE1  | 4:Ja:607:GLY:H    | 2.18                     | 0.62              |
| 4:Ja:620:ALA:HB2  | 4:Ja:703:ASP:HB2  | 1.80                     | 0.62              |
| 4:Ja:687:ASN:HB3  | 4:Ja:710:ARG:HG2  | 1.81                     | 0.62              |
| 8:Vb:30:PRO:O     | 8:Vb:109:LYS:NZ   | 2.33                     | 0.62              |
| 8:Va:47:PRO:HA    | 8:Va:80:THR:HG23  | 1.81                     | 0.61              |
| 5:Lc:166:ARG:HH12 | 5:Lc:175:TRP:HE1  | 1.47                     | 0.61              |
| 8:Vd:83:THR:HG22  | 8:Vd:137:THR:HG22 | 1.82                     | 0.61              |
| 4:Ja:147:TRP:CD1  | 4:Ja:180:ARG:HE   | 2.18                     | 0.61              |
| 7:Mc:84:VAL:HG21  | 7:Mc:104:PHE:HB3  | 1.81                     | 0.61              |
| 8:Vf:122:GLY:HA2  | 8:Vf:143:VAL:HG12 | 1.80                     | 0.61              |
| 6:Tc:55:TYR:HA    | 6:Tc:77:VAL:HB    | 1.82                     | 0.61              |
| 4:Jb:471:LEU:HB3  | 4:Jb:472:ARG:NH2  | 2.15                     | 0.61              |
| 6:Ti:23:GLN:HB2   | 6:Ti:61:ILE:HG23  | 1.83                     | 0.61              |
| 8:Va:143:VAL:HG23 | 8:Vf:69:ALA:HA    | 1.81                     | 0.61              |
| 8:Vf:147:SER:OG   | 8:Vf:152:ARG:NH2  | 2.33                     | 0.61              |
| 2:Ia:188:VAL:HG11 | 5:Lb:164:PRO:HB2  | 1.82                     | 0.61              |
| 4:Ja:512:THR:HG21 | 4:Ja:545:LYS:HE2  | 1.83                     | 0.61              |
| 8:Ve:131:VAL:HA   | 8:Ve:134:ILE:HD13 | 1.82                     | 0.61              |
| 4:Ja:62:SER:OG    | 4:Ja:63:GLY:N     | 2.32                     | 0.61              |
| 4:Ja:471:LEU:HD13 | 4:Ja:585:ALA:HB2  | 1.83                     | 0.61              |
| 4:Ja:687:ASN:HA   | 4:Ja:710:ARG:HA   | 1.82                     | 0.61              |
| 4:Jb:211:CYS:SG   | 4:Jb:212:TYR:N    | 2.74                     | 0.61              |
| 4:Jc:718:SER:H    | 4:Jc:735:LEU:HA   | 1.65                     | 0.61              |
| 8:Ve:47:PRO:HA    | 8:Ve:80:THR:HG23  | 1.81                     | 0.61              |
| 4:Jc:745:GLU:OE1  | 4:Jc:768:THR:OG1  | 2.19                     | 0.61              |
| 2:Ib:197:ARG:HD3  | 4:Jb:410:TRP:CD1  | 2.36                     | 0.61              |
| 4:Jc:574:VAL:HA   | 4:Jc:589:VAL:HG12 | 1.81                     | 0.61              |
| 5:La:1:MET:HE3    | 5:La:1:MET:HA     | 1.83                     | 0.60              |
| 4:Jb:594:GLU:HG2  | 4:Jb:595:LYS:HD3  | 1.82                     | 0.60              |
| 4:Ja:175:ARG:HH21 | 4:Ja:177:PHE:HB3  | 1.65                     | 0.60              |
| 5:Lc:144:SER:OG   | 5:Lc:145:ALA:N    | 2.34                     | 0.60              |
| 7:Md:13:ASP:HB2   | 7:Md:45:SER:HB2   | 1.84                     | 0.60              |
| 4:Ja:111:ARG:HB2  | 4:Ja:205:ILE:HD11 | 1.83                     | 0.60              |
| 8:Va:10:VAL:HG23  | 8:Vb:134:ILE:HD13 | 1.82                     | 0.60              |
| 2:Ia:205:GLN:H    | 5:Lb:229:LYS:NZ   | 1.99                     | 0.60              |
| 4:Jb:31:SER:OG    | 4:Jb:32:GLU:N     | 2.35                     | 0.60              |
| 4:Jb:115:THR:OG1  | 4:Jb:201:SER:O    | 2.18                     | 0.60              |
| 8:Vc:147:SER:HG   | 8:Vc:152:ARG:HH22 | 1.47                     | 0.60              |
| 4:Jb:723:THR:HB   | 4:Jb:730:THR:HB   | 1.82                     | 0.60              |
| 5:La:5:ARG:NH1    | 5:La:128:GLU:O    | 2.34                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Ma:14:VAL:HG13  | 7:Ma:44:TYR:HE1   | 1.66                     | 0.60              |
| 4:Jc:615:GLY:C    | 4:Jc:617:THR:H    | 2.09                     | 0.60              |
| 8:Vb:36:TRP:CD2   | 8:Vb:109:LYS:HE2  | 2.36                     | 0.59              |
| 2:Ia:165:GLN:N    | 2:Ia:165:GLN:OE1  | 2.35                     | 0.59              |
| 4:Jc:142:GLN:NE2  | 4:Jc:178:ASN:OD1  | 2.34                     | 0.59              |
| 7:Md:22:LYS:NZ    | 7:Me:105:GLU:OE2  | 2.34                     | 0.59              |
| 4:Ja:122:VAL:HG21 | 4:Ja:130:ARG:HH11 | 1.68                     | 0.59              |
| 4:Jb:576:ILE:HB   | 4:Jb:588:ALA:HB3  | 1.83                     | 0.59              |
| 4:Jc:287:MET:HE1  | 4:Jc:335:ALA:HB1  | 1.84                     | 0.59              |
| 6:Tc:71:HIS:ND1   | 8:Va:63:GLU:OE1   | 2.35                     | 0.59              |
| 7:Ma:40:ASN:O     | 7:Ma:40:ASN:ND2   | 2.34                     | 0.59              |
| 4:Ja:247:SER:HA   | 4:Ja:265:LYS:HD2  | 1.84                     | 0.59              |
| 4:Jc:64:VAL:HG22  | 4:Jc:222:VAL:HG22 | 1.85                     | 0.59              |
| 8:Ve:42:VAL:HG23  | 8:Ve:84:LEU:HG    | 1.83                     | 0.59              |
| 4:Ja:79:GLU:N     | 4:Ja:79:GLU:OE1   | 2.35                     | 0.59              |
| 4:Jc:282:HIS:HB3  | 4:Jc:286:GLY:HA3  | 1.84                     | 0.59              |
| 6:Tb:32:THR:HG23  | 6:Tb:33:VAL:HG13  | 1.85                     | 0.59              |
| 6:Td:71:HIS:NE2   | 8:Vb:63:GLU:HB2   | 2.18                     | 0.59              |
| 6:Tf:23:GLN:HB2   | 6:Tf:61:ILE:HB    | 1.84                     | 0.59              |
| 6:Tl:44:ASP:OD1   | 6:Tl:48:ARG:N     | 2.34                     | 0.59              |
| 4:Jc:719:ARG:NH1  | 4:Jc:721:GLU:OE1  | 2.34                     | 0.59              |
| 7:Ma:40:ASN:ND2   | 7:Ma:40:ASN:C     | 2.59                     | 0.59              |
| 8:Ve:44:ASP:OD1   | 8:Ve:83:THR:OG1   | 2.18                     | 0.59              |
| 4:Ja:125:THR:OG1  | 4:Ja:129:ASP:OD1  | 2.16                     | 0.59              |
| 4:Ja:577:ARG:HH21 | 5:Lc:68:LEU:HG    | 1.68                     | 0.59              |
| 4:Ja:628:VAL:HG12 | 4:Ja:637:VAL:HG12 | 1.85                     | 0.59              |
| 4:Jb:523:LEU:HB3  | 4:Jb:533:VAL:HG12 | 1.84                     | 0.59              |
| 4:Jb:647:VAL:HG12 | 4:Jb:648:LYS:HG2  | 1.85                     | 0.59              |
| 6:Th:20:CYS:SG    | 6:Th:21:THR:N     | 2.76                     | 0.59              |
| 4:Jc:183:ARG:NH2  | 4:Jc:195:ASN:O    | 2.36                     | 0.58              |
| 1:Hc:843:ARG:HH12 | 5:La:76:ARG:HD2   | 1.68                     | 0.58              |
| 4:Ja:471:LEU:HG   | 4:Ja:472:ARG:HD3  | 1.84                     | 0.58              |
| 8:Vf:46:THR:OG1   | 8:Vf:81:SER:OG    | 2.20                     | 0.58              |
| 2:Ia:210:ALA:HB2  | 4:Jc:23:LEU:HB2   | 1.84                     | 0.58              |
| 4:Ja:475:PRO:HB3  | 5:Lc:2:GLN:HG2    | 1.85                     | 0.58              |
| 4:Jc:616:VAL:HG21 | 5:Lc:232:GLN:HB2  | 1.86                     | 0.58              |
| 7:Md:21:ARG:HB3   | 7:Md:33:ALA:HB3   | 1.85                     | 0.58              |
| 4:Ja:248:ASN:ND2  | 4:Ja:257:SER:O    | 2.36                     | 0.58              |
| 4:Jb:141:ILE:HG22 | 4:Jb:179:ILE:HG22 | 1.85                     | 0.58              |
| 5:Lc:166:ARG:NH1  | 5:Lc:175:TRP:HE1  | 2.01                     | 0.58              |
| 4:Jb:401:VAL:HG12 | 4:Jb:433:MET:HB3  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Lc:173:CYS:SG   | 5:Lc:174:THR:N    | 2.75                     | 0.58              |
| 7:Mc:99:GLU:OE1   | 7:Mc:99:GLU:N     | 2.37                     | 0.58              |
| 8:Vd:41:LYS:HG3   | 8:Vd:43:LYS:HZ3   | 1.68                     | 0.58              |
| 4:Jb:226:GLN:O    | 4:Jb:672:ARG:NH1  | 2.36                     | 0.58              |
| 8:Va:44:ASP:OD1   | 8:Va:83:THR:OG1   | 2.17                     | 0.58              |
| 2:Ib:176:PHE:HA   | 4:Jb:328:TYR:H    | 1.69                     | 0.58              |
| 2:Ia:219:VAL:HG21 | 4:Jc:152:ASP:O    | 2.04                     | 0.58              |
| 4:Ja:749:SER:HB3  | 4:Ja:763:THR:HG22 | 1.85                     | 0.58              |
| 4:Jc:508:ASP:HB2  | 4:Jc:543:LYS:HZ1  | 1.68                     | 0.58              |
| 8:Va:150:GLU:OE1  | 8:Va:150:GLU:N    | 2.33                     | 0.58              |
| 8:Vb:33:ASP:OD2   | 8:Vb:111:ARG:NH1  | 2.36                     | 0.58              |
| 4:Ja:788:TYR:HE1  | 4:Ja:802:GLU:HG3  | 1.68                     | 0.58              |
| 4:Jc:537:SER:OG   | 4:Jc:548:ARG:NH1  | 2.36                     | 0.58              |
| 4:Jc:625:THR:HG23 | 4:Jc:640:ARG:HG3  | 1.85                     | 0.58              |
| 4:Jc:747:TRP:HZ3  | 4:Jc:765:TYR:HA   | 1.69                     | 0.58              |
| 8:Vf:134:ILE:HD12 | 8:Vf:134:ILE:H    | 1.68                     | 0.58              |
| 2:Ib:197:ARG:HH21 | 4:Jb:235:ASN:HD22 | 1.50                     | 0.57              |
| 4:Jb:381:ASP:OD2  | 4:Jb:386:ARG:NH2  | 2.37                     | 0.57              |
| 4:Jc:472:ARG:HD2  | 5:Lb:107:LYS:HD2  | 1.85                     | 0.57              |
| 6:Tb:1:MET:HE1    | 6:Tb:3:VAL:HG22   | 1.86                     | 0.57              |
| 6:Ti:66:GLY:HA2   | 7:Me:79:TRP:CG    | 2.39                     | 0.57              |
| 7:Ma:40:ASN:O     | 7:Ma:41:LEU:HD23  | 2.04                     | 0.57              |
| 7:Mb:13:ASP:OD1   | 7:Mb:14:VAL:N     | 2.37                     | 0.57              |
| 3:Ic:190:PRO:HB3  | 4:Ja:330:THR:HA   | 1.86                     | 0.57              |
| 5:Lc:61:ILE:HG13  | 5:Lc:81:VAL:HG22  | 1.85                     | 0.57              |
| 7:Mc:54:GLU:N     | 7:Mc:54:GLU:OE1   | 2.36                     | 0.57              |
| 4:Jb:40:ASP:OD2   | 4:Jb:43:LYS:HG3   | 2.04                     | 0.57              |
| 6:Td:44:ASP:OD1   | 6:Td:48:ARG:N     | 2.35                     | 0.57              |
| 7:Mf:84:VAL:HG21  | 7:Mf:104:PHE:HB3  | 1.85                     | 0.57              |
| 8:Vc:150:GLU:N    | 8:Vc:150:GLU:OE2  | 2.37                     | 0.57              |
| 8:Vd:33:ASP:OD2   | 8:Vd:111:ARG:NH1  | 2.37                     | 0.57              |
| 8:Vf:33:ASP:OD2   | 8:Vf:111:ARG:NH1  | 2.37                     | 0.57              |
| 2:Ib:185:GLN:HB3  | 5:La:230:LEU:HD21 | 1.85                     | 0.57              |
| 5:Lb:48:PRO:HB3   | 5:Lb:57:GLN:HA    | 1.84                     | 0.57              |
| 5:La:173:CYS:SG   | 5:La:174:THR:N    | 2.76                     | 0.57              |
| 6:Tf:13:THR:HG22  | 6:Tg:24:LEU:HD12  | 1.86                     | 0.57              |
| 6:Ti:66:GLY:HA2   | 7:Me:79:TRP:CD1   | 2.39                     | 0.57              |
| 8:Ve:31:LEU:O     | 8:Ve:111:ARG:NH2  | 2.37                     | 0.57              |
| 7:Me:70:SER:HA    | 7:Me:85:THR:HG22  | 1.87                     | 0.57              |
| 2:Ia:192:LEU:HD13 | 4:Jc:328:TYR:CD1  | 2.39                     | 0.57              |
| 4:Ja:1:MET:HB2    | 4:Ja:3:LYS:HZ1    | 1.70                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:371:TYR:HE2  | 4:Ja:466:VAL:HG22 | 1.69                     | 0.57              |
| 4:Ja:490:SER:OG   | 4:Ja:491:THR:N    | 2.38                     | 0.57              |
| 4:Jb:466:VAL:HB   | 4:Jb:585:ALA:HB3  | 1.86                     | 0.57              |
| 4:Jb:689:ARG:HH11 | 4:Jb:706:SER:HB2  | 1.70                     | 0.57              |
| 4:Jc:541:GLY:C    | 4:Jc:543:LYS:H    | 2.13                     | 0.57              |
| 1:Hb:847:LEU:H    | 1:Hb:847:LEU:HD23 | 1.70                     | 0.57              |
| 4:Jc:147:TRP:HD1  | 4:Jc:180:ARG:HE   | 1.53                     | 0.57              |
| 6:Te:13:THR:HG23  | 6:Te:15:LYS:HG2   | 1.87                     | 0.57              |
| 7:Md:75:PRO:HB2   | 7:Md:78:GLU:HG3   | 1.85                     | 0.57              |
| 8:Vb:83:THR:HG22  | 8:Vb:137:THR:HG22 | 1.85                     | 0.57              |
| 2:Ib:185:GLN:HG2  | 5:La:230:LEU:HD11 | 1.86                     | 0.56              |
| 4:Jb:357:LEU:HB2  | 5:La:156:THR:HG21 | 1.86                     | 0.56              |
| 4:Jc:490:SER:OG   | 4:Jc:491:THR:N    | 2.38                     | 0.56              |
| 5:Lb:17:GLN:NE2   | 7:Md:31:GLN:OE1   | 2.38                     | 0.56              |
| 8:Vb:72:GLN:HB3   | 8:Vc:123:TRP:CE3  | 2.40                     | 0.56              |
| 4:Ja:574:VAL:HA   | 4:Ja:589:VAL:HG12 | 1.86                     | 0.56              |
| 4:Jb:827:LEU:HA   | 4:Jc:822:ILE:HD11 | 1.86                     | 0.56              |
| 4:Jc:407:ASN:OD1  | 4:Jc:408:ASN:ND2  | 2.37                     | 0.56              |
| 6:Tk:68:PRO:HD3   | 7:Mf:77:TYR:HD1   | 1.70                     | 0.56              |
| 8:Vb:148:MET:HE3  | 8:Vb:148:MET:HA   | 1.88                     | 0.56              |
| 8:Vc:44:ASP:OD1   | 8:Vc:83:THR:OG1   | 2.16                     | 0.56              |
| 8:Vd:46:THR:OG1   | 8:Vd:81:SER:OG    | 2.23                     | 0.56              |
| 8:Vf:148:MET:HE3  | 8:Vf:148:MET:HA   | 1.87                     | 0.56              |
| 4:Ja:75:GLN:NE2   | 4:Ja:212:TYR:O    | 2.35                     | 0.56              |
| 4:Jc:125:THR:OG1  | 4:Jc:129:ASP:OD1  | 2.18                     | 0.56              |
| 4:Jc:495:VAL:HB   | 4:Jc:509:ARG:NH2  | 2.21                     | 0.56              |
| 6:Tl:82:GLN:OE1   | 6:Tl:82:GLN:N     | 2.38                     | 0.56              |
| 2:Ib:142:LEU:HB3  | 2:Ib:146:MET:HE3  | 1.87                     | 0.56              |
| 6:Tc:42:ASN:OD1   | 6:Tc:42:ASN:N     | 2.37                     | 0.56              |
| 4:Ja:594:GLU:HG2  | 4:Ja:595:LYS:HD3  | 1.86                     | 0.56              |
| 4:Ja:723:THR:HB   | 4:Ja:730:THR:HB   | 1.87                     | 0.56              |
| 4:Jc:543:LYS:O    | 4:Jc:543:LYS:NZ   | 2.34                     | 0.56              |
| 4:Jb:132:PRO:HG3  | 4:Jb:158:LYS:HB2  | 1.88                     | 0.56              |
| 4:Jc:391:ALA:HB3  | 4:Jc:394:ASP:HB2  | 1.87                     | 0.56              |
| 6:Tc:18:GLN:CD    | 6:Tc:18:GLN:H     | 2.13                     | 0.56              |
| 7:Mc:25:PHE:CE2   | 7:Mc:30:SER:HA    | 2.40                     | 0.56              |
| 8:Vf:36:TRP:CD2   | 8:Vf:109:LYS:HE2  | 2.41                     | 0.56              |
| 8:Vc:47:PRO:HA    | 8:Vc:80:THR:HG23  | 1.88                     | 0.56              |
| 4:Ja:523:LEU:HB3  | 4:Ja:533:VAL:HG12 | 1.88                     | 0.56              |
| 4:Jc:40:ASP:OD2   | 4:Jc:43:LYS:HG3   | 2.05                     | 0.56              |
| 7:Mf:14:VAL:HG22  | 7:Mf:44:TYR:HD1   | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Jb:184:MET:N    | 4:Jb:184:MET:HE2  | 2.21                     | 0.56              |
| 2:Ia:139:LEU:H    | 2:Ia:139:LEU:HD23 | 1.71                     | 0.55              |
| 4:Ja:475:PRO:HG3  | 5:Lc:1:MET:HA     | 1.87                     | 0.55              |
| 4:Jb:621:VAL:HG12 | 4:Jb:644:PRO:HD3  | 1.89                     | 0.55              |
| 5:Lc:177:TYR:CD1  | 5:Lc:178:ARG:HG3  | 2.40                     | 0.55              |
| 5:Lc:226:SER:O    | 5:Lc:228:ASN:N    | 2.39                     | 0.55              |
| 4:Jb:411:GLU:HG3  | 5:Lb:230:LEU:HB3  | 1.88                     | 0.55              |
| 2:Ib:146:MET:HE1  | 4:Jb:576:ILE:HG13 | 1.88                     | 0.55              |
| 3:Ic:196:MET:HG3  | 3:Ic:196:MET:O    | 2.06                     | 0.55              |
| 6:Tl:29:ASN:OD1   | 6:Tl:35:VAL:N     | 2.38                     | 0.55              |
| 8:Vf:47:PRO:HA    | 8:Vf:80:THR:HG23  | 1.87                     | 0.55              |
| 4:Jc:681:THR:HG22 | 4:Jc:682:GLN:HG3  | 1.89                     | 0.55              |
| 8:Vd:147:SER:OG   | 8:Vd:152:ARG:NH2  | 2.39                     | 0.55              |
| 2:Ia:196:MET:O    | 2:Ia:198:VAL:HG13 | 2.07                     | 0.55              |
| 6:Tc:20:CYS:HB3   | 6:Tc:43:PRO:HD2   | 1.88                     | 0.55              |
| 8:Va:123:TRP:CE3  | 8:Vf:72:GLN:HB2   | 2.42                     | 0.55              |
| 2:Ia:211:ASP:OD1  | 2:Ia:212:GLU:N    | 2.39                     | 0.55              |
| 4:Jb:75:GLN:NE2   | 4:Jb:212:TYR:O    | 2.30                     | 0.55              |
| 4:Jb:222:VAL:HG12 | 4:Jb:224:SER:H    | 1.72                     | 0.55              |
| 4:Jb:360:VAL:HG11 | 4:Jb:477:ASP:HB2  | 1.88                     | 0.55              |
| 5:La:69:ASN:OD1   | 5:La:70:GLY:N     | 2.40                     | 0.55              |
| 6:Te:41:GLU:HB3   | 6:Te:51:MET:HE1   | 1.89                     | 0.55              |
| 2:Ia:180:ASP:OD1  | 2:Ia:181:ASN:N    | 2.39                     | 0.55              |
| 4:Jb:757:ARG:HB2  | 4:Jb:758:GLN:NE2  | 2.22                     | 0.55              |
| 4:Jc:175:ARG:HG2  | 4:Jc:176:PRO:HD2  | 1.89                     | 0.55              |
| 4:Jc:628:VAL:HG22 | 4:Jc:637:VAL:HG12 | 1.89                     | 0.55              |
| 6:Td:25:LYS:NZ    | 6:Td:36:ASN:OD1   | 2.38                     | 0.55              |
| 7:Ma:14:VAL:HG13  | 7:Ma:44:TYR:CE1   | 2.41                     | 0.55              |
| 4:Jb:490:SER:OG   | 4:Jb:491:THR:N    | 2.39                     | 0.55              |
| 6:Tk:68:PRO:HD3   | 7:Mf:77:TYR:CD1   | 2.42                     | 0.55              |
| 7:Ma:52:ARG:NH2   | 7:Ma:95:MET:O     | 2.40                     | 0.55              |
| 4:Jc:222:VAL:HG12 | 4:Jc:224:SER:H    | 1.71                     | 0.55              |
| 4:Jb:372:ASN:OD1  | 4:Jb:375:ASN:ND2  | 2.38                     | 0.54              |
| 4:Jb:623:HIS:ND1  | 4:Jb:642:ASP:OD2  | 2.38                     | 0.54              |
| 5:Lc:11:GLU:HG3   | 5:Lc:111:ARG:HD3  | 1.88                     | 0.54              |
| 4:Jb:556:TYR:CZ   | 7:Mc:109:ASN:HB2  | 2.42                     | 0.54              |
| 4:Jc:282:HIS:ND1  | 4:Jc:283:PRO:O    | 2.39                     | 0.54              |
| 5:La:19:ALA:HB3   | 5:La:110:ALA:HB2  | 1.89                     | 0.54              |
| 4:Ja:223:ASP:OD2  | 4:Ja:223:ASP:N    | 2.38                     | 0.54              |
| 4:Ja:604:HIS:NE2  | 4:Ja:606:ASP:HB3  | 2.22                     | 0.54              |
| 6:Tl:55:TYR:HA    | 6:Tl:77:VAL:HB    | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Jb:282:HIS:ND1  | 4:Jb:283:PRO:O    | 2.41                     | 0.54              |
| 4:Jb:823:THR:HG22 | 4:Jb:824:GLU:H    | 1.73                     | 0.54              |
| 4:Ja:279:MET:HG2  | 5:Lc:163:PHE:CE1  | 2.42                     | 0.54              |
| 6:Tb:63:GLN:HE22  | 6:Tb:69:PRO:HG3   | 1.72                     | 0.54              |
| 8:Vc:147:SER:OG   | 8:Vc:152:ARG:NH2  | 2.28                     | 0.54              |
| 5:La:226:SER:O    | 5:La:228:ASN:N    | 2.37                     | 0.54              |
| 6:Ti:24:LEU:HD23  | 6:Ti:58:TYR:HD2   | 1.72                     | 0.54              |
| 4:Ja:396:HIS:HA   | 4:Ja:429:ASN:HB2  | 1.89                     | 0.54              |
| 4:Ja:818:PHE:HA   | 4:Ja:821:LYS:HD3  | 1.90                     | 0.54              |
| 4:Jb:498:VAL:HG23 | 4:Jb:507:LEU:HD13 | 1.90                     | 0.54              |
| 5:Lb:25:GLU:OE2   | 5:Lb:35:ARG:NH2   | 2.40                     | 0.54              |
| 5:Lb:226:SER:O    | 5:Lb:228:ASN:N    | 2.40                     | 0.54              |
| 6:Tc:41:GLU:HG2   | 6:Tc:51:MET:SD    | 2.48                     | 0.54              |
| 8:Vc:100:PHE:HD1  | 8:Vc:124:VAL:HG13 | 1.73                     | 0.54              |
| 4:Jc:495:VAL:HA   | 4:Jc:559:TRP:HA   | 1.88                     | 0.54              |
| 5:Lb:60:PRO:HB3   | 7:Mc:25:PHE:CE1   | 2.43                     | 0.54              |
| 5:Lb:192:GLU:HG3  | 5:Lb:204:LYS:HG2  | 1.89                     | 0.54              |
| 8:Vc:52:ALA:HA    | 8:Vc:75:LYS:HA    | 1.88                     | 0.54              |
| 8:Vd:17:LEU:HD13  | 8:Vd:110:ILE:HG22 | 1.89                     | 0.54              |
| 3:Ic:189:LEU:HD22 | 4:Ja:32:GLU:HB2   | 1.90                     | 0.54              |
| 5:La:48:PRO:HB3   | 5:La:57:GLN:HA    | 1.89                     | 0.54              |
| 5:Lc:107:LYS:HG2  | 5:Lc:131:VAL:HB   | 1.91                     | 0.54              |
| 8:Va:72:GLN:HB2   | 8:Vb:123:TRP:CE3  | 2.43                     | 0.54              |
| 6:Tk:82:GLN:N     | 6:Tk:82:GLN:OE1   | 2.41                     | 0.53              |
| 4:Ja:118:VAL:O    | 4:Ja:162:GLN:HA   | 2.08                     | 0.53              |
| 4:Jb:695:VAL:HG12 | 4:Jb:701:GLN:HA   | 1.90                     | 0.53              |
| 8:Vc:78:GLY:O     | 8:Vc:142:ASN:ND2  | 2.37                     | 0.53              |
| 4:Ja:583:THR:HG22 | 4:Ja:583:THR:O    | 2.09                     | 0.53              |
| 4:Jc:162:GLN:OE1  | 4:Jc:162:GLN:N    | 2.34                     | 0.53              |
| 4:Ja:411:GLU:HG3  | 5:La:230:LEU:HB2  | 1.89                     | 0.53              |
| 4:Jc:494:ARG:HG3  | 4:Jc:509:ARG:HE   | 1.73                     | 0.53              |
| 4:Ja:248:ASN:HD21 | 4:Ja:257:SER:C    | 2.17                     | 0.53              |
| 4:Ja:577:ARG:NH2  | 5:Lc:68:LEU:H     | 2.05                     | 0.53              |
| 4:Jb:759:VAL:O    | 4:Jb:763:THR:OG1  | 2.25                     | 0.53              |
| 6:Ti:41:GLU:HG2   | 6:Ti:51:MET:SD    | 2.48                     | 0.53              |
| 6:Tk:61:ILE:HG23  | 6:Tk:69:PRO:HB3   | 1.91                     | 0.53              |
| 4:Jb:508:ASP:OD1  | 4:Jb:508:ASP:N    | 2.42                     | 0.53              |
| 6:Ti:55:TYR:HA    | 6:Ti:77:VAL:HB    | 1.90                     | 0.53              |
| 8:Vd:72:GLN:HB2   | 8:Ve:123:TRP:CE3  | 2.44                     | 0.53              |
| 4:Ja:2:GLY:O      | 4:Ja:3:LYS:HG2    | 2.09                     | 0.53              |
| 4:Jb:315:GLY:HA2  | 4:Jb:605:PHE:HA   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Ti:71:HIS:CE1   | 8:Ve:63:GLU:HB3   | 2.44                     | 0.53              |
| 8:Vd:47:PRO:HA    | 8:Vd:80:THR:HG23  | 1.90                     | 0.53              |
| 4:Ja:241:ARG:NH2  | 4:Ja:278:ASP:OD1  | 2.42                     | 0.53              |
| 7:Ma:7:LYS:HD2    | 8:Va:59:TYR:CD2   | 2.43                     | 0.53              |
| 4:Jb:745:GLU:OE1  | 4:Jb:768:THR:OG1  | 2.26                     | 0.52              |
| 8:Ve:46:THR:HG1   | 8:Ve:81:SER:HG    | 1.57                     | 0.52              |
| 2:Ia:176:PHE:HB2  | 4:Jc:327:ALA:HA   | 1.91                     | 0.52              |
| 2:Ib:222:GLY:HA3  | 4:Jb:156:LYS:HB2  | 1.92                     | 0.52              |
| 4:Ja:31:SER:OG    | 4:Ja:32:GLU:N     | 2.41                     | 0.52              |
| 4:Ja:526:GLY:H    | 4:Ja:530:PRO:HD2  | 1.74                     | 0.52              |
| 4:Jc:548:ARG:HD2  | 4:Jc:548:ARG:N    | 2.25                     | 0.52              |
| 6:Ta:38:VAL:HG22  | 6:Tc:67:PHE:HZ    | 1.75                     | 0.52              |
| 8:Vc:69:ALA:HA    | 8:Vd:143:VAL:HG23 | 1.90                     | 0.52              |
| 4:Jb:535:VAL:HG13 | 4:Jb:548:ARG:HG3  | 1.91                     | 0.52              |
| 8:Vb:18:TRP:HB2   | 8:Vb:109:LYS:HG3  | 1.90                     | 0.52              |
| 8:Vb:49:GLU:H     | 8:Vb:78:GLY:HA3   | 1.74                     | 0.52              |
| 8:Ve:150:GLU:OE2  | 8:Ve:150:GLU:N    | 2.36                     | 0.52              |
| 4:Ja:222:VAL:HG12 | 4:Ja:224:SER:H    | 1.74                     | 0.52              |
| 7:Ma:54:GLU:OE2   | 7:Ma:54:GLU:N     | 2.33                     | 0.52              |
| 8:Vf:49:GLU:H     | 8:Vf:78:GLY:HA3   | 1.75                     | 0.52              |
| 7:Mc:40:ASN:ND2   | 7:Md:63:GLU:OE2   | 2.43                     | 0.52              |
| 8:Vf:46:THR:HG1   | 8:Vf:81:SER:HG    | 1.53                     | 0.52              |
| 4:Jb:261:ASP:OD1  | 4:Jb:261:ASP:N    | 2.43                     | 0.52              |
| 6:Th:67:PHE:CE2   | 7:Me:5:ARG:HG3    | 2.45                     | 0.52              |
| 8:Va:46:THR:OG1   | 8:Va:81:SER:OG    | 2.27                     | 0.52              |
| 8:Vb:52:ALA:HA    | 8:Vb:75:LYS:HA    | 1.91                     | 0.52              |
| 8:Vd:47:PRO:HG2   | 8:Ve:129:LYS:HB3  | 1.92                     | 0.52              |
| 4:Jb:113:ARG:HB2  | 4:Jb:168:VAL:HG22 | 1.91                     | 0.52              |
| 8:Va:93:GLN:HA    | 8:Va:96:LEU:HB3   | 1.92                     | 0.52              |
| 8:Vc:36:TRP:CD2   | 8:Vc:109:LYS:HE2  | 2.44                     | 0.52              |
| 8:Vc:68:THR:OG1   | 8:Vd:76:SER:OG    | 2.24                     | 0.52              |
| 8:Vc:72:GLN:HB2   | 8:Vd:123:TRP:CE3  | 2.45                     | 0.52              |
| 8:Vc:87:MET:HB2   | 8:Vc:93:GLN:HE22  | 1.75                     | 0.52              |
| 8:Vd:69:ALA:HA    | 8:Ve:143:VAL:HG23 | 1.92                     | 0.52              |
| 4:Ja:282:HIS:ND1  | 4:Ja:283:PRO:O    | 2.37                     | 0.52              |
| 4:Ja:381:ASP:OD1  | 4:Ja:381:ASP:N    | 2.38                     | 0.52              |
| 4:Jc:32:GLU:OE2   | 5:Lb:166:ARG:NH1  | 2.39                     | 0.52              |
| 8:Vb:69:ALA:HA    | 8:Vc:143:VAL:HG23 | 1.92                     | 0.52              |
| 4:Ja:535:VAL:H    | 4:Ja:548:ARG:NH2  | 1.99                     | 0.52              |
| 4:Ja:624:LEU:HD12 | 4:Ja:707:VAL:HB   | 1.91                     | 0.52              |
| 6:Tg:5:ILE:HG22   | 6:Tg:49:TYR:HE2   | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Va:69:ALA:HA    | 8:Vb:143:VAL:HG23 | 1.92                     | 0.52              |
| 4:Jb:528:GLY:HA2  | 5:La:6:GLN:NE2    | 2.25                     | 0.51              |
| 4:Jc:536:GLN:NE2  | 4:Jc:546:VAL:O    | 2.37                     | 0.51              |
| 5:Lb:41:GLU:HA    | 7:Mc:27:ASP:OD1   | 2.10                     | 0.51              |
| 6:Ti:28:ARG:HH21  | 6:Ti:56:GLY:HA2   | 1.75                     | 0.51              |
| 6:Tj:90:LEU:HB3   | 6:Tk:29:ASN:HD22  | 1.75                     | 0.51              |
| 8:Vc:18:TRP:CE2   | 8:Vc:38:ARG:HG3   | 2.46                     | 0.51              |
| 4:Jc:118:VAL:O    | 4:Jc:162:GLN:HA   | 2.09                     | 0.51              |
| 4:Jc:637:VAL:CG2  | 4:Jc:680:PHE:HB2  | 2.40                     | 0.51              |
| 8:Vb:47:PRO:HG2   | 8:Vc:129:LYS:HB3  | 1.92                     | 0.51              |
| 8:Vf:22:GLY:N     | 8:Vf:35:ASP:OD1   | 2.42                     | 0.51              |
| 3:Ic:196:MET:O    | 3:Ic:198:VAL:HG13 | 2.09                     | 0.51              |
| 5:La:25:GLU:OE2   | 5:La:35:ARG:NH2   | 2.43                     | 0.51              |
| 4:Jb:175:ARG:HG2  | 4:Jb:176:PRO:HD2  | 1.93                     | 0.51              |
| 4:Jc:656:LEU:HB3  | 4:Jc:668:VAL:HG13 | 1.92                     | 0.51              |
| 6:Tg:87:ASN:ND2   | 6:Ti:31:THR:O     | 2.42                     | 0.51              |
| 7:Mc:52:ARG:NH1   | 7:Mc:95:MET:O     | 2.44                     | 0.51              |
| 4:Jc:18:LEU:HD11  | 4:Jc:159:THR:HG21 | 1.93                     | 0.51              |
| 4:Jc:162:GLN:H    | 4:Jc:162:GLN:CD   | 2.17                     | 0.51              |
| 5:La:60:PRO:HG3   | 7:Ma:25:PHE:CZ    | 2.44                     | 0.51              |
| 7:Mc:74:THR:OG1   | 7:Mc:81:GLN:OE1   | 2.22                     | 0.51              |
| 8:Va:36:TRP:N     | 8:Va:36:TRP:CD1   | 2.79                     | 0.51              |
| 2:Ia:212:GLU:N    | 2:Ia:212:GLU:OE1  | 2.44                     | 0.51              |
| 4:Jb:574:VAL:HA   | 4:Jb:589:VAL:HG12 | 1.91                     | 0.51              |
| 7:Mc:70:SER:HA    | 7:Mc:85:THR:HG22  | 1.93                     | 0.51              |
| 2:Ia:186:GLY:HA3  | 2:Ib:170:GLY:HA2  | 1.92                     | 0.51              |
| 6:Tf:44:ASP:OD1   | 6:Tf:48:ARG:N     | 2.44                     | 0.51              |
| 7:Md:79:TRP:HB3   | 7:Md:80:ARG:NH2   | 2.26                     | 0.51              |
| 4:Jb:782:GLY:H    | 4:Jb:806:ARG:NH2  | 2.08                     | 0.51              |
| 5:Lc:182:CYS:SG   | 5:Lc:217:ASN:ND2  | 2.83                     | 0.51              |
| 6:Te:67:PHE:CE1   | 7:Mc:5:ARG:HG3    | 2.46                     | 0.51              |
| 8:Va:99:TRP:NE1   | 8:Va:104:ASP:O    | 2.40                     | 0.51              |
| 8:Vc:53:GLU:HB3   | 8:Vc:73:GLY:O     | 2.11                     | 0.51              |
| 4:Ja:503:ARG:HE   | 4:Ja:546:VAL:HG21 | 1.76                     | 0.50              |
| 6:Te:22:ILE:HD11  | 6:Te:60:VAL:HG23  | 1.92                     | 0.50              |
| 6:Tk:29:ASN:OD1   | 6:Tk:35:VAL:HG13  | 2.10                     | 0.50              |
| 8:Vc:42:VAL:HA    | 8:Vc:84:LEU:HB3   | 1.92                     | 0.50              |
| 8:Ve:78:GLY:O     | 8:Ve:142:ASN:ND2  | 2.43                     | 0.50              |
| 4:Ja:454:THR:OG1  | 4:Ja:458:GLU:OE1  | 2.20                     | 0.50              |
| 4:Jb:513:LEU:HD12 | 4:Jb:514:PRO:HD2  | 1.93                     | 0.50              |
| 4:Jc:523:LEU:HB3  | 4:Jc:533:VAL:HG12 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Tk:28:ARG:HH21  | 6:Tk:57:GLN:HE21  | 1.59                     | 0.50              |
| 1:Ha:831:ARG:HH22 | 1:Hb:836:ASP:HB3  | 1.76                     | 0.50              |
| 4:Ja:752:GLN:HB2  | 4:Ja:786:TYR:CZ   | 2.46                     | 0.50              |
| 4:Ja:162:GLN:H    | 4:Ja:162:GLN:CD   | 2.19                     | 0.50              |
| 4:Jc:752:GLN:HB2  | 4:Jc:786:TYR:CZ   | 2.46                     | 0.50              |
| 7:Mc:32:ARG:HH21  | 7:Md:107:VAL:HG21 | 1.76                     | 0.50              |
| 4:Jc:576:ILE:HB   | 4:Jc:588:ALA:HB3  | 1.94                     | 0.50              |
| 5:La:177:TYR:HD1  | 5:La:178:ARG:N    | 2.09                     | 0.50              |
| 7:Me:25:PHE:HB2   | 7:Me:28:GLY:O     | 2.12                     | 0.50              |
| 2:Ia:196:MET:HE2  | 4:Jc:326:ASN:HB3  | 1.93                     | 0.50              |
| 5:Lb:107:LYS:HG2  | 5:Lb:131:VAL:HB   | 1.94                     | 0.50              |
| 7:Mf:13:ASP:HB3   | 7:Mf:45:SER:HB2   | 1.93                     | 0.50              |
| 2:Ia:188:VAL:HG13 | 5:Lb:166:ARG:O    | 2.12                     | 0.50              |
| 4:Jc:279:MET:HE2  | 4:Jc:338:VAL:HG12 | 1.94                     | 0.50              |
| 4:Ja:748:PHE:HE2  | 4:Ja:785:TYR:HB3  | 1.77                     | 0.50              |
| 4:Jc:380:ASP:N    | 4:Jc:380:ASP:OD1  | 2.44                     | 0.50              |
| 6:Ti:25:LYS:HZ1   | 6:Ti:37:THR:N     | 2.10                     | 0.50              |
| 7:Md:76:PRO:HG3   | 8:Vd:60:LEU:HD23  | 1.94                     | 0.50              |
| 7:Ma:25:PHE:CE2   | 7:Ma:30:SER:HA    | 2.47                     | 0.50              |
| 4:Ja:373:ARG:HH12 | 7:Mf:27:ASP:CG    | 2.20                     | 0.49              |
| 4:Jc:617:THR:OG1  | 4:Jc:700:GLN:OE1  | 2.23                     | 0.49              |
| 4:Jc:732:THR:O    | 4:Jc:732:THR:OG1  | 2.23                     | 0.49              |
| 4:Jc:747:TRP:CZ3  | 4:Jc:765:TYR:HA   | 2.47                     | 0.49              |
| 7:Ma:77:TYR:CG    | 7:Ma:78:GLU:N     | 2.80                     | 0.49              |
| 8:Va:72:GLN:NE2   | 8:Va:75:LYS:HE3   | 2.27                     | 0.49              |
| 8:Vb:90:GLU:CD    | 8:Vb:92:GLY:H     | 2.19                     | 0.49              |
| 2:Ib:164:ILE:HD12 | 2:Ib:164:ILE:H    | 1.76                     | 0.49              |
| 4:Ja:110:ASP:HB2  | 4:Ja:206:ILE:HA   | 1.93                     | 0.49              |
| 4:Jc:788:TYR:HE1  | 4:Jc:802:GLU:HG3  | 1.77                     | 0.49              |
| 6:Ta:22:ILE:HD11  | 6:Ta:43:PRO:HG3   | 1.94                     | 0.49              |
| 4:Jb:719:ARG:NH1  | 4:Jb:721:GLU:OE1  | 2.36                     | 0.49              |
| 6:Td:82:GLN:OE1   | 6:Td:82:GLN:N     | 2.44                     | 0.49              |
| 8:Va:36:TRP:CD2   | 8:Va:109:LYS:HE2  | 2.48                     | 0.49              |
| 2:Ia:136:THR:HG21 | 4:Jc:580:ASP:HB2  | 1.94                     | 0.49              |
| 4:Ja:373:ARG:NH1  | 7:Mf:27:ASP:OD2   | 2.40                     | 0.49              |
| 4:Jb:822:ILE:HG13 | 4:Jb:826:HIS:HB2  | 1.94                     | 0.49              |
| 4:Jc:260:TRP:NE1  | 4:Jc:261:ASP:O    | 2.45                     | 0.49              |
| 4:Jc:664:SER:OG   | 4:Jc:665:GLU:N    | 2.45                     | 0.49              |
| 5:Lb:19:ALA:HB3   | 5:Lb:110:ALA:HB2  | 1.93                     | 0.49              |
| 6:Tf:55:TYR:HA    | 6:Tf:77:VAL:HB    | 1.92                     | 0.49              |
| 7:Ma:17:VAL:HG22  | 7:Mb:88:LYS:HG2   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Vf:93:GLN:HA    | 8:Vf:96:LEU:HB3   | 1.92                     | 0.49              |
| 2:Ib:189:LEU:HA   | 5:La:168:MET:HE1  | 1.94                     | 0.49              |
| 4:Ja:371:TYR:CE2  | 4:Ja:466:VAL:HG22 | 2.48                     | 0.49              |
| 4:Jb:64:VAL:HG22  | 4:Jb:222:VAL:HG22 | 1.94                     | 0.49              |
| 4:Jb:247:SER:HA   | 4:Jb:265:LYS:HD3  | 1.93                     | 0.49              |
| 4:Jb:628:VAL:HG12 | 4:Jb:637:VAL:HG22 | 1.94                     | 0.49              |
| 4:Jc:541:GLY:O    | 4:Jc:543:LYS:N    | 2.43                     | 0.49              |
| 5:Lb:61:ILE:HG13  | 5:Lb:81:VAL:HG22  | 1.94                     | 0.49              |
| 4:Jb:353:ASN:ND2  | 4:Jb:475:PRO:HB2  | 2.28                     | 0.49              |
| 5:Lc:114:ASP:OD1  | 5:Lc:115:ALA:N    | 2.45                     | 0.49              |
| 6:Tb:60:VAL:HG13  | 6:Tb:72:ALA:HB3   | 1.95                     | 0.49              |
| 3:Ic:208:SER:OG   | 3:Ic:209:THR:N    | 2.46                     | 0.49              |
| 3:Ic:210:ALA:HB2  | 4:Ja:23:LEU:HB2   | 1.93                     | 0.49              |
| 4:Ja:81:PHE:HD2   | 4:Ja:221:GLN:HE21 | 1.59                     | 0.49              |
| 4:Ja:380:ASP:OD1  | 4:Ja:380:ASP:N    | 2.45                     | 0.49              |
| 4:Ja:575:SER:HB2  | 4:Ja:590:GLN:NE2  | 2.26                     | 0.49              |
| 4:Jb:98:THR:O     | 4:Jb:98:THR:OG1   | 2.30                     | 0.49              |
| 6:Tf:15:LYS:HD2   | 6:Tf:16:PRO:HD2   | 1.95                     | 0.49              |
| 6:Ti:61:ILE:HD11  | 6:Ti:69:PRO:HB3   | 1.94                     | 0.49              |
| 8:Vc:7:THR:O      | 8:Vc:8:MET:HE2    | 2.12                     | 0.49              |
| 2:Ib:210:ALA:HB2  | 4:Jb:23:LEU:HB2   | 1.94                     | 0.49              |
| 4:Ja:718:SER:H    | 4:Ja:735:LEU:HA   | 1.78                     | 0.49              |
| 4:Jc:570:LEU:HB3  | 4:Jc:572:ARG:HH12 | 1.76                     | 0.49              |
| 6:Tl:13:THR:HG22  | 6:Th:24:LEU:HD13  | 1.93                     | 0.49              |
| 6:Th:22:ILE:HD11  | 6:Th:60:VAL:HG23  | 1.93                     | 0.49              |
| 7:Me:52:ARG:NH2   | 7:Me:95:MET:O     | 2.46                     | 0.49              |
| 4:Ja:494:ARG:HH12 | 7:Ma:37:LEU:HD13  | 1.77                     | 0.49              |
| 4:Jb:625:THR:HG23 | 4:Jb:640:ARG:HG3  | 1.94                     | 0.49              |
| 4:Jb:752:GLN:HB2  | 4:Jb:786:TYR:CZ   | 2.47                     | 0.49              |
| 6:Td:55:TYR:HA    | 6:Td:77:VAL:HB    | 1.94                     | 0.49              |
| 5:Lc:19:ALA:HB3   | 5:Lc:110:ALA:HB2  | 1.95                     | 0.49              |
| 5:Lb:16:GLU:OE2   | 7:Md:32:ARG:NH2   | 2.33                     | 0.49              |
| 7:Mc:23:VAL:HG13  | 7:Mc:25:PHE:CZ    | 2.48                     | 0.49              |
| 8:Ve:43:LYS:N     | 8:Ve:83:THR:O     | 2.45                     | 0.49              |
| 8:Vf:30:PRO:HB2   | 8:Vf:117:VAL:HG21 | 1.95                     | 0.49              |
| 3:Ic:192:LEU:HD13 | 4:Ja:328:TYR:HD1  | 1.78                     | 0.48              |
| 4:Ja:354:GLY:O    | 4:Ja:355:GLN:NE2  | 2.46                     | 0.48              |
| 4:Jb:594:GLU:N    | 4:Jb:594:GLU:OE2  | 2.46                     | 0.48              |
| 4:Jc:471:LEU:HD13 | 4:Jc:585:ALA:HB2  | 1.94                     | 0.48              |
| 4:Jc:562:LYS:NZ   | 4:Jc:564:PRO:HB3  | 2.28                     | 0.48              |
| 7:Mf:14:VAL:HG22  | 7:Mf:44:TYR:CD1   | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Me:8:VAL:HG13   | 7:Me:46:VAL:HG13  | 1.95                     | 0.48              |
| 4:Jb:175:ARG:HD2  | 4:Jb:176:PRO:O    | 2.13                     | 0.48              |
| 4:Jc:583:THR:HG21 | 7:Md:21:ARG:HH11  | 1.79                     | 0.48              |
| 4:Jc:646:VAL:HG13 | 4:Jc:650:VAL:HG13 | 1.95                     | 0.48              |
| 5:Lc:25:GLU:OE2   | 5:Lc:35:ARG:NH2   | 2.46                     | 0.48              |
| 7:Mc:23:VAL:HG22  | 7:Mc:25:PHE:CE1   | 2.47                     | 0.48              |
| 8:Va:72:GLN:HE22  | 8:Va:75:LYS:HE3   | 1.77                     | 0.48              |
| 8:Va:114:ASN:OD1  | 8:Va:116:THR:OG1  | 2.21                     | 0.48              |
| 4:Ja:378:MET:O    | 4:Ja:378:MET:HG2  | 2.13                     | 0.48              |
| 4:Ja:391:ALA:HB3  | 4:Ja:394:ASP:HB2  | 1.94                     | 0.48              |
| 6:Ti:42:ASN:OD1   | 6:Ti:42:ASN:N     | 2.40                     | 0.48              |
| 7:Me:77:TYR:O     | 7:Me:77:TYR:CD1   | 2.67                     | 0.48              |
| 8:Vb:147:SER:OG   | 8:Vb:152:ARG:NH2  | 2.46                     | 0.48              |
| 4:Ja:132:PRO:HG3  | 4:Ja:158:LYS:HB2  | 1.94                     | 0.48              |
| 4:Jb:528:GLY:HA2  | 5:La:6:GLN:HE21   | 1.78                     | 0.48              |
| 6:Tb:22:ILE:HD11  | 6:Tb:60:VAL:HG23  | 1.95                     | 0.48              |
| 6:Th:60:VAL:HG13  | 6:Th:72:ALA:HB3   | 1.93                     | 0.48              |
| 8:Vc:10:VAL:HG23  | 8:Vd:134:ILE:HD13 | 1.95                     | 0.48              |
| 8:Vc:46:THR:HG1   | 8:Vc:81:SER:HG    | 1.57                     | 0.48              |
| 8:Ve:69:ALA:HA    | 8:Vf:143:VAL:HG23 | 1.95                     | 0.48              |
| 4:Jb:260:TRP:NE1  | 4:Jb:261:ASP:O    | 2.47                     | 0.48              |
| 4:Jb:615:GLY:O    | 4:Jb:617:THR:OG1  | 2.30                     | 0.48              |
| 6:Th:18:GLN:OE1   | 6:Th:18:GLN:N     | 2.46                     | 0.48              |
| 7:Ma:49:SER:O     | 7:Ma:97:ARG:NH2   | 2.46                     | 0.48              |
| 1:Ha:831:ARG:HB2  | 1:Ha:831:ARG:NH1  | 2.29                     | 0.48              |
| 4:Jc:472:ARG:CZ   | 4:Jc:472:ARG:HA   | 2.43                     | 0.48              |
| 4:Jc:650:VAL:HA   | 4:Jc:695:VAL:O    | 2.14                     | 0.48              |
| 5:Lc:43:ASN:HD21  | 5:Lc:47:GLU:HB2   | 1.78                     | 0.48              |
| 6:Ta:5:ILE:HG22   | 6:Ta:49:TYR:HE2   | 1.77                     | 0.48              |
| 6:Tc:27:ARG:NH2   | 6:Tc:57:GLN:OE1   | 2.38                     | 0.48              |
| 7:Ma:77:TYR:OH    | 7:Mb:56:THR:N     | 2.46                     | 0.48              |
| 3:Ic:144:ALA:HA   | 3:Ic:147:VAL:HB   | 1.94                     | 0.48              |
| 4:Ja:64:VAL:HG22  | 4:Ja:222:VAL:HG22 | 1.95                     | 0.48              |
| 4:Ja:572:ARG:HE   | 4:Ja:591:HIS:HA   | 1.79                     | 0.48              |
| 4:Ja:749:SER:OG   | 4:Ja:786:TYR:HB2  | 2.13                     | 0.48              |
| 5:La:59:TYR:CG    | 5:La:60:PRO:HD2   | 2.49                     | 0.48              |
| 7:Mc:1:MET:SD     | 7:Mc:83:LYS:NZ    | 2.87                     | 0.48              |
| 8:Vf:6:PRO:O      | 8:Vf:7:THR:OG1    | 2.29                     | 0.48              |
| 4:Ja:143:ARG:NH1  | 4:Ja:148:VAL:HG13 | 2.29                     | 0.48              |
| 4:Jc:612:THR:O    | 4:Jc:614:ASN:N    | 2.47                     | 0.48              |
| 6:Tb:21:THR:HB    | 6:Tb:63:GLN:HB3   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Md:7:LYS:HE2    | 8:Vd:59:TYR:CD2   | 2.49                     | 0.48              |
| 8:Vb:47:PRO:HA    | 8:Vb:80:THR:HG23  | 1.95                     | 0.48              |
| 5:La:43:ASN:HD21  | 5:La:47:GLU:HB2   | 1.78                     | 0.47              |
| 6:Tc:15:LYS:HD2   | 6:Tc:16:PRO:HD2   | 1.96                     | 0.47              |
| 6:Tg:16:PRO:HG2   | 6:Tg:18:GLN:HE22  | 1.79                     | 0.47              |
| 6:Tl:28:ARG:NE    | 6:Tl:57:GLN:OE1   | 2.38                     | 0.47              |
| 6:Tk:55:TYR:HA    | 6:Tk:77:VAL:HB    | 1.94                     | 0.47              |
| 7:Me:75:PRO:HB2   | 7:Me:78:GLU:HB2   | 1.94                     | 0.47              |
| 4:Jb:757:ARG:HB2  | 4:Jb:758:GLN:HE21 | 1.79                     | 0.47              |
| 4:Jc:116:PHE:CZ   | 4:Jc:153:ILE:HD12 | 2.49                     | 0.47              |
| 4:Jc:152:ASP:O    | 4:Jc:153:ILE:HG12 | 2.14                     | 0.47              |
| 7:Ma:44:TYR:HD2   | 7:Ma:73:TRP:HZ3   | 1.62                     | 0.47              |
| 4:Ja:556:TYR:CZ   | 7:Ma:109:ASN:HB2  | 2.49                     | 0.47              |
| 4:Ja:750:GLU:HG2  | 4:Ja:785:TYR:HE1  | 1.79                     | 0.47              |
| 4:Ja:787:PHE:HB3  | 4:Ja:789:ILE:HD11 | 1.97                     | 0.47              |
| 4:Jc:134:GLU:HA   | 4:Jc:155:ILE:O    | 2.14                     | 0.47              |
| 5:La:139:GLN:HE21 | 5:La:141:SER:HB3  | 1.80                     | 0.47              |
| 7:Mf:75:PRO:HB2   | 7:Mf:78:GLU:HB2   | 1.96                     | 0.47              |
| 8:Ve:6:PRO:HB3    | 8:Vf:88:PRO:HG2   | 1.96                     | 0.47              |
| 2:Ib:197:ARG:NH2  | 4:Jb:235:ASN:HD22 | 2.12                     | 0.47              |
| 4:Ja:495:VAL:HA   | 4:Ja:559:TRP:HA   | 1.95                     | 0.47              |
| 4:Jc:98:THR:O     | 4:Jc:98:THR:OG1   | 2.30                     | 0.47              |
| 6:Ta:93:MET:SD    | 6:Ta:94:THR:N     | 2.87                     | 0.47              |
| 8:Vf:36:TRP:H     | 8:Vf:36:TRP:CD1   | 2.32                     | 0.47              |
| 1:Hc:829:MET:HA   | 3:Ic:140:PHE:HE2  | 1.79                     | 0.47              |
| 4:Jb:210:GLN:NE2  | 4:Jb:211:CYS:O    | 2.48                     | 0.47              |
| 4:Jc:360:VAL:HG11 | 4:Jc:477:ASP:HB2  | 1.97                     | 0.47              |
| 4:Jc:727:PHE:HE1  | 4:Jc:781:PRO:HD3  | 1.78                     | 0.47              |
| 6:Ta:29:ASN:HD21  | 6:Tc:90:LEU:HD13  | 1.78                     | 0.47              |
| 8:Va:18:TRP:HB2   | 8:Va:109:LYS:HG3  | 1.94                     | 0.47              |
| 8:Va:100:PHE:HD1  | 8:Va:124:VAL:HG13 | 1.80                     | 0.47              |
| 5:Lc:177:TYR:HD1  | 5:Lc:178:ARG:HG3  | 1.80                     | 0.47              |
| 6:Ti:4:LYS:HZ3    | 6:Ti:51:MET:H     | 1.62                     | 0.47              |
| 2:Ia:220:VAL:HA   | 4:Jc:154:THR:HG23 | 1.96                     | 0.47              |
| 4:Ja:30:ILE:HG21  | 4:Ja:238:LEU:HD12 | 1.96                     | 0.47              |
| 4:Ja:104:ILE:O    | 4:Ja:176:PRO:HA   | 2.14                     | 0.47              |
| 4:Ja:627:GLU:OE1  | 4:Jb:160:THR:HG23 | 2.15                     | 0.47              |
| 4:Jb:188:SER:HA   | 4:Jb:193:LEU:HD11 | 1.96                     | 0.47              |
| 4:Jb:443:GLN:HA   | 4:Jb:446:ARG:NH1  | 2.29                     | 0.47              |
| 5:La:226:SER:OG   | 5:La:227:ILE:N    | 2.47                     | 0.47              |
| 6:Tb:18:GLN:N     | 6:Tb:18:GLN:OE1   | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Ma:8:VAL:HG12   | 7:Ma:46:VAL:HG13  | 1.96                     | 0.47              |
| 7:Me:32:ARG:HH12  | 7:Mf:107:VAL:HG21 | 1.79                     | 0.47              |
| 8:Vd:49:GLU:H     | 8:Vd:78:GLY:HA3   | 1.80                     | 0.47              |
| 1:Hc:842:MET:HA   | 1:Hc:848:PHE:HA   | 1.97                     | 0.47              |
| 4:Ja:378:MET:HE1  | 7:Mf:26:GLY:HA2   | 1.96                     | 0.47              |
| 4:Jc:454:THR:HG23 | 4:Jc:458:GLU:OE1  | 2.15                     | 0.47              |
| 4:Jc:637:VAL:HG22 | 4:Jc:680:PHE:HB2  | 1.97                     | 0.47              |
| 4:Jc:733:PRO:HG2  | 4:Jc:744:PHE:CD2  | 2.44                     | 0.47              |
| 6:Tf:18:GLN:N     | 6:Tf:18:GLN:OE1   | 2.48                     | 0.47              |
| 6:Ti:23:GLN:NE2   | 6:Ti:63:GLN:OE1   | 2.47                     | 0.47              |
| 6:Tk:61:ILE:HD12  | 6:Tk:69:PRO:HB3   | 1.96                     | 0.47              |
| 7:Mc:10:PRO:HA    | 8:Vc:60:LEU:HD21  | 1.97                     | 0.47              |
| 4:Jc:31:SER:OG    | 4:Jc:32:GLU:N     | 2.47                     | 0.47              |
| 4:Jc:90:LEU:HD23  | 4:Jc:90:LEU:HA    | 1.81                     | 0.47              |
| 4:Jc:472:ARG:HD3  | 5:Lb:131:VAL:HG21 | 1.97                     | 0.47              |
| 6:Tl:68:PRO:HD3   | 7:Md:77:TYR:HD1   | 1.79                     | 0.47              |
| 6:Th:63:GLN:HE22  | 7:Me:57:VAL:HG11  | 1.80                     | 0.47              |
| 8:Vb:72:GLN:NE2   | 8:Vc:103:GLY:HA3  | 2.30                     | 0.47              |
| 4:Jc:136:ARG:HD2  | 4:Jc:184:MET:HG3  | 1.97                     | 0.47              |
| 5:La:180:ASP:OD1  | 5:La:180:ASP:N    | 2.34                     | 0.47              |
| 4:Ja:469:GLU:HB3  | 5:Lc:12:CYS:O     | 2.15                     | 0.46              |
| 4:Jb:26:VAL:HG21  | 4:Jb:234:ARG:NH2  | 2.30                     | 0.46              |
| 4:Jb:122:VAL:HG23 | 4:Jb:194:GLN:HE21 | 1.80                     | 0.46              |
| 4:Jb:342:PHE:O    | 4:Jb:346:MET:HE2  | 2.14                     | 0.46              |
| 5:La:173:CYS:N    | 5:La:207:LYS:O    | 2.41                     | 0.46              |
| 6:Tc:4:LYS:HZ3    | 6:Tc:51:MET:H     | 1.63                     | 0.46              |
| 7:Mc:27:ASP:HB2   | 7:Md:38:ASN:OD1   | 2.15                     | 0.46              |
| 8:Vc:18:TRP:CZ3   | 8:Vc:33:ASP:HB3   | 2.50                     | 0.46              |
| 2:Ib:165:GLN:N    | 2:Ib:165:GLN:OE1  | 2.48                     | 0.46              |
| 4:Jc:130:ARG:HB3  | 4:Jc:158:LYS:HE3  | 1.96                     | 0.46              |
| 7:Mb:75:PRO:HB2   | 7:Mb:78:GLU:HG2   | 1.98                     | 0.46              |
| 4:Ja:745:GLU:OE2  | 4:Ja:790:ARG:NE   | 2.48                     | 0.46              |
| 4:Jb:118:VAL:HG22 | 4:Jb:197:THR:HG22 | 1.97                     | 0.46              |
| 4:Jb:651:SER:HB3  | 4:Jb:695:VAL:HG23 | 1.97                     | 0.46              |
| 6:Tl:64:VAL:HG12  | 6:Tl:64:VAL:O     | 2.16                     | 0.46              |
| 6:Td:61:ILE:HD11  | 6:Td:69:PRO:HB3   | 1.98                     | 0.46              |
| 8:Vf:10:VAL:HG22  | 8:Vf:12:GLY:H     | 1.80                     | 0.46              |
| 4:Jb:782:GLY:H    | 4:Jb:806:ARG:CZ   | 2.29                     | 0.46              |
| 4:Jc:109:ILE:HB   | 4:Jc:171:ASN:HD22 | 1.79                     | 0.46              |
| 4:Jb:494:ARG:NE   | 4:Jb:510:GLU:OE1  | 2.27                     | 0.46              |
| 4:Jb:562:LYS:NZ   | 4:Jb:564:PRO:HB3  | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Md:2:LYS:HD3    | 7:Md:65:HIS:NE2   | 2.30                     | 0.46              |
| 7:Md:49:SER:O     | 7:Md:97:ARG:NH2   | 2.49                     | 0.46              |
| 8:Vb:11:LYS:HD2   | 8:Vb:11:LYS:O     | 2.15                     | 0.46              |
| 8:Vd:100:PHE:HB2  | 8:Vd:124:VAL:HG21 | 1.98                     | 0.46              |
| 8:Ve:109:LYS:HB2  | 8:Ve:119:VAL:HG22 | 1.97                     | 0.46              |
| 2:Ib:219:VAL:HG21 | 4:Jb:152:ASP:O    | 2.16                     | 0.46              |
| 4:Ja:102:ARG:HA   | 4:Ja:102:ARG:HD3  | 1.77                     | 0.46              |
| 4:Ja:367:LYS:HG3  | 4:Ja:481:ILE:HG22 | 1.98                     | 0.46              |
| 4:Jb:138:LEU:HG   | 4:Jb:184:MET:HE3  | 1.96                     | 0.46              |
| 4:Jc:42:LEU:HD23  | 4:Jc:42:LEU:O     | 2.15                     | 0.46              |
| 6:Tc:5:ILE:HD11   | 6:Tc:89:PHE:HE2   | 1.81                     | 0.46              |
| 8:Vc:87:MET:HB2   | 8:Vc:93:GLN:NE2   | 2.31                     | 0.46              |
| 4:Ja:16:ASP:OD2   | 4:Ja:666:ARG:HB3  | 2.15                     | 0.46              |
| 4:Ja:373:ARG:HG3  | 4:Ja:486:TYR:CE2  | 2.46                     | 0.46              |
| 6:Te:60:VAL:HG13  | 6:Te:72:ALA:HB3   | 1.97                     | 0.46              |
| 4:Jc:12:ARG:HB3   | 4:Jc:63:GLY:HA3   | 1.97                     | 0.46              |
| 6:Tg:42:ASN:OD1   | 6:Tg:42:ASN:N     | 2.49                     | 0.46              |
| 7:Md:14:VAL:HG12  | 7:Md:44:TYR:HD1   | 1.81                     | 0.46              |
| 8:Va:66:ASP:HA    | 8:Vb:74:GLN:HE21  | 1.81                     | 0.46              |
| 4:Ja:121:LEU:HD22 | 4:Ja:157:GLY:O    | 2.16                     | 0.45              |
| 4:Jc:102:ARG:HD3  | 4:Jc:102:ARG:HA   | 1.77                     | 0.45              |
| 1:Ha:837:GLU:OE1  | 1:Hc:831:ARG:NH2  | 2.37                     | 0.45              |
| 4:Ja:657:THR:O    | 4:Ja:688:TYR:HB2  | 2.15                     | 0.45              |
| 4:Jb:308:CYS:SG   | 4:Jb:323:ILE:HD11 | 2.57                     | 0.45              |
| 4:Jb:572:ARG:HD3  | 4:Jb:591:HIS:HA   | 1.98                     | 0.45              |
| 4:Jb:620:ALA:HB2  | 4:Jb:703:ASP:HB2  | 1.98                     | 0.45              |
| 5:Lc:73:THR:OG1   | 5:Lc:74:SER:N     | 2.48                     | 0.45              |
| 5:Lc:181:GLU:OE1  | 5:Lc:181:GLU:N    | 2.49                     | 0.45              |
| 6:Te:63:GLN:HE22  | 7:Mc:57:VAL:HG11  | 1.80                     | 0.45              |
| 7:Ma:77:TYR:O     | 7:Ma:78:GLU:HB2   | 2.16                     | 0.45              |
| 7:Md:80:ARG:HB3   | 7:Md:82:ILE:HG23  | 1.98                     | 0.45              |
| 8:Va:67:TRP:CE2   | 8:Vb:145:ARG:HB3  | 2.51                     | 0.45              |
| 4:Ja:373:ARG:HH22 | 7:Mf:27:ASP:CG    | 2.24                     | 0.45              |
| 4:Jb:62:SER:OG    | 4:Jb:63:GLY:N     | 2.43                     | 0.45              |
| 4:Jb:227:PHE:CD2  | 4:Jb:232:VAL:HG11 | 2.52                     | 0.45              |
| 4:Jb:271:ASN:O    | 4:Jb:275:CYS:HB2  | 2.16                     | 0.45              |
| 4:Jb:502:THR:OG1  | 4:Jb:503:ARG:N    | 2.49                     | 0.45              |
| 4:Jb:695:VAL:HB   | 4:Jb:699:GLY:HA2  | 1.98                     | 0.45              |
| 4:Jc:188:SER:HA   | 4:Jc:193:LEU:HD11 | 1.98                     | 0.45              |
| 6:Tg:27:ARG:HD2   | 6:Tg:59:SER:HB2   | 1.97                     | 0.45              |
| 6:Th:42:ASN:OD1   | 6:Th:42:ASN:N     | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Md:9:LYS:HE2    | 7:Md:10:PRO:HD2   | 1.98                     | 0.45              |
| 4:Ja:472:ARG:HH21 | 5:Lc:107:LYS:HE3  | 1.81                     | 0.45              |
| 4:Jc:396:HIS:HA   | 4:Jc:429:ASN:HB2  | 1.98                     | 0.45              |
| 4:Jc:397:ASN:OD1  | 4:Jc:397:ASN:N    | 2.49                     | 0.45              |
| 4:Jc:401:VAL:HA   | 4:Jc:433:MET:O    | 2.16                     | 0.45              |
| 5:Lb:226:SER:OG   | 5:Lb:227:ILE:N    | 2.49                     | 0.45              |
| 6:Tf:45:GLU:N     | 6:Tf:45:GLU:OE1   | 2.48                     | 0.45              |
| 6:Tg:35:VAL:HG13  | 6:Tg:36:ASN:OD1   | 2.17                     | 0.45              |
| 8:Va:31:LEU:O     | 8:Va:111:ARG:NH2  | 2.49                     | 0.45              |
| 8:Vb:10:VAL:HG21  | 8:Vb:113:PRO:HG2  | 1.97                     | 0.45              |
| 8:Vb:36:TRP:H     | 8:Vb:36:TRP:CD1   | 2.34                     | 0.45              |
| 4:Ja:36:GLU:OE2   | 4:Ja:268:TYR:HB2  | 2.17                     | 0.45              |
| 4:Jb:162:GLN:H    | 4:Jb:162:GLN:CD   | 2.21                     | 0.45              |
| 4:Jc:397:ASN:ND2  | 4:Jc:423:ILE:HD13 | 2.31                     | 0.45              |
| 6:Tl:61:ILE:HD12  | 6:Tl:69:PRO:HB3   | 1.99                     | 0.45              |
| 6:Ti:4:LYS:HZ3    | 6:Ti:51:MET:N     | 2.15                     | 0.45              |
| 7:Ma:32:ARG:HB3   | 7:Mb:68:TRP:HB2   | 1.98                     | 0.45              |
| 7:Md:62:LEU:HD23  | 7:Md:62:LEU:HA    | 1.71                     | 0.45              |
| 7:Me:9:LYS:HB3    | 7:Me:9:LYS:HE3    | 1.76                     | 0.45              |
| 4:Ja:395:ARG:HA   | 4:Ja:455:GLU:OE1  | 2.16                     | 0.45              |
| 4:Ja:540:ASP:OD1  | 4:Ja:540:ASP:N    | 2.50                     | 0.45              |
| 4:Ja:815:LEU:HD21 | 4:Jc:821:LYS:HE2  | 1.98                     | 0.45              |
| 4:Jb:42:LEU:HD23  | 4:Jb:42:LEU:O     | 2.16                     | 0.45              |
| 4:Jb:353:ASN:HD21 | 4:Jb:475:PRO:HB2  | 1.80                     | 0.45              |
| 4:Jc:227:PHE:HA   | 4:Jc:672:ARG:HH11 | 1.81                     | 0.45              |
| 1:Hc:836:ASP:O    | 1:Hc:840:THR:HG22 | 2.17                     | 0.45              |
| 4:Jb:601:ASN:C    | 4:Jb:601:ASN:OD1  | 2.59                     | 0.45              |
| 4:Jc:212:TYR:HD2  | 4:Jc:217:LEU:HD22 | 1.82                     | 0.45              |
| 5:Lb:1:MET:HE3    | 5:Lb:2:GLN:H      | 1.80                     | 0.45              |
| 6:Tc:25:LYS:HD2   | 6:Tc:38:VAL:HG12  | 1.99                     | 0.45              |
| 6:Tj:93:MET:SD    | 6:Tj:94:THR:N     | 2.90                     | 0.45              |
| 7:Mb:9:LYS:HG2    | 7:Mb:10:PRO:HD2   | 1.99                     | 0.45              |
| 7:Md:4:PHE:CE1    | 7:Md:6:TRP:HB2    | 2.52                     | 0.45              |
| 8:Vd:10:VAL:HG21  | 8:Vd:113:PRO:HG2  | 1.99                     | 0.45              |
| 8:Vf:10:VAL:HG21  | 8:Vf:113:PRO:HG2  | 1.99                     | 0.45              |
| 4:Jb:332:GLN:OE1  | 5:La:162:VAL:HG21 | 2.16                     | 0.45              |
| 4:Jc:18:LEU:HD12  | 4:Jc:163:TYR:CD1  | 2.52                     | 0.45              |
| 4:Jc:395:ARG:HA   | 4:Jc:455:GLU:OE1  | 2.17                     | 0.45              |
| 4:Jc:458:GLU:HG2  | 4:Jc:592:VAL:HA   | 1.99                     | 0.45              |
| 4:Jc:748:PHE:HE1  | 4:Jc:785:TYR:HB3  | 1.81                     | 0.45              |
| 6:Te:86:LEU:HD12  | 6:Te:90:LEU:HD11  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Tg:67:PHE:CE2   | 7:Md:5:ARG:HG3    | 2.52                     | 0.45              |
| 6:Tg:93:MET:SD    | 6:Tg:94:THR:N     | 2.90                     | 0.45              |
| 6:Th:61:ILE:HD13  | 6:Th:71:HIS:HA    | 1.98                     | 0.45              |
| 8:Vd:10:VAL:HG22  | 8:Vd:12:GLY:H     | 1.82                     | 0.45              |
| 8:Ve:93:GLN:HA    | 8:Ve:96:LEU:HB3   | 1.99                     | 0.45              |
| 3:Ic:198:VAL:HG11 | 4:Ja:328:TYR:CG   | 2.52                     | 0.45              |
| 4:Ja:562:LYS:NZ   | 4:Ja:564:PRO:HB3  | 2.32                     | 0.45              |
| 4:Jb:367:LYS:HB3  | 4:Jb:367:LYS:HE3  | 1.80                     | 0.45              |
| 4:Jb:556:TYR:OH   | 7:Mc:109:ASN:HB2  | 2.17                     | 0.45              |
| 4:Jc:723:THR:HB   | 4:Jc:730:THR:HB   | 1.99                     | 0.45              |
| 6:Tf:66:GLY:HA2   | 7:Mc:79:TRP:CG    | 2.52                     | 0.45              |
| 6:Tj:29:ASN:OD1   | 6:Tj:35:VAL:N     | 2.48                     | 0.45              |
| 7:Mc:25:PHE:HE2   | 7:Mc:31:GLN:H     | 1.64                     | 0.45              |
| 3:Ic:146:MET:HE1  | 4:Ja:576:ILE:HG13 | 1.99                     | 0.44              |
| 4:Ja:1:MET:HB2    | 4:Ja:3:LYS:NZ     | 2.31                     | 0.44              |
| 4:Ja:40:ASP:OD1   | 4:Ja:43:LYS:HD2   | 2.17                     | 0.44              |
| 4:Ja:572:ARG:HD3  | 4:Ja:590:GLN:O    | 2.17                     | 0.44              |
| 4:Jc:203:THR:HG22 | 4:Jc:205:ILE:HG23 | 1.98                     | 0.44              |
| 4:Jc:503:ARG:HG3  | 4:Jc:503:ARG:O    | 2.17                     | 0.44              |
| 4:Jc:527:SER:HB3  | 4:Jc:553:VAL:HG11 | 1.99                     | 0.44              |
| 4:Jc:539:THR:OG1  | 4:Jc:545:LYS:NZ   | 2.49                     | 0.44              |
| 5:Lb:71:LYS:HB2   | 5:Lb:71:LYS:HE3   | 1.72                     | 0.44              |
| 8:Vc:72:GLN:HB2   | 8:Vd:123:TRP:CD2  | 2.51                     | 0.44              |
| 2:Ib:220:VAL:HG13 | 4:Jb:156:LYS:NZ   | 2.31                     | 0.44              |
| 3:Ic:222:GLY:HA3  | 4:Ja:156:LYS:HE2  | 1.99                     | 0.44              |
| 4:Ja:14:ALA:H     | 4:Ja:15:LYS:NZ    | 2.07                     | 0.44              |
| 4:Jc:348:CYS:SG   | 4:Jc:361:GLN:HB3  | 2.57                     | 0.44              |
| 4:Jc:383:ALA:HB2  | 5:Lc:146:VAL:HG13 | 1.98                     | 0.44              |
| 4:Jc:590:GLN:N    | 4:Jc:590:GLN:CD   | 2.75                     | 0.44              |
| 4:Jc:594:GLU:N    | 4:Jc:594:GLU:OE2  | 2.50                     | 0.44              |
| 5:Lb:120:ASN:OD1  | 5:Lb:121:GLY:N    | 2.50                     | 0.44              |
| 5:La:38:PHE:HE1   | 5:La:57:GLN:HE21  | 1.64                     | 0.44              |
| 6:Ta:44:ASP:OD1   | 6:Ta:48:ARG:N     | 2.46                     | 0.44              |
| 7:Ma:53:GLU:HA    | 7:Ma:53:GLU:OE1   | 2.16                     | 0.44              |
| 8:Vc:109:LYS:HB3  | 8:Vc:119:VAL:HG12 | 1.98                     | 0.44              |
| 8:Vf:87:MET:HB2   | 8:Vf:93:GLN:NE2   | 2.32                     | 0.44              |
| 4:Ja:462:VAL:HG13 | 4:Ja:589:VAL:CG2  | 2.48                     | 0.44              |
| 4:Jc:110:ASP:HB2  | 4:Jc:206:ILE:HA   | 1.98                     | 0.44              |
| 4:Jc:541:GLY:O    | 4:Jc:542:VAL:HG12 | 2.18                     | 0.44              |
| 6:Tj:41:GLU:OE1   | 6:Tj:51:MET:HG2   | 2.18                     | 0.44              |
| 7:Md:59:GLU:O     | 7:Md:63:GLU:N     | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Vd:30:PRO:HB2   | 8:Vd:117:VAL:HG21 | 2.00                     | 0.44              |
| 8:Vd:31:LEU:H     | 8:Vd:31:LEU:HD22  | 1.82                     | 0.44              |
| 8:Vf:36:TRP:CD1   | 8:Vf:36:TRP:N     | 2.85                     | 0.44              |
| 3:Ic:217:GLN:HB3  | 4:Ja:152:ASP:OD2  | 2.18                     | 0.44              |
| 4:Jc:30:ILE:HG21  | 4:Jc:238:LEU:HD12 | 1.99                     | 0.44              |
| 5:La:54:ARG:HG2   | 5:La:55:GLN:H     | 1.82                     | 0.44              |
| 5:La:194:ASP:OD1  | 5:La:194:ASP:N    | 2.50                     | 0.44              |
| 6:Tb:35:VAL:HG22  | 6:Tb:36:ASN:OD1   | 2.18                     | 0.44              |
| 6:Td:18:GLN:OE1   | 6:Td:18:GLN:N     | 2.50                     | 0.44              |
| 8:Va:21:LYS:HD3   | 8:Va:35:ASP:O     | 2.18                     | 0.44              |
| 4:Ja:61:ILE:HG22  | 4:Ja:62:SER:H     | 1.81                     | 0.44              |
| 4:Ja:572:ARG:HD3  | 4:Ja:590:GLN:C    | 2.42                     | 0.44              |
| 4:Jb:121:LEU:N    | 4:Jb:159:THR:O    | 2.48                     | 0.44              |
| 4:Jb:367:LYS:HG3  | 4:Jb:481:ILE:HG22 | 2.00                     | 0.44              |
| 4:Jc:687:ASN:HA   | 4:Jc:710:ARG:HA   | 2.00                     | 0.44              |
| 5:Lc:77:PRO:HG2   | 5:Lc:152:LEU:HB2  | 1.99                     | 0.44              |
| 5:La:191:ASP:OD1  | 5:La:195:GLN:N    | 2.40                     | 0.44              |
| 6:Tj:49:TYR:OH    | 6:Tj:86:LEU:N     | 2.36                     | 0.44              |
| 7:Me:25:PHE:CD1   | 7:Me:30:SER:HA    | 2.53                     | 0.44              |
| 8:Ve:36:TRP:CD1   | 8:Ve:36:TRP:N     | 2.85                     | 0.44              |
| 8:Vf:72:GLN:HG2   | 8:Vf:73:GLY:N     | 2.32                     | 0.44              |
| 4:Jb:540:ASP:O    | 4:Jb:544:VAL:HB   | 2.18                     | 0.44              |
| 4:Jb:572:ARG:HB3  | 4:Jb:589:VAL:HG21 | 1.98                     | 0.44              |
| 4:Jc:308:CYS:SG   | 4:Jc:323:ILE:HD11 | 2.58                     | 0.44              |
| 6:Tf:35:VAL:HG13  | 6:Tf:36:ASN:OD1   | 2.18                     | 0.44              |
| 6:Tl:12:GLY:HA3   | 6:Th:58:TYR:HE2   | 1.83                     | 0.44              |
| 6:Ti:15:LYS:NZ    | 6:Ti:18:GLN:OE1   | 2.51                     | 0.44              |
| 6:Ti:35:VAL:HG22  | 6:Ti:36:ASN:OD1   | 2.18                     | 0.44              |
| 6:Tk:13:THR:OG1   | 6:Tk:15:LYS:HD3   | 2.17                     | 0.44              |
| 7:Mb:21:ARG:HB3   | 7:Mb:33:ALA:HB3   | 1.98                     | 0.44              |
| 7:Mf:4:PHE:CE1    | 7:Mf:6:TRP:HB2    | 2.53                     | 0.44              |
| 8:Vc:114:ASN:OD1  | 8:Vc:115:GLY:N    | 2.50                     | 0.44              |
| 2:Ib:192:LEU:HG   | 4:Jb:328:TYR:HD1  | 1.82                     | 0.44              |
| 4:Jb:124:THR:HG23 | 4:Jb:128:GLY:HA2  | 2.00                     | 0.44              |
| 4:Jb:399:VAL:HG23 | 4:Jb:452:ILE:HD11 | 1.99                     | 0.44              |
| 4:Jc:279:MET:HG2  | 5:Lb:163:PHE:CE1  | 2.53                     | 0.44              |
| 4:Jc:485:ASP:N    | 4:Jc:485:ASP:OD1  | 2.48                     | 0.44              |
| 4:Jc:556:TYR:CZ   | 7:Me:109:ASN:HB2  | 2.52                     | 0.44              |
| 5:Lb:60:PRO:HG3   | 7:Mc:25:PHE:CZ    | 2.53                     | 0.44              |
| 5:Lb:167:ILE:HD13 | 5:Lb:167:ILE:HA   | 1.83                     | 0.44              |
| 6:Tb:64:VAL:HB    | 6:Tb:67:PHE:HB2   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Tj:5:ILE:HG22   | 6:Tj:49:TYR:CE1   | 2.46                     | 0.44              |
| 7:Mf:40:ASN:O     | 7:Mf:41:LEU:HD23  | 2.18                     | 0.44              |
| 8:Vd:36:TRP:CE3   | 8:Vd:109:LYS:HG2  | 2.53                     | 0.44              |
| 1:Hb:844:ASP:OD1  | 1:Hb:845:GLY:N    | 2.50                     | 0.44              |
| 4:Jc:61:ILE:HG22  | 4:Jc:62:SER:H     | 1.82                     | 0.44              |
| 4:Jc:112:LEU:HD11 | 4:Jc:202:TYR:HD2  | 1.83                     | 0.44              |
| 7:Ma:40:ASN:C     | 7:Ma:40:ASN:HD22  | 2.16                     | 0.44              |
| 7:Mf:10:PRO:HD3   | 8:Vf:59:TYR:HA    | 2.00                     | 0.44              |
| 8:Va:126:SER:OG   | 8:Va:139:LYS:HG2  | 2.17                     | 0.44              |
| 8:Vc:124:VAL:HG23 | 8:Vc:140:VAL:HG12 | 2.00                     | 0.44              |
| 4:Ja:259:ILE:HD13 | 4:Ja:259:ILE:HA   | 1.87                     | 0.44              |
| 4:Ja:462:VAL:O    | 4:Ja:589:VAL:HG22 | 2.18                     | 0.44              |
| 6:Tb:85:THR:OG1   | 6:Tb:88:ASP:OD2   | 2.13                     | 0.44              |
| 7:Mc:9:LYS:HD2    | 7:Mc:49:SER:HB3   | 2.00                     | 0.44              |
| 3:Ic:158:LYS:HG3  | 3:Ic:159:ALA:H    | 1.83                     | 0.43              |
| 3:Ic:196:MET:HE3  | 3:Ic:196:MET:HB2  | 1.70                     | 0.43              |
| 4:Ja:245:VAL:HG21 | 4:Ja:269:SER:HB2  | 1.99                     | 0.43              |
| 4:Ja:372:ASN:HD22 | 4:Ja:561:LEU:HD11 | 1.82                     | 0.43              |
| 4:Ja:472:ARG:NH2  | 5:Lc:107:LYS:HE3  | 2.33                     | 0.43              |
| 4:Ja:657:THR:OG1  | 4:Ja:665:GLU:HG3  | 2.18                     | 0.43              |
| 4:Jb:101:THR:HG22 | 4:Jb:180:ARG:HG2  | 1.99                     | 0.43              |
| 4:Jb:654:LEU:HD22 | 4:Jb:692:VAL:HG22 | 2.00                     | 0.43              |
| 6:Ti:65:ASP:N     | 6:Ti:65:ASP:OD1   | 2.48                     | 0.43              |
| 4:Jb:61:ILE:HG22  | 4:Jb:62:SER:H     | 1.83                     | 0.43              |
| 5:Lc:229:LYS:HA   | 5:Lc:229:LYS:HE2  | 1.98                     | 0.43              |
| 8:Vd:36:TRP:N     | 8:Vd:36:TRP:CD1   | 2.86                     | 0.43              |
| 4:Jb:578:GLU:HB2  | 4:Jb:586:ILE:HB   | 2.00                     | 0.43              |
| 8:Va:18:TRP:NE1   | 8:Va:111:ARG:HD2  | 2.33                     | 0.43              |
| 8:Va:145:ARG:HG2  | 8:Vf:67:TRP:CE2   | 2.53                     | 0.43              |
| 2:Ib:212:GLU:N    | 2:Ib:212:GLU:OE2  | 2.52                     | 0.43              |
| 2:Ib:221:ILE:HG21 | 4:Jb:18:LEU:HD13  | 2.01                     | 0.43              |
| 8:Vb:36:TRP:CD1   | 8:Vb:36:TRP:N     | 2.86                     | 0.43              |
| 8:Vb:61:ASP:OD2   | 8:Vb:61:ASP:C     | 2.61                     | 0.43              |
| 8:Vd:67:TRP:HA    | 8:Ve:75:LYS:O     | 2.19                     | 0.43              |
| 4:Ja:320:GLU:HG3  | 4:Ja:321:PRO:O    | 2.18                     | 0.43              |
| 4:Ja:542:VAL:HG23 | 4:Ja:543:LYS:H    | 1.83                     | 0.43              |
| 4:Jb:181:MET:HE1  | 4:Jb:199:TRP:CE3  | 2.53                     | 0.43              |
| 4:Jb:463:ASP:OD1  | 4:Jb:463:ASP:C    | 2.61                     | 0.43              |
| 4:Jc:387:TYR:CD2  | 4:Jc:462:VAL:HB   | 2.53                     | 0.43              |
| 5:Lb:230:LEU:HD23 | 5:Lb:230:LEU:HA   | 1.81                     | 0.43              |
| 5:La:37:PHE:CE2   | 5:La:54:ARG:HD3   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Ma:25:PHE:HB2   | 7:Ma:28:GLY:O     | 2.18                     | 0.43              |
| 8:Va:36:TRP:CZ3   | 8:Va:109:LYS:HG2  | 2.53                     | 0.43              |
| 8:Vd:59:TYR:HB2   | 8:Vd:62:ASP:OD2   | 2.18                     | 0.43              |
| 8:Vf:109:LYS:HB3  | 8:Vf:119:VAL:HG12 | 1.99                     | 0.43              |
| 4:Ja:193:LEU:HD13 | 4:Ja:193:LEU:HA   | 1.91                     | 0.43              |
| 4:Ja:595:LYS:HE2  | 4:Ja:595:LYS:HB2  | 1.84                     | 0.43              |
| 4:Ja:817:PHE:CE1  | 4:Jb:781:PRO:HG2  | 2.54                     | 0.43              |
| 4:Jb:494:ARG:HE   | 4:Jb:510:GLU:CD   | 2.21                     | 0.43              |
| 4:Jb:577:ARG:HG2  | 4:Jb:578:GLU:N    | 2.34                     | 0.43              |
| 4:Jc:369:TRP:O    | 4:Jc:480:GLU:HB2  | 2.18                     | 0.43              |
| 5:Lc:25:GLU:OE1   | 5:Lc:106:ARG:NH2  | 2.39                     | 0.43              |
| 5:La:40:ASN:OD1   | 7:Ma:25:PHE:HB3   | 2.18                     | 0.43              |
| 6:Tk:78:TYR:HB3   | 6:Tk:80:ASP:OD1   | 2.19                     | 0.43              |
| 1:Ha:844:ASP:C    | 1:Ha:844:ASP:OD1  | 2.61                     | 0.43              |
| 4:Jb:529:ASN:N    | 4:Jb:530:PRO:HD3  | 2.34                     | 0.43              |
| 4:Jc:393:LYS:HE3  | 5:Lc:159:ASP:HB3  | 2.01                     | 0.43              |
| 7:Me:88:LYS:HE3   | 7:Me:88:LYS:HB3   | 1.76                     | 0.43              |
| 8:Vc:36:TRP:CD1   | 8:Vc:36:TRP:N     | 2.87                     | 0.43              |
| 2:Ib:188:VAL:CG1  | 5:La:164:PRO:HB2  | 2.49                     | 0.43              |
| 4:Ja:141:ILE:O    | 4:Ja:143:ARG:NH2  | 2.30                     | 0.43              |
| 4:Jb:56:GLU:OE1   | 4:Jb:56:GLU:N     | 2.51                     | 0.43              |
| 4:Jb:199:TRP:HZ2  | 4:Jb:202:TYR:CD1  | 2.36                     | 0.43              |
| 4:Jc:355:GLN:HB2  | 5:Lb:134:ARG:HG2  | 2.01                     | 0.43              |
| 4:Jc:472:ARG:HA   | 4:Jc:472:ARG:NE   | 2.33                     | 0.43              |
| 4:Jc:572:ARG:HD2  | 4:Jc:589:VAL:HG23 | 2.00                     | 0.43              |
| 6:Td:65:ASP:OD1   | 6:Td:65:ASP:N     | 2.50                     | 0.43              |
| 7:Ma:94:SER:O     | 7:Mf:10:PRO:HB3   | 2.19                     | 0.43              |
| 4:Ja:406:PRO:HB3  | 4:Ja:410:TRP:CH2  | 2.54                     | 0.43              |
| 4:Jc:433:MET:O    | 4:Jc:433:MET:HG3  | 2.19                     | 0.43              |
| 4:Jc:481:ILE:HG13 | 4:Jc:570:LEU:O    | 2.19                     | 0.43              |
| 4:Jc:727:PHE:CE1  | 4:Jc:781:PRO:HD3  | 2.53                     | 0.43              |
| 6:Td:68:PRO:HD3   | 7:Mb:77:TYR:HD1   | 1.84                     | 0.43              |
| 6:Tk:18:GLN:OE1   | 6:Tk:18:GLN:N     | 2.52                     | 0.43              |
| 8:Vd:42:VAL:HG22  | 8:Vd:84:LEU:HD22  | 1.99                     | 0.43              |
| 2:Ia:165:GLN:NE2  | 2:Ib:166:THR:OG1  | 2.51                     | 0.43              |
| 1:Hb:843:ARG:NH1  | 5:Lb:76:ARG:HD2   | 2.34                     | 0.43              |
| 4:Ja:810:ASP:N    | 4:Ja:810:ASP:OD1  | 2.51                     | 0.43              |
| 4:Jb:50:THR:HG21  | 4:Jb:701:GLN:HG2  | 2.01                     | 0.43              |
| 4:Jb:595:LYS:HE2  | 4:Jb:595:LYS:HB2  | 1.85                     | 0.43              |
| 4:Jb:623:HIS:NE2  | 4:Jc:164:LEU:HD12 | 2.34                     | 0.43              |
| 4:Jb:806:ARG:NH1  | 4:Jb:807:ALA:H    | 2.16                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Jc:646:VAL:HG22 | 4:Jc:650:VAL:HG11 | 2.00                     | 0.43              |
| 6:Tb:62:LEU:HD23  | 6:Tb:62:LEU:HA    | 1.84                     | 0.43              |
| 6:Tf:20:CYS:SG    | 6:Tf:21:THR:N     | 2.92                     | 0.43              |
| 6:Th:62:LEU:HD23  | 6:Th:62:LEU:HA    | 1.78                     | 0.43              |
| 8:Vb:7:THR:C      | 8:Vc:87:MET:HE1   | 2.44                     | 0.43              |
| 8:Vd:36:TRP:CZ3   | 8:Vd:109:LYS:HG2  | 2.54                     | 0.43              |
| 8:Ve:112:PHE:C    | 8:Ve:114:ASN:N    | 2.70                     | 0.43              |
| 8:Vf:18:TRP:CE2   | 8:Vf:38:ARG:HG3   | 2.54                     | 0.43              |
| 2:Ia:188:VAL:CG1  | 5:Lb:164:PRO:HB2  | 2.48                     | 0.42              |
| 4:Ja:52:VAL:HG12  | 4:Ja:61:ILE:HG13  | 2.01                     | 0.42              |
| 4:Ja:98:THR:O     | 4:Ja:98:THR:OG1   | 2.34                     | 0.42              |
| 4:Ja:520:LEU:HD12 | 4:Ja:562:LYS:HE2  | 2.01                     | 0.42              |
| 4:Jb:111:ARG:HG2  | 4:Jb:170:GLY:HA2  | 2.01                     | 0.42              |
| 4:Jc:18:LEU:HD12  | 4:Jc:163:TYR:CG   | 2.54                     | 0.42              |
| 4:Jc:227:PHE:CD2  | 4:Jc:232:VAL:HG11 | 2.54                     | 0.42              |
| 4:Jc:693:ARG:HD2  | 4:Jc:701:GLN:HB3  | 2.01                     | 0.42              |
| 2:Ib:160:ARG:HD3  | 2:Ib:160:ARG:HA   | 1.69                     | 0.42              |
| 4:Ja:36:GLU:HB3   | 4:Ja:239:ARG:HB2  | 2.01                     | 0.42              |
| 4:Ja:227:PHE:CD2  | 4:Ja:232:VAL:HG11 | 2.53                     | 0.42              |
| 4:Ja:315:GLY:HA2  | 4:Ja:605:PHE:H    | 1.83                     | 0.42              |
| 4:Ja:746:PHE:CE2  | 4:Ja:772:TRP:HB2  | 2.53                     | 0.42              |
| 4:Jc:556:TYR:OH   | 7:Me:109:ASN:HB2  | 2.19                     | 0.42              |
| 6:Tc:25:LYS:HZ1   | 6:Tc:36:ASN:HA    | 1.83                     | 0.42              |
| 6:Tf:24:LEU:HB3   | 6:Tf:58:TYR:HD2   | 1.84                     | 0.42              |
| 6:Th:44:ASP:OD1   | 6:Th:48:ARG:N     | 2.52                     | 0.42              |
| 6:Tj:23:GLN:HB2   | 6:Tj:61:ILE:HB    | 2.00                     | 0.42              |
| 6:Tj:35:VAL:HG22  | 6:Tj:36:ASN:OD1   | 2.20                     | 0.42              |
| 7:Md:7:LYS:HD2    | 8:Vd:61:ASP:OD1   | 2.19                     | 0.42              |
| 8:Va:3:VAL:HA     | 8:Va:4:PRO:HD3    | 1.90                     | 0.42              |
| 8:Ve:89:GLY:O     | 8:Ve:94:GLN:NE2   | 2.52                     | 0.42              |
| 8:Vf:18:TRP:HB2   | 8:Vf:109:LYS:HG3  | 1.99                     | 0.42              |
| 3:Ic:151:VAL:O    | 3:Ic:154:MET:HG2  | 2.20                     | 0.42              |
| 4:Ja:583:THR:HG21 | 7:Mf:21:ARG:NH1   | 2.34                     | 0.42              |
| 4:Ja:594:GLU:OE2  | 4:Ja:594:GLU:N    | 2.52                     | 0.42              |
| 4:Jb:116:PHE:CZ   | 4:Jb:153:ILE:HG21 | 2.54                     | 0.42              |
| 4:Jb:125:THR:OG1  | 4:Jb:129:ASP:OD1  | 2.19                     | 0.42              |
| 4:Jb:454:THR:HG23 | 4:Jb:458:GLU:OE2  | 2.19                     | 0.42              |
| 4:Jb:719:ARG:HG2  | 4:Jb:734:HIS:HB2  | 2.01                     | 0.42              |
| 4:Jc:572:ARG:HH11 | 4:Jc:572:ARG:HG2  | 1.83                     | 0.42              |
| 8:Vd:124:VAL:HG12 | 8:Vd:140:VAL:HG12 | 2.00                     | 0.42              |
| 3:Ic:190:PRO:O    | 4:Ja:31:SER:HA    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:175:ARG:NE   | 4:Ja:176:PRO:O    | 2.53                     | 0.42              |
| 4:Ja:479:ILE:HD12 | 4:Ja:572:ARG:O    | 2.20                     | 0.42              |
| 4:Jb:539:THR:O    | 4:Jb:539:THR:OG1  | 2.34                     | 0.42              |
| 4:Jb:780:LYS:HB3  | 4:Jb:780:LYS:HE3  | 1.86                     | 0.42              |
| 4:Jc:494:ARG:NH1  | 7:Md:27:ASP:OD2   | 2.51                     | 0.42              |
| 5:Lc:163:PHE:HB3  | 5:Lc:164:PRO:HD3  | 2.00                     | 0.42              |
| 7:Ma:108:VAL:CG1  | 7:Mf:28:GLY:HA3   | 2.48                     | 0.42              |
| 7:Ma:109:ASN:ND2  | 7:Ma:109:ASN:H    | 2.18                     | 0.42              |
| 8:Vd:56:ASP:OD1   | 8:Vd:57:ASP:N     | 2.53                     | 0.42              |
| 8:Ve:21:LYS:HD3   | 8:Ve:35:ASP:O     | 2.19                     | 0.42              |
| 3:Ic:219:VAL:HG21 | 4:Ja:152:ASP:O    | 2.20                     | 0.42              |
| 4:Ja:26:VAL:HG21  | 4:Ja:234:ARG:NH2  | 2.35                     | 0.42              |
| 4:Ja:372:ASN:HA   | 4:Ja:483:ASP:O    | 2.19                     | 0.42              |
| 4:Ja:387:TYR:CD1  | 4:Ja:462:VAL:HB   | 2.55                     | 0.42              |
| 4:Jb:109:ILE:HD12 | 4:Jb:171:ASN:ND2  | 2.35                     | 0.42              |
| 4:Jb:203:THR:HG22 | 4:Jb:205:ILE:HG23 | 2.01                     | 0.42              |
| 4:Jb:536:GLN:NE2  | 4:Jb:546:VAL:O    | 2.51                     | 0.42              |
| 4:Jc:322:ARG:NH2  | 4:Jc:601:ASN:HD21 | 2.18                     | 0.42              |
| 4:Jc:508:ASP:HB2  | 4:Jc:543:LYS:NZ   | 2.34                     | 0.42              |
| 6:Ti:44:ASP:OD1   | 6:Ti:48:ARG:N     | 2.50                     | 0.42              |
| 4:Ja:556:TYR:OH   | 7:Ma:109:ASN:HB2  | 2.19                     | 0.42              |
| 4:Jc:137:LEU:O    | 4:Jc:138:LEU:HD23 | 2.20                     | 0.42              |
| 4:Jc:227:PHE:HA   | 4:Jc:672:ARG:NH1  | 2.34                     | 0.42              |
| 6:Ti:5:ILE:HD13   | 6:Ti:5:ILE:HA     | 1.82                     | 0.42              |
| 8:Ve:17:LEU:HD12  | 8:Ve:18:TRP:N     | 2.34                     | 0.42              |
| 2:Ib:198:VAL:HG21 | 4:Jb:328:TYR:CD2  | 2.54                     | 0.42              |
| 2:Ib:207:ILE:HD13 | 4:Ja:648:LYS:O    | 2.20                     | 0.42              |
| 4:Ja:272:MET:SD   | 4:Ja:325:CYS:HB2  | 2.60                     | 0.42              |
| 4:Jb:572:ARG:HG2  | 4:Jb:572:ARG:HH11 | 1.84                     | 0.42              |
| 4:Jb:781:PRO:HA   | 4:Jb:806:ARG:HH12 | 1.85                     | 0.42              |
| 4:Jc:254:ARG:NH2  | 4:Jc:270:ASN:OD1  | 2.53                     | 0.42              |
| 4:Jc:367:LYS:HE3  | 4:Jc:367:LYS:HB3  | 1.83                     | 0.42              |
| 4:Jc:577:ARG:HH21 | 5:Lb:68:LEU:HG    | 1.85                     | 0.42              |
| 5:La:177:TYR:CD2  | 5:La:205:CYS:HB2  | 2.54                     | 0.42              |
| 6:Ta:24:LEU:O     | 6:Ta:38:VAL:HA    | 2.20                     | 0.42              |
| 6:Tb:27:ARG:NH1   | 6:Tb:74:THR:OG1   | 2.53                     | 0.42              |
| 6:Tf:68:PRO:HD3   | 7:Mc:77:TYR:CD1   | 2.54                     | 0.42              |
| 6:Tg:65:ASP:OD1   | 6:Tg:65:ASP:O     | 2.38                     | 0.42              |
| 7:Md:10:PRO:HA    | 8:Vd:60:LEU:HD11  | 2.01                     | 0.42              |
| 7:Me:22:LYS:HD3   | 7:Me:22:LYS:HA    | 1.86                     | 0.42              |
| 2:Ia:147:VAL:HG22 | 2:Ia:154:MET:HE1  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:578:GLU:HG2  | 5:Lc:67:GLU:OE1   | 2.19                     | 0.42              |
| 4:Ja:714:PRO:O    | 4:Ja:798:SER:HB3  | 2.20                     | 0.42              |
| 4:Jc:647:VAL:HG12 | 4:Jc:648:LYS:HG2  | 2.02                     | 0.42              |
| 6:Tc:9:LEU:HD11   | 6:Tc:20:CYS:SG    | 2.60                     | 0.42              |
| 6:Th:41:GLU:C     | 6:Th:41:GLU:OE1   | 2.63                     | 0.42              |
| 8:Va:33:ASP:OD1   | 8:Va:33:ASP:N     | 2.53                     | 0.42              |
| 8:Vb:6:PRO:O      | 8:Vb:7:THR:OG1    | 2.31                     | 0.42              |
| 1:Ha:841:GLN:NE2  | 1:Ha:847:LEU:HD22 | 2.35                     | 0.42              |
| 3:Ic:165:GLN:N    | 3:Ic:165:GLN:OE1  | 2.53                     | 0.42              |
| 4:Ja:576:ILE:HG23 | 5:Lc:69:ASN:OD1   | 2.20                     | 0.42              |
| 4:Jb:381:ASP:OD1  | 4:Jb:381:ASP:N    | 2.36                     | 0.42              |
| 4:Jc:529:ASN:N    | 4:Jc:530:PRO:HD3  | 2.35                     | 0.42              |
| 7:Mb:7:LYS:HB2    | 7:Mb:7:LYS:HE2    | 1.78                     | 0.42              |
| 8:Vb:126:SER:HB3  | 8:Vb:139:LYS:HB3  | 2.01                     | 0.42              |
| 8:Vf:129:LYS:HE2  | 8:Vf:129:LYS:HB3  | 1.73                     | 0.42              |
| 4:Ja:115:THR:HG22 | 4:Ja:166:SER:HB3  | 2.02                     | 0.41              |
| 4:Ja:529:ASN:N    | 4:Ja:530:PRO:HD3  | 2.35                     | 0.41              |
| 4:Ja:698:TRP:CZ3  | 5:La:232:GLN:HA   | 2.55                     | 0.41              |
| 4:Jb:830:GLU:H    | 4:Jb:830:GLU:CD   | 2.28                     | 0.41              |
| 6:Tb:55:TYR:HA    | 6:Tb:77:VAL:HG13  | 2.01                     | 0.41              |
| 6:Td:62:LEU:HD12  | 6:Te:34:VAL:HG11  | 2.02                     | 0.41              |
| 6:Te:20:CYS:SG    | 6:Te:21:THR:N     | 2.93                     | 0.41              |
| 6:Ti:23:GLN:C     | 6:Ti:24:LEU:HD12  | 2.44                     | 0.41              |
| 4:Ja:213:PRO:HG2  | 5:Lc:175:TRP:CZ2  | 2.56                     | 0.41              |
| 4:Jb:109:ILE:HD12 | 4:Jb:171:ASN:HD21 | 1.86                     | 0.41              |
| 4:Jb:495:VAL:HA   | 4:Jb:559:TRP:HA   | 2.01                     | 0.41              |
| 4:Jc:104:ILE:O    | 4:Jc:176:PRO:HB3  | 2.19                     | 0.41              |
| 4:Jc:784:ASP:OD1  | 4:Jc:806:ARG:NH1  | 2.50                     | 0.41              |
| 6:Ta:65:ASP:N     | 6:Ta:65:ASP:OD1   | 2.51                     | 0.41              |
| 7:Md:54:GLU:N     | 7:Md:54:GLU:OE2   | 2.53                     | 0.41              |
| 7:Md:91:SER:HB3   | 7:Md:100:PHE:CE1  | 2.56                     | 0.41              |
| 7:Mf:22:LYS:HB3   | 7:Mf:22:LYS:HE3   | 1.77                     | 0.41              |
| 8:Ve:3:VAL:HA     | 8:Ve:4:PRO:HD3    | 1.88                     | 0.41              |
| 1:Ha:827:TYR:HB2  | 1:Hb:829:MET:HE2  | 2.01                     | 0.41              |
| 4:Ja:475:PRO:HG3  | 5:Lc:1:MET:CA     | 2.49                     | 0.41              |
| 4:Jc:819:LYS:HA   | 4:Jc:819:LYS:HD3  | 1.80                     | 0.41              |
| 5:Lc:38:PHE:HE1   | 5:Lc:57:GLN:HE21  | 1.68                     | 0.41              |
| 6:Te:44:ASP:OD1   | 6:Te:48:ARG:N     | 2.51                     | 0.41              |
| 6:Tl:23:GLN:HB2   | 6:Tl:61:ILE:HB    | 2.02                     | 0.41              |
| 7:Mf:62:LEU:HD23  | 7:Mf:62:LEU:HA    | 1.89                     | 0.41              |
| 8:Vc:7:THR:C      | 8:Vc:8:MET:HE2    | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Vf:41:LYS:HA    | 8:Vf:41:LYS:HD2   | 1.70                     | 0.41              |
| 1:Ha:847:LEU:HD12 | 1:Hc:842:MET:HE1  | 2.03                     | 0.41              |
| 4:Ja:369:TRP:HD1  | 4:Ja:371:TYR:CE1  | 2.39                     | 0.41              |
| 4:Ja:823:THR:H    | 4:Ja:826:HIS:HE1  | 1.68                     | 0.41              |
| 4:Jb:739:ASP:N    | 4:Jb:739:ASP:OD1  | 2.52                     | 0.41              |
| 4:Jc:89:VAL:HB    | 4:Jc:201:SER:HB3  | 2.03                     | 0.41              |
| 4:Jc:478:VAL:H    | 4:Jc:574:VAL:CG1  | 2.33                     | 0.41              |
| 4:Jc:605:PHE:O    | 4:Jc:607:GLY:N    | 2.53                     | 0.41              |
| 6:Td:61:ILE:HD11  | 6:Td:69:PRO:CB    | 2.50                     | 0.41              |
| 7:Mc:23:VAL:HG13  | 7:Mc:25:PHE:HZ    | 1.85                     | 0.41              |
| 2:Ib:176:PHE:HB3  | 4:Jb:327:ALA:HA   | 2.02                     | 0.41              |
| 4:Ja:115:THR:OG1  | 4:Ja:201:SER:O    | 2.21                     | 0.41              |
| 4:Ja:308:CYS:SG   | 4:Ja:323:ILE:HD11 | 2.60                     | 0.41              |
| 4:Jb:92:THR:HG23  | 4:Jb:199:TRP:HB3  | 2.02                     | 0.41              |
| 4:Jb:276:LEU:HD22 | 4:Jb:346:MET:HE1  | 2.01                     | 0.41              |
| 6:Tc:61:ILE:HG23  | 6:Tc:69:PRO:HB3   | 2.01                     | 0.41              |
| 6:Td:67:PHE:CD2   | 6:Td:68:PRO:HD2   | 2.55                     | 0.41              |
| 6:Te:67:PHE:HE1   | 7:Mc:5:ARG:HG3    | 1.84                     | 0.41              |
| 6:Tf:68:PRO:HD3   | 7:Mc:77:TYR:HD1   | 1.86                     | 0.41              |
| 8:Vb:16:THR:OG1   | 8:Vb:18:TRP:NE1   | 2.51                     | 0.41              |
| 4:Ja:495:VAL:O    | 4:Ja:509:ARG:HG2  | 2.20                     | 0.41              |
| 4:Jb:453:LYS:HE2  | 4:Jb:599:VAL:HG11 | 2.03                     | 0.41              |
| 6:Tb:12:GLY:HA3   | 6:Tc:58:TYR:HE2   | 1.86                     | 0.41              |
| 7:Md:84:VAL:HG23  | 7:Md:105:GLU:O    | 2.20                     | 0.41              |
| 7:Md:88:LYS:HE3   | 7:Md:88:LYS:HB3   | 1.78                     | 0.41              |
| 7:Me:9:LYS:HD2    | 7:Me:49:SER:HB3   | 2.01                     | 0.41              |
| 8:Va:43:LYS:N     | 8:Va:83:THR:O     | 2.48                     | 0.41              |
| 8:Vc:66:ASP:OD2   | 8:Vd:75:LYS:NZ    | 2.52                     | 0.41              |
| 8:Vd:91:GLN:OE1   | 8:Vd:91:GLN:HA    | 2.20                     | 0.41              |
| 8:Ve:46:THR:O     | 8:Ve:46:THR:OG1   | 2.39                     | 0.41              |
| 1:Ha:830:ALA:HB1  | 1:Hb:830:ALA:HA   | 2.03                     | 0.41              |
| 3:Ic:221:ILE:HD12 | 4:Ja:154:THR:O    | 2.21                     | 0.41              |
| 4:Ja:138:LEU:HG   | 4:Ja:184:MET:SD   | 2.60                     | 0.41              |
| 4:Ja:276:LEU:O    | 4:Ja:276:LEU:HD12 | 2.20                     | 0.41              |
| 4:Ja:819:LYS:HE2  | 4:Ja:819:LYS:HB2  | 1.89                     | 0.41              |
| 4:Ja:830:GLU:HA   | 4:Ja:833:GLU:HG3  | 2.01                     | 0.41              |
| 4:Jb:756:ILE:O    | 4:Jb:759:VAL:HG13 | 2.21                     | 0.41              |
| 4:Jc:495:VAL:HB   | 4:Jc:509:ARG:CZ   | 2.51                     | 0.41              |
| 4:Jc:595:LYS:HE2  | 4:Jc:595:LYS:HB2  | 1.85                     | 0.41              |
| 5:Lc:190:ALA:HB3  | 5:Lc:215:ARG:NH2  | 2.36                     | 0.41              |
| 5:La:199:ASP:OD2  | 5:La:201:THR:HG23 | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Tf:49:TYR:OH    | 6:Tf:85:THR:OG1   | 2.33                     | 0.41              |
| 6:Th:5:ILE:HG22   | 6:Th:49:TYR:HE2   | 1.86                     | 0.41              |
| 8:Vc:83:THR:HG22  | 8:Vc:137:THR:HB   | 2.02                     | 0.41              |
| 8:Vd:6:PRO:O      | 8:Vd:7:THR:OG1    | 2.31                     | 0.41              |
| 8:Ve:109:LYS:HG3  | 8:Ve:117:VAL:HG23 | 2.01                     | 0.41              |
| 8:Vf:5:ASN:OD1    | 8:Vf:5:ASN:C      | 2.62                     | 0.41              |
| 2:Ia:180:ASP:OD1  | 2:Ia:180:ASP:C    | 2.64                     | 0.41              |
| 2:Ib:211:ASP:O    | 4:Jb:12:ARG:NH1   | 2.53                     | 0.41              |
| 1:Hc:818:ILE:HG13 | 1:Hc:821:ALA:HB3  | 2.02                     | 0.41              |
| 3:Jc:207:ILE:HD12 | 4:Jc:646:VAL:HG11 | 2.03                     | 0.41              |
| 4:Ja:211:CYS:SG   | 4:Ja:212:TYR:N    | 2.93                     | 0.41              |
| 4:Jb:122:VAL:HG23 | 4:Jb:194:GLN:NE2  | 2.36                     | 0.41              |
| 4:Jb:246:PRO:HG2  | 4:Jb:249:TYR:HB2  | 2.03                     | 0.41              |
| 4:Jb:476:GLY:O    | 4:Jb:478:VAL:HG13 | 2.20                     | 0.41              |
| 4:Jc:181:MET:SD   | 4:Jc:199:TRP:CD1  | 3.14                     | 0.41              |
| 4:Jc:249:TYR:HD1  | 4:Jc:256:TYR:CE2  | 2.39                     | 0.41              |
| 4:Jc:477:ASP:H    | 4:Jc:574:VAL:HG13 | 1.85                     | 0.41              |
| 4:Jc:696:ASN:HD21 | 4:Jc:700:GLN:HB3  | 1.86                     | 0.41              |
| 5:Lc:24:TRP:CD1   | 5:Lc:61:ILE:HG21  | 2.56                     | 0.41              |
| 7:Ma:14:VAL:HG12  | 7:Ma:14:VAL:O     | 2.21                     | 0.41              |
| 8:Va:33:ASP:OD1   | 8:Va:111:ARG:NH2  | 2.45                     | 0.41              |
| 2:Ia:197:ARG:HA   | 4:Jc:236:TYR:O    | 2.21                     | 0.41              |
| 4:Ja:164:LEU:HD12 | 4:Jc:623:HIS:CE1  | 2.56                     | 0.41              |
| 4:Ja:471:LEU:HD13 | 4:Ja:585:ALA:CB   | 2.49                     | 0.41              |
| 4:Ja:813:GLY:HA3  | 4:Jb:777:ILE:HD11 | 2.03                     | 0.41              |
| 4:Jb:369:TRP:O    | 4:Jb:480:GLU:HB2  | 2.21                     | 0.41              |
| 4:Jb:472:ARG:HD2  | 5:La:107:LYS:HE3  | 2.02                     | 0.41              |
| 4:Jc:14:ALA:H     | 4:Jc:15:LYS:HZ3   | 1.68                     | 0.41              |
| 4:Jc:54:ASP:OD2   | 4:Jc:54:ASP:N     | 2.39                     | 0.41              |
| 4:Jc:418:GLU:OE1  | 4:Jc:428:ARG:NH2  | 2.53                     | 0.41              |
| 4:Jc:541:GLY:C    | 4:Jc:543:LYS:N    | 2.79                     | 0.41              |
| 4:Jc:758:GLN:OE1  | 4:Jc:762:SER:OG   | 2.39                     | 0.41              |
| 5:Lb:11:GLU:HG2   | 5:Lb:14:ARG:HH21  | 1.86                     | 0.41              |
| 5:La:11:GLU:HG3   | 5:La:111:ARG:HD3  | 2.02                     | 0.41              |
| 5:La:156:THR:O    | 5:La:156:THR:OG1  | 2.36                     | 0.41              |
| 6:Ta:88:ASP:HA    | 6:Ta:91:CYS:SG    | 2.60                     | 0.41              |
| 6:Tc:71:HIS:CE1   | 8:Va:63:GLU:HB2   | 2.56                     | 0.41              |
| 7:Me:32:ARG:NH1   | 7:Mf:85:THR:HG21  | 2.35                     | 0.41              |
| 8:Vc:43:LYS:H     | 8:Vc:84:LEU:HA    | 1.86                     | 0.41              |
| 2:Ia:151:VAL:HG13 | 4:Jc:455:GLU:HG2  | 2.03                     | 0.41              |
| 1:Hc:823:LEU:HD13 | 1:Hc:823:LEU:HA   | 1.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Ja:50:THR:HG21  | 4:Ja:701:GLN:HG2  | 2.03                     | 0.41              |
| 4:Jb:636:GLN:OE1  | 4:Jb:636:GLN:HA   | 2.19                     | 0.41              |
| 4:Jc:26:VAL:HG13  | 4:Jc:220:VAL:HG13 | 2.02                     | 0.41              |
| 4:Jc:200:SER:OG   | 4:Jc:201:SER:N    | 2.53                     | 0.41              |
| 5:La:163:PHE:HB3  | 5:La:164:PRO:HD3  | 2.02                     | 0.41              |
| 7:Ma:70:SER:HA    | 7:Ma:85:THR:HG22  | 2.02                     | 0.41              |
| 7:Mf:54:GLU:H     | 7:Mf:54:GLU:CD    | 2.29                     | 0.41              |
| 8:Vf:97:LEU:HD12  | 8:Vf:97:LEU:HA    | 1.85                     | 0.41              |
| 4:Ja:195:ASN:OD1  | 4:Ja:195:ASN:N    | 2.54                     | 0.40              |
| 4:Ja:247:SER:HG   | 4:Ja:263:THR:HG1  | 1.69                     | 0.40              |
| 4:Ja:823:THR:H    | 4:Ja:826:HIS:CE1  | 2.39                     | 0.40              |
| 5:Lb:24:TRP:CD1   | 5:Lb:61:ILE:HG21  | 2.56                     | 0.40              |
| 6:Tb:86:LEU:O     | 6:Tb:90:LEU:HD12  | 2.21                     | 0.40              |
| 6:Tg:8:VAL:HG22   | 6:Tg:48:ARG:HG3   | 2.03                     | 0.40              |
| 6:Tj:87:ASN:ND2   | 6:Tk:30:SER:O     | 2.54                     | 0.40              |
| 8:Vb:91:GLN:HA    | 8:Vb:91:GLN:OE1   | 2.21                     | 0.40              |
| 8:Vc:43:LYS:N     | 8:Vc:83:THR:O     | 2.52                     | 0.40              |
| 8:Ve:110:ILE:HG13 | 8:Ve:118:ASP:HB3  | 2.03                     | 0.40              |
| 1:Ha:831:ARG:NH2  | 1:Hb:836:ASP:HB3  | 2.36                     | 0.40              |
| 2:Ia:153:GLN:C    | 2:Ia:153:GLN:OE1  | 2.64                     | 0.40              |
| 4:Ja:32:GLU:OE2   | 5:Lc:166:ARG:HD3  | 2.22                     | 0.40              |
| 4:Ja:111:ARG:HB2  | 4:Ja:205:ILE:CD1  | 2.51                     | 0.40              |
| 4:Ja:525:ASP:OD2  | 4:Ja:525:ASP:C    | 2.64                     | 0.40              |
| 4:Ja:834:LYS:HA   | 4:Ja:834:LYS:HE2  | 2.04                     | 0.40              |
| 4:Jb:360:VAL:HG11 | 4:Jb:477:ASP:CB   | 2.50                     | 0.40              |
| 4:Jb:601:ASN:OD1  | 4:Jb:602:GLY:N    | 2.54                     | 0.40              |
| 4:Jb:649:GLY:O    | 4:Jb:696:ASN:HA   | 2.20                     | 0.40              |
| 4:Jc:16:ASP:O     | 4:Jc:17:ASN:HB3   | 2.20                     | 0.40              |
| 4:Jc:582:GLY:HA3  | 4:Jc:584:TYR:CE1  | 2.56                     | 0.40              |
| 6:Tj:11:ASP:OD1   | 6:Tj:15:LYS:N     | 2.38                     | 0.40              |
| 6:Tk:11:ASP:OD1   | 6:Tk:13:THR:OG1   | 2.34                     | 0.40              |
| 7:Me:13:ASP:OD1   | 7:Me:14:VAL:N     | 2.54                     | 0.40              |
| 7:Me:25:PHE:HE1   | 7:Me:31:GLN:H     | 1.68                     | 0.40              |
| 8:Vc:6:PRO:O      | 8:Vc:7:THR:OG1    | 2.32                     | 0.40              |
| 8:Vf:3:VAL:HA     | 8:Vf:4:PRO:HD3    | 1.88                     | 0.40              |
| 1:Hb:837:GLU:HA   | 1:Hb:840:THR:HG22 | 2.02                     | 0.40              |
| 4:Ja:472:ARG:HH12 | 4:Ja:579:ASN:ND2  | 2.08                     | 0.40              |
| 4:Ja:650:VAL:HA   | 4:Ja:695:VAL:O    | 2.21                     | 0.40              |
| 4:Jb:320:GLU:HG3  | 4:Jb:321:PRO:O    | 2.21                     | 0.40              |
| 4:Jc:259:ILE:HD13 | 4:Jc:259:ILE:HA   | 1.87                     | 0.40              |
| 4:Jc:393:LYS:HB2  | 4:Jc:393:LYS:HE2  | 1.77                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Jc:669:SER:OG   | 4:Jc:670:THR:N    | 2.53                     | 0.40              |
| 5:La:24:TRP:CD1   | 5:La:61:ILE:HG21  | 2.56                     | 0.40              |
| 6:Tc:61:ILE:HD13  | 6:Tc:69:PRO:HB3   | 2.02                     | 0.40              |
| 6:Tg:29:ASN:OD1   | 6:Tg:35:VAL:N     | 2.54                     | 0.40              |
| 6:Tj:9:LEU:HD11   | 6:Tj:17:VAL:HB    | 2.02                     | 0.40              |
| 7:Mf:8:VAL:HG13   | 7:Mf:46:VAL:HG23  | 2.02                     | 0.40              |
| 4:Ja:463:ASP:OD2  | 4:Ja:464:PHE:N    | 2.54                     | 0.40              |
| 4:Ja:818:PHE:O    | 4:Jc:826:HIS:HA   | 2.22                     | 0.40              |
| 4:Jb:397:ASN:O    | 4:Jb:418:GLU:HA   | 2.22                     | 0.40              |
| 4:Jb:423:ILE:HD13 | 4:Jb:423:ILE:HA   | 1.91                     | 0.40              |
| 4:Jb:747:TRP:HB2  | 4:Jb:788:TYR:HB2  | 2.03                     | 0.40              |
| 5:Lc:19:ALA:HB2   | 7:Mf:34:PRO:HG2   | 2.04                     | 0.40              |
| 5:Lb:173:CYS:SG   | 5:Lb:174:THR:N    | 2.94                     | 0.40              |
| 6:Td:15:LYS:HE2   | 6:Td:15:LYS:HB3   | 1.94                     | 0.40              |
| 7:Mb:51:PRO:HG2   | 7:Mb:54:GLU:OE2   | 2.21                     | 0.40              |
| 8:Va:36:TRP:CE3   | 8:Va:109:LYS:HE2  | 2.56                     | 0.40              |
| 8:Vc:41:LYS:HD2   | 8:Vc:41:LYS:HA    | 1.77                     | 0.40              |
| 4:Ja:137:LEU:C    | 4:Ja:138:LEU:HD23 | 2.47                     | 0.40              |
| 4:Jc:326:ASN:O    | 4:Jc:437:GLY:HA2  | 2.22                     | 0.40              |
| 5:Lb:40:ASN:OD1   | 7:Mc:25:PHE:HB3   | 2.21                     | 0.40              |
| 6:Tb:82:GLN:N     | 6:Tb:82:GLN:OE1   | 2.54                     | 0.40              |
| 6:Tk:30:SER:OG    | 6:Tk:33:VAL:HB    | 2.21                     | 0.40              |
| 7:Ma:9:LYS:HG3    | 7:Ma:10:PRO:HD2   | 2.03                     | 0.40              |
| 8:Ve:134:ILE:H    | 8:Ve:134:ILE:HG12 | 1.71                     | 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   | Ha    | 30/32 (94%) | 28 (93%) | 2 (7%)  | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | Hb    | 30/32 (94%)    | 25 (83%)  | 5 (17%)  | 0        | 100         | 100 |
| 1   | Hc    | 30/32 (94%)    | 27 (90%)  | 3 (10%)  | 0        | 100         | 100 |
| 2   | Ia    | 87/90 (97%)    | 75 (86%)  | 11 (13%) | 1 (1%)   | 12          | 37  |
| 2   | Ib    | 88/90 (98%)    | 77 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 3   | Ic    | 88/90 (98%)    | 78 (89%)  | 10 (11%) | 0        | 100         | 100 |
| 4   | Ja    | 833/835 (100%) | 744 (89%) | 85 (10%) | 4 (0%)   | 25          | 54  |
| 4   | Jb    | 833/835 (100%) | 751 (90%) | 81 (10%) | 1 (0%)   | 48          | 77  |
| 4   | Jc    | 833/835 (100%) | 759 (91%) | 70 (8%)  | 4 (0%)   | 25          | 54  |
| 5   | La    | 230/232 (99%)  | 215 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 5   | Lb    | 230/232 (99%)  | 214 (93%) | 15 (6%)  | 1 (0%)   | 30          | 60  |
| 5   | Lc    | 230/232 (99%)  | 209 (91%) | 20 (9%)  | 1 (0%)   | 30          | 60  |
| 6   | Ta    | 92/94 (98%)    | 91 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 6   | Tb    | 92/94 (98%)    | 89 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 6   | Tc    | 92/94 (98%)    | 85 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 6   | Td    | 92/94 (98%)    | 85 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 6   | Te    | 92/94 (98%)    | 89 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 6   | Tf    | 92/94 (98%)    | 81 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 6   | Tg    | 92/94 (98%)    | 91 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 6   | Th    | 92/94 (98%)    | 89 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 6   | Ti    | 92/94 (98%)    | 84 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 6   | Tj    | 92/94 (98%)    | 92 (100%) | 0        | 0        | 100         | 100 |
| 6   | Tk    | 92/94 (98%)    | 83 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 6   | Tl    | 92/94 (98%)    | 83 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 7   | Ma    | 107/109 (98%)  | 95 (89%)  | 11 (10%) | 1 (1%)   | 14          | 41  |
| 7   | Mb    | 107/109 (98%)  | 100 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 7   | Mc    | 107/109 (98%)  | 97 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 7   | Md    | 107/109 (98%)  | 97 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 7   | Me    | 107/109 (98%)  | 97 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 7   | Mf    | 107/109 (98%)  | 101 (94%) | 6 (6%)   | 0        | 100         | 100 |
| 8   | Va    | 150/152 (99%)  | 137 (91%) | 12 (8%)  | 1 (1%)   | 19          | 47  |
| 8   | Vb    | 150/152 (99%)  | 140 (93%) | 9 (6%)   | 1 (1%)   | 19          | 47  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 8   | Vc    | 150/152 (99%)   | 140 (93%)  | 9 (6%)   | 1 (1%)   | 19          | 47  |
| 8   | Vd    | 150/152 (99%)   | 141 (94%)  | 8 (5%)   | 1 (1%)   | 19          | 47  |
| 8   | Ve    | 150/152 (99%)   | 140 (93%)  | 9 (6%)   | 1 (1%)   | 19          | 47  |
| 8   | Vf    | 150/152 (99%)   | 141 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| All | All   | 6188/6261 (99%) | 5670 (92%) | 500 (8%) | 18 (0%)  | 38          | 66  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Jc    | 542 | VAL  |
| 4   | Jc    | 616 | VAL  |
| 4   | Ja    | 613 | VAL  |
| 4   | Jb    | 613 | VAL  |
| 4   | Jc    | 606 | ASP  |
| 4   | Jc    | 613 | VAL  |
| 2   | Ia    | 185 | GLN  |
| 4   | Ja    | 608 | GLU  |
| 5   | Lc    | 227 | ILE  |
| 5   | Lb    | 168 | MET  |
| 7   | Ma    | 78  | GLU  |
| 8   | Vc    | 133 | VAL  |
| 8   | Ve    | 133 | VAL  |
| 8   | Vd    | 133 | VAL  |
| 4   | Ja    | 822 | ILE  |
| 8   | Va    | 133 | VAL  |
| 8   | Vb    | 133 | VAL  |
| 4   | Ja    | 379 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | Ha    | 22/23 (96%)  | 22 (100%) | 0        | 100         | 100 |
| 1   | Hb    | 23/23 (100%) | 22 (96%)  | 1 (4%)   | 25          | 51  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | Hc    | 23/23 (100%)   | 21 (91%)  | 2 (9%)   | 8           | 28 |
| 2   | Ia    | 69/70 (99%)    | 62 (90%)  | 7 (10%)  | 6           | 22 |
| 2   | Ib    | 68/70 (97%)    | 63 (93%)  | 5 (7%)   | 11          | 36 |
| 3   | Ic    | 70/70 (100%)   | 67 (96%)  | 3 (4%)   | 25          | 51 |
| 4   | Ja    | 709/711 (100%) | 681 (96%) | 28 (4%)  | 27          | 54 |
| 4   | Jb    | 709/711 (100%) | 683 (96%) | 26 (4%)  | 29          | 55 |
| 4   | Jc    | 707/711 (99%)  | 687 (97%) | 20 (3%)  | 38          | 63 |
| 5   | La    | 195/198 (98%)  | 187 (96%) | 8 (4%)   | 26          | 52 |
| 5   | Lb    | 194/198 (98%)  | 192 (99%) | 2 (1%)   | 73          | 84 |
| 5   | Lc    | 194/198 (98%)  | 192 (99%) | 2 (1%)   | 73          | 84 |
| 6   | Ta    | 80/80 (100%)   | 75 (94%)  | 5 (6%)   | 15          | 40 |
| 6   | Tb    | 80/80 (100%)   | 77 (96%)  | 3 (4%)   | 28          | 54 |
| 6   | Tc    | 80/80 (100%)   | 74 (92%)  | 6 (8%)   | 11          | 35 |
| 6   | Td    | 80/80 (100%)   | 79 (99%)  | 1 (1%)   | 65          | 79 |
| 6   | Te    | 80/80 (100%)   | 76 (95%)  | 4 (5%)   | 20          | 47 |
| 6   | Tf    | 80/80 (100%)   | 72 (90%)  | 8 (10%)  | 6           | 23 |
| 6   | Tg    | 80/80 (100%)   | 76 (95%)  | 4 (5%)   | 20          | 47 |
| 6   | Th    | 80/80 (100%)   | 77 (96%)  | 3 (4%)   | 28          | 54 |
| 6   | Ti    | 80/80 (100%)   | 74 (92%)  | 6 (8%)   | 11          | 35 |
| 6   | Tj    | 80/80 (100%)   | 73 (91%)  | 7 (9%)   | 8           | 28 |
| 6   | Tk    | 80/80 (100%)   | 76 (95%)  | 4 (5%)   | 20          | 47 |
| 6   | Tl    | 80/80 (100%)   | 76 (95%)  | 4 (5%)   | 20          | 47 |
| 7   | Ma    | 96/96 (100%)   | 92 (96%)  | 4 (4%)   | 25          | 51 |
| 7   | Mb    | 94/96 (98%)    | 91 (97%)  | 3 (3%)   | 34          | 60 |
| 7   | Mc    | 96/96 (100%)   | 93 (97%)  | 3 (3%)   | 35          | 61 |
| 7   | Md    | 96/96 (100%)   | 93 (97%)  | 3 (3%)   | 35          | 61 |
| 7   | Me    | 96/96 (100%)   | 93 (97%)  | 3 (3%)   | 35          | 61 |
| 7   | Mf    | 95/96 (99%)    | 90 (95%)  | 5 (5%)   | 19          | 45 |
| 8   | Va    | 124/124 (100%) | 114 (92%) | 10 (8%)  | 9           | 31 |
| 8   | Vb    | 124/124 (100%) | 116 (94%) | 8 (6%)   | 14          | 40 |
| 8   | Vc    | 124/124 (100%) | 118 (95%) | 6 (5%)   | 21          | 48 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 8   | Vd    | 124/124 (100%)   | 120 (97%)  | 4 (3%)   | 34          | 60 |
| 8   | Ve    | 124/124 (100%)   | 117 (94%)  | 7 (6%)   | 17          | 44 |
| 8   | Vf    | 124/124 (100%)   | 115 (93%)  | 9 (7%)   | 11          | 36 |
| All | All   | 5260/5286 (100%) | 5036 (96%) | 224 (4%) | 27          | 51 |

All (224) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Ia    | 174 | THR  |
| 2   | Ia    | 175 | TYR  |
| 2   | Ia    | 192 | LEU  |
| 2   | Ia    | 203 | VAL  |
| 2   | Ia    | 207 | ILE  |
| 2   | Ia    | 212 | GLU  |
| 2   | Ia    | 221 | ILE  |
| 1   | Hb    | 848 | PHE  |
| 2   | Ib    | 136 | THR  |
| 2   | Ib    | 168 | ASP  |
| 2   | Ib    | 174 | THR  |
| 2   | Ib    | 176 | PHE  |
| 2   | Ib    | 208 | SER  |
| 1   | Hc    | 823 | LEU  |
| 1   | Hc    | 847 | LEU  |
| 3   | Ic    | 140 | PHE  |
| 3   | Ic    | 161 | THR  |
| 3   | Ic    | 221 | ILE  |
| 4   | Ja    | 6   | SER  |
| 4   | Ja    | 18  | LEU  |
| 4   | Ja    | 49  | SER  |
| 4   | Ja    | 81  | PHE  |
| 4   | Ja    | 88  | THR  |
| 4   | Ja    | 94  | VAL  |
| 4   | Ja    | 153 | ILE  |
| 4   | Ja    | 154 | THR  |
| 4   | Ja    | 159 | THR  |
| 4   | Ja    | 217 | LEU  |
| 4   | Ja    | 220 | VAL  |
| 4   | Ja    | 312 | VAL  |
| 4   | Ja    | 331 | THR  |
| 4   | Ja    | 333 | ARG  |
| 4   | Ja    | 360 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Ja    | 377 | VAL  |
| 4   | Ja    | 438 | CYS  |
| 4   | Ja    | 462 | VAL  |
| 4   | Ja    | 518 | THR  |
| 4   | Ja    | 529 | ASN  |
| 4   | Ja    | 549 | VAL  |
| 4   | Ja    | 612 | THR  |
| 4   | Ja    | 624 | LEU  |
| 4   | Ja    | 634 | GLU  |
| 4   | Ja    | 646 | VAL  |
| 4   | Ja    | 668 | VAL  |
| 4   | Ja    | 710 | ARG  |
| 4   | Ja    | 761 | THR  |
| 4   | Jb    | 49  | SER  |
| 4   | Jb    | 81  | PHE  |
| 4   | Jb    | 88  | THR  |
| 4   | Jb    | 94  | VAL  |
| 4   | Jb    | 139 | VAL  |
| 4   | Jb    | 153 | ILE  |
| 4   | Jb    | 160 | THR  |
| 4   | Jb    | 245 | VAL  |
| 4   | Jb    | 312 | VAL  |
| 4   | Jb    | 340 | SER  |
| 4   | Jb    | 353 | ASN  |
| 4   | Jb    | 377 | VAL  |
| 4   | Jb    | 454 | THR  |
| 4   | Jb    | 462 | VAL  |
| 4   | Jb    | 481 | ILE  |
| 4   | Jb    | 508 | ASP  |
| 4   | Jb    | 518 | THR  |
| 4   | Jb    | 529 | ASN  |
| 4   | Jb    | 531 | VAL  |
| 4   | Jb    | 549 | VAL  |
| 4   | Jb    | 584 | TYR  |
| 4   | Jb    | 587 | THR  |
| 4   | Jb    | 591 | HIS  |
| 4   | Jb    | 668 | VAL  |
| 4   | Jb    | 687 | ASN  |
| 4   | Jb    | 779 | ILE  |
| 4   | Jc    | 17  | ASN  |
| 4   | Jc    | 26  | VAL  |
| 4   | Jc    | 49  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Jc    | 81  | PHE  |
| 4   | Jc    | 88  | THR  |
| 4   | Jc    | 94  | VAL  |
| 4   | Jc    | 148 | VAL  |
| 4   | Jc    | 217 | LEU  |
| 4   | Jc    | 245 | VAL  |
| 4   | Jc    | 312 | VAL  |
| 4   | Jc    | 331 | THR  |
| 4   | Jc    | 377 | VAL  |
| 4   | Jc    | 423 | ILE  |
| 4   | Jc    | 454 | THR  |
| 4   | Jc    | 462 | VAL  |
| 4   | Jc    | 466 | VAL  |
| 4   | Jc    | 477 | ASP  |
| 4   | Jc    | 542 | VAL  |
| 4   | Jc    | 621 | VAL  |
| 4   | Jc    | 629 | THR  |
| 5   | Lc    | 143 | LEU  |
| 5   | Lc    | 230 | LEU  |
| 5   | Lb    | 73  | THR  |
| 5   | Lb    | 180 | ASP  |
| 5   | La    | 4   | ILE  |
| 5   | La    | 73  | THR  |
| 5   | La    | 81  | VAL  |
| 5   | La    | 82  | SER  |
| 5   | La    | 167 | ILE  |
| 5   | La    | 169 | LEU  |
| 5   | La    | 180 | ASP  |
| 5   | La    | 208 | CYS  |
| 6   | Ta    | 32  | THR  |
| 6   | Ta    | 37  | THR  |
| 6   | Ta    | 65  | ASP  |
| 6   | Ta    | 70  | SER  |
| 6   | Ta    | 76  | THR  |
| 6   | Tb    | 52  | ASP  |
| 6   | Tb    | 77  | VAL  |
| 6   | Tb    | 81  | SER  |
| 6   | Tc    | 31  | THR  |
| 6   | Tc    | 42  | ASN  |
| 6   | Tc    | 52  | ASP  |
| 6   | Tc    | 61  | ILE  |
| 6   | Tc    | 76  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | Tc    | 86  | LEU  |
| 6   | Td    | 17  | VAL  |
| 6   | Te    | 3   | VAL  |
| 6   | Te    | 42  | ASN  |
| 6   | Te    | 65  | ASP  |
| 6   | Te    | 86  | LEU  |
| 6   | Tf    | 40  | SER  |
| 6   | Tf    | 42  | ASN  |
| 6   | Tf    | 52  | ASP  |
| 6   | Tf    | 67  | PHE  |
| 6   | Tf    | 70  | SER  |
| 6   | Tf    | 74  | THR  |
| 6   | Tf    | 76  | THR  |
| 6   | Tf    | 81  | SER  |
| 6   | Tg    | 57  | GLN  |
| 6   | Tg    | 70  | SER  |
| 6   | Tg    | 79  | GLU  |
| 6   | Tg    | 87  | ASN  |
| 6   | Tl    | 17  | VAL  |
| 6   | Tl    | 67  | PHE  |
| 6   | Tl    | 76  | THR  |
| 6   | Tl    | 85  | THR  |
| 6   | Th    | 19  | ASN  |
| 6   | Th    | 42  | ASN  |
| 6   | Th    | 80  | ASP  |
| 6   | Ti    | 31  | THR  |
| 6   | Ti    | 42  | ASN  |
| 6   | Ti    | 61  | ILE  |
| 6   | Ti    | 76  | THR  |
| 6   | Ti    | 78  | TYR  |
| 6   | Ti    | 85  | THR  |
| 6   | Tj    | 1   | MET  |
| 6   | Tj    | 9   | LEU  |
| 6   | Tj    | 32  | THR  |
| 6   | Tj    | 40  | SER  |
| 6   | Tj    | 52  | ASP  |
| 6   | Tj    | 70  | SER  |
| 6   | Tj    | 76  | THR  |
| 6   | Tk    | 52  | ASP  |
| 6   | Tk    | 67  | PHE  |
| 6   | Tk    | 71  | HIS  |
| 6   | Tk    | 76  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Ma    | 12  | MET  |
| 7   | Ma    | 24  | ARG  |
| 7   | Ma    | 40  | ASN  |
| 7   | Ma    | 103 | GLU  |
| 7   | Mb    | 12  | MET  |
| 7   | Mb    | 23  | VAL  |
| 7   | Mb    | 99  | GLU  |
| 7   | Mc    | 90  | SER  |
| 7   | Mc    | 98  | VAL  |
| 7   | Mc    | 103 | GLU  |
| 7   | Md    | 74  | THR  |
| 7   | Md    | 90  | SER  |
| 7   | Md    | 91  | SER  |
| 7   | Me    | 7   | LYS  |
| 7   | Me    | 80  | ARG  |
| 7   | Me    | 86  | CYS  |
| 7   | Mf    | 23  | VAL  |
| 7   | Mf    | 48  | LEU  |
| 7   | Mf    | 58  | LEU  |
| 7   | Mf    | 60  | SER  |
| 7   | Mf    | 91  | SER  |
| 8   | Va    | 33  | ASP  |
| 8   | Va    | 34  | VAL  |
| 8   | Va    | 36  | TRP  |
| 8   | Va    | 42  | VAL  |
| 8   | Va    | 51  | THR  |
| 8   | Va    | 70  | THR  |
| 8   | Va    | 114 | ASN  |
| 8   | Va    | 135 | THR  |
| 8   | Va    | 138 | VAL  |
| 8   | Va    | 140 | VAL  |
| 8   | Vb    | 3   | VAL  |
| 8   | Vb    | 19  | VAL  |
| 8   | Vb    | 60  | LEU  |
| 8   | Vb    | 96  | LEU  |
| 8   | Vb    | 114 | ASN  |
| 8   | Vb    | 124 | VAL  |
| 8   | Vb    | 143 | VAL  |
| 8   | Vb    | 154 | THR  |
| 8   | Vc    | 25  | ASP  |
| 8   | Vc    | 70  | THR  |
| 8   | Vc    | 125 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | Vc    | 139 | LYS  |
| 8   | Vc    | 140 | VAL  |
| 8   | Vc    | 147 | SER  |
| 8   | Vd    | 3   | VAL  |
| 8   | Vd    | 96  | LEU  |
| 8   | Vd    | 124 | VAL  |
| 8   | Vd    | 142 | ASN  |
| 8   | Ve    | 33  | ASP  |
| 8   | Ve    | 37  | SER  |
| 8   | Ve    | 46  | THR  |
| 8   | Ve    | 84  | LEU  |
| 8   | Ve    | 116 | THR  |
| 8   | Ve    | 124 | VAL  |
| 8   | Ve    | 135 | THR  |
| 8   | Vf    | 3   | VAL  |
| 8   | Vf    | 10  | VAL  |
| 8   | Vf    | 33  | ASP  |
| 8   | Vf    | 58  | SER  |
| 8   | Vf    | 80  | THR  |
| 8   | Vf    | 93  | GLN  |
| 8   | Vf    | 96  | LEU  |
| 8   | Vf    | 124 | VAL  |
| 8   | Vf    | 154 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Ia    | 173 | ASN  |
| 2   | Ia    | 205 | GLN  |
| 2   | Ib    | 217 | GLN  |
| 3   | Ic    | 172 | GLN  |
| 4   | Ja    | 178 | ASN  |
| 4   | Ja    | 221 | GLN  |
| 4   | Ja    | 248 | ASN  |
| 4   | Ja    | 326 | ASN  |
| 4   | Ja    | 353 | ASN  |
| 4   | Ja    | 355 | GLN  |
| 4   | Ja    | 579 | ASN  |
| 4   | Ja    | 590 | GLN  |
| 4   | Ja    | 604 | HIS  |
| 4   | Ja    | 623 | HIS  |
| 4   | Jb    | 119 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Jb    | 140 | GLN  |
| 4   | Jb    | 178 | ASN  |
| 4   | Jb    | 194 | GLN  |
| 4   | Jb    | 353 | ASN  |
| 4   | Jb    | 529 | ASN  |
| 4   | Jc    | 140 | GLN  |
| 4   | Jc    | 214 | ASN  |
| 4   | Jc    | 375 | ASN  |
| 4   | Jc    | 408 | ASN  |
| 4   | Jc    | 601 | ASN  |
| 4   | Jc    | 604 | HIS  |
| 5   | Lc    | 6   | GLN  |
| 5   | Lc    | 129 | GLN  |
| 5   | Lc    | 171 | ASN  |
| 5   | Lb    | 17  | GLN  |
| 6   | Ta    | 63  | GLN  |
| 6   | Tc    | 23  | GLN  |
| 6   | Tc    | 63  | GLN  |
| 6   | Td    | 19  | ASN  |
| 6   | Tf    | 23  | GLN  |
| 6   | Tl    | 19  | ASN  |
| 6   | Ti    | 23  | GLN  |
| 6   | Tk    | 19  | ASN  |
| 6   | Tk    | 42  | ASN  |
| 7   | Mb    | 81  | GLN  |
| 7   | Me    | 109 | ASN  |
| 8   | Vd    | 94  | GLN  |
| 8   | Vf    | 29  | ASN  |
| 8   | Vf    | 114 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 9   | SF4  | Lb    | 301 | 5    | 0,12,12      | -    | -           | -           |      |             |
| 9   | SF4  | La    | 301 | 5    | 0,12,12      | -    | -           | -           |      |             |
| 9   | SF4  | Lc    | 301 | 5    | 0,12,12      | -    | -           | -           |      |             |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 9   | SF4  | Lb    | 301 | 5    | -       | -        | 0/6/5/5 |
| 9   | SF4  | La    | 301 | 5    | -       | -        | 0/6/5/5 |
| 9   | SF4  | Lc    | 301 | 5    | -       | -        | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

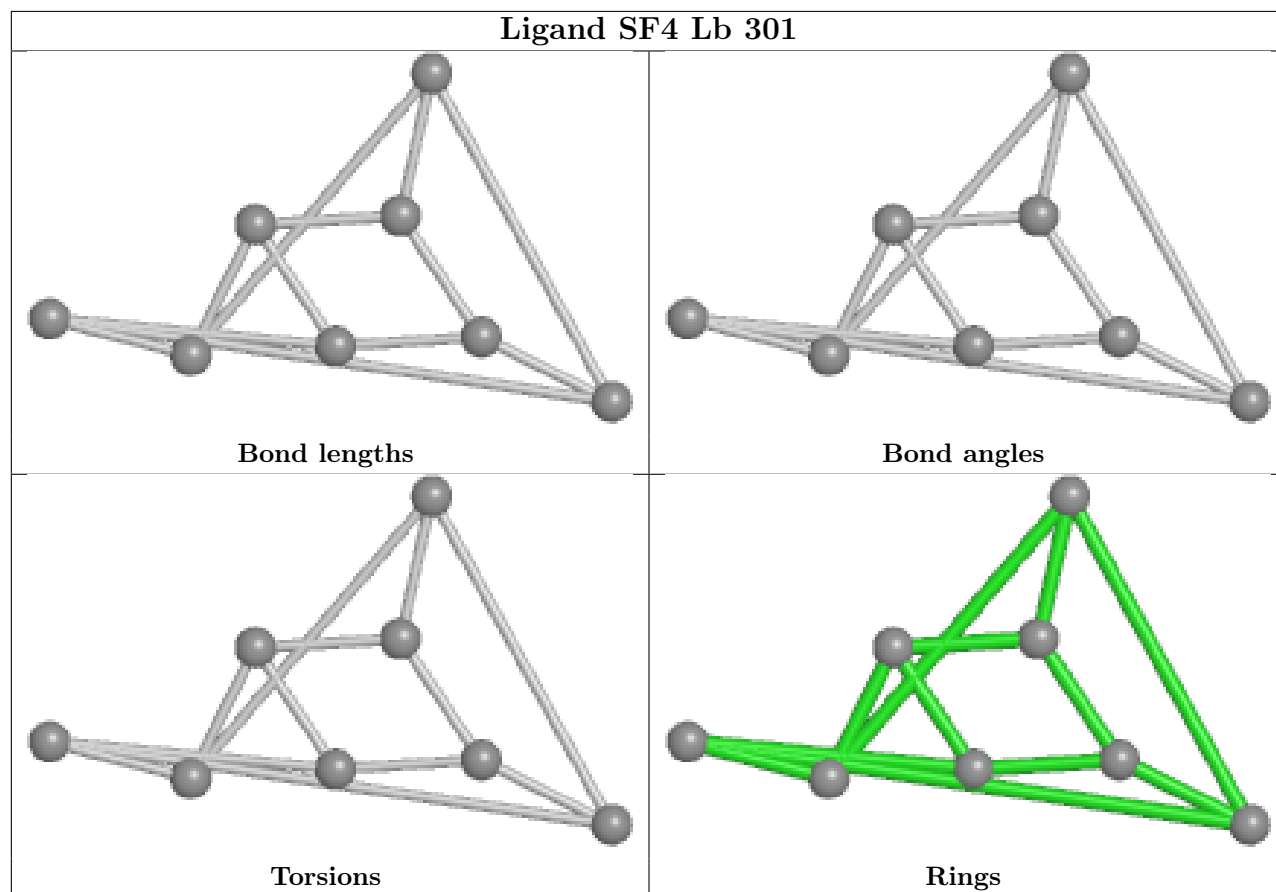
There are no torsion outliers.

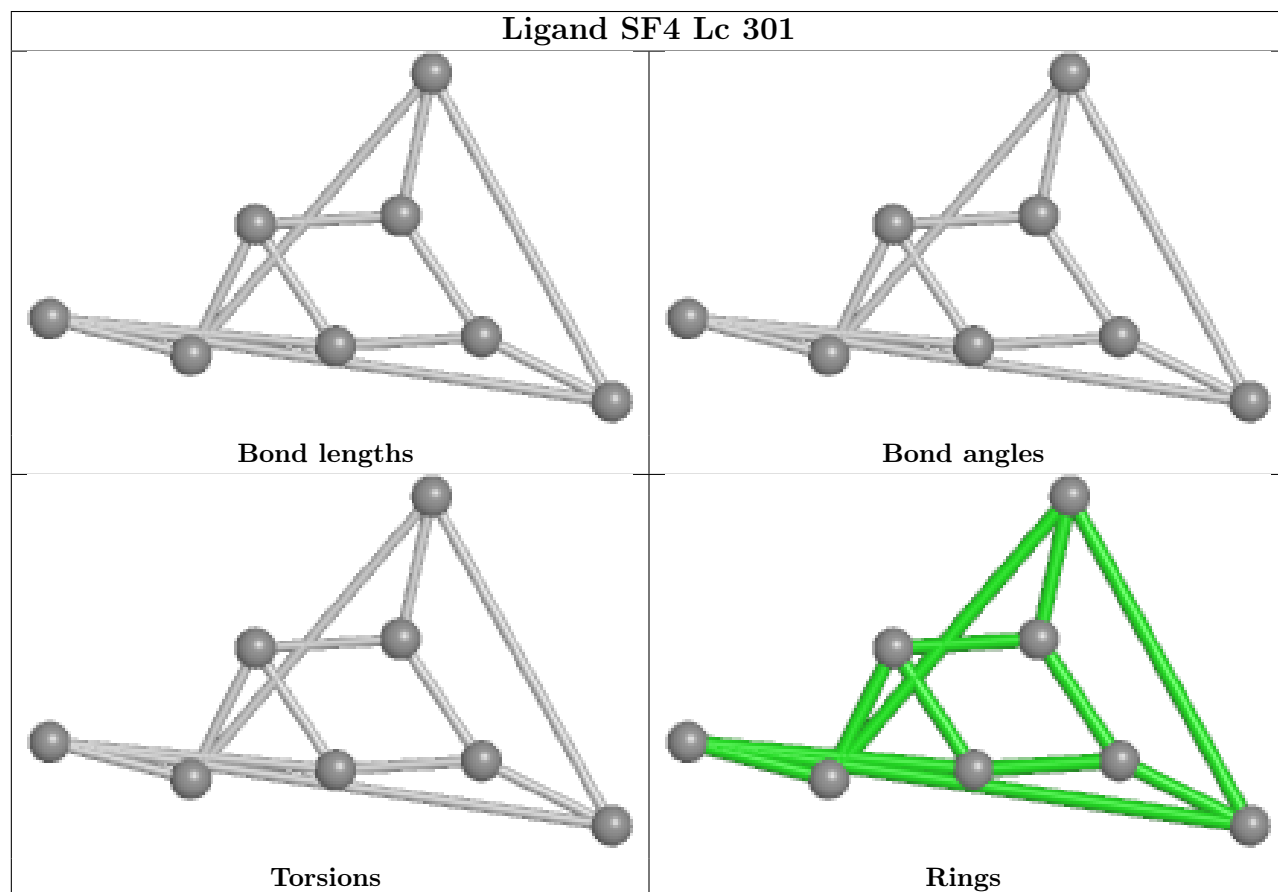
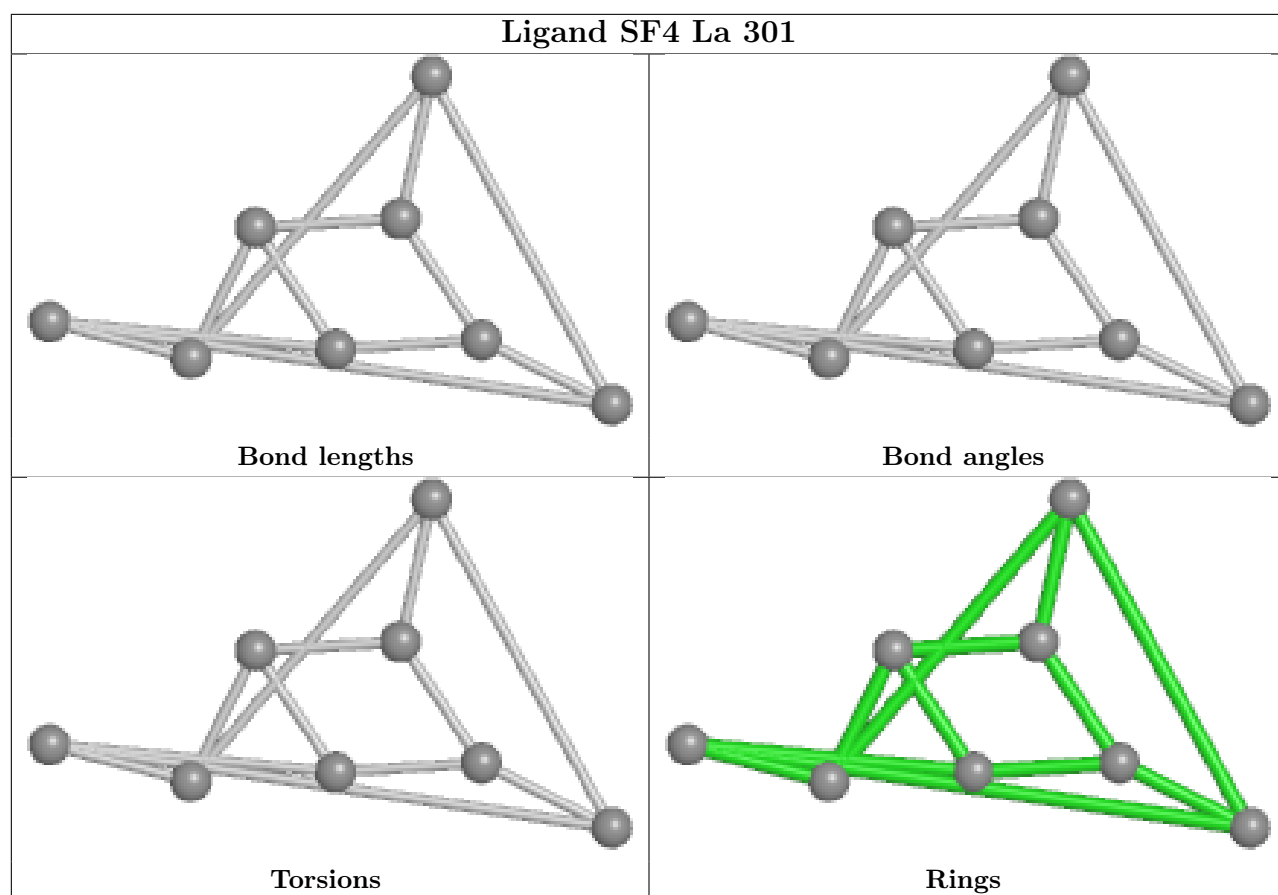
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.



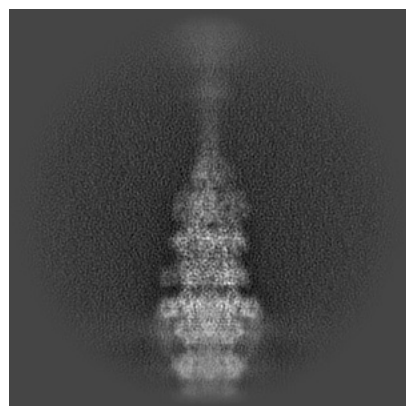
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47685. These allow visual inspection of the internal detail of the map and identification of artifacts.

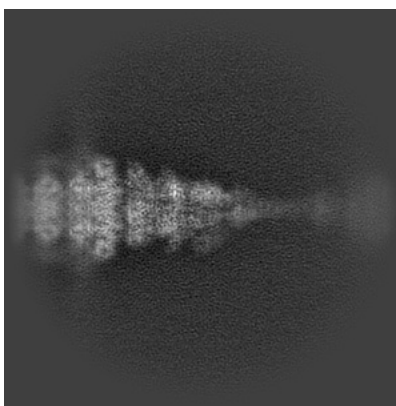
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

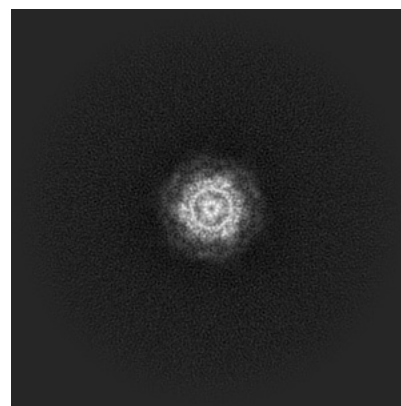
#### 6.1.1 Primary map



X

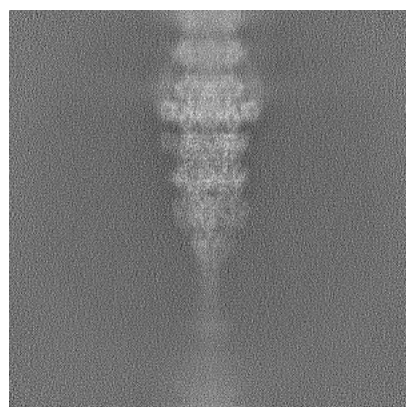


Y

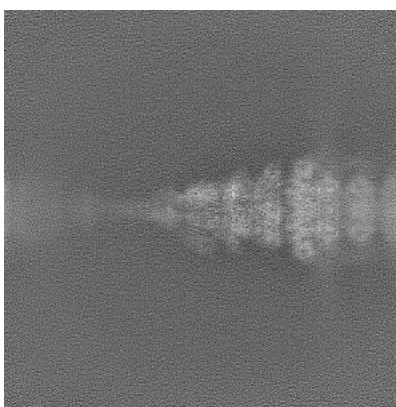


Z

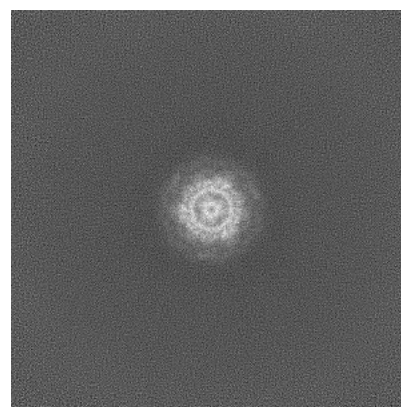
#### 6.1.2 Raw map



X



Y

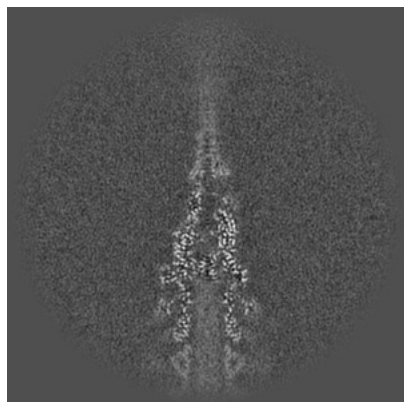


Z

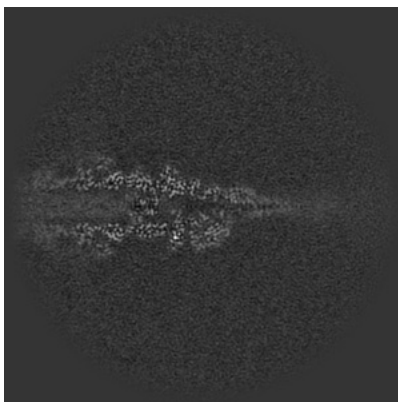
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

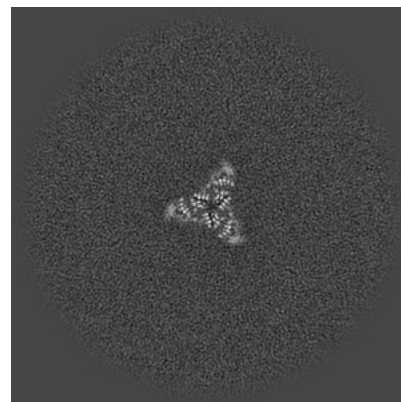
### 6.2.1 Primary map



X Index: 224

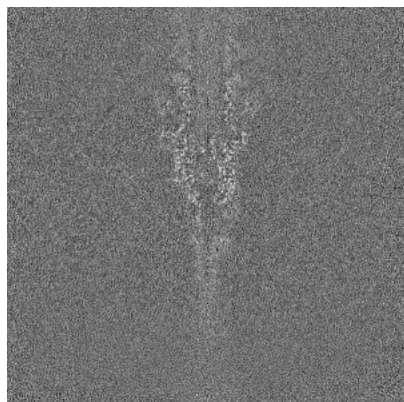


Y Index: 224

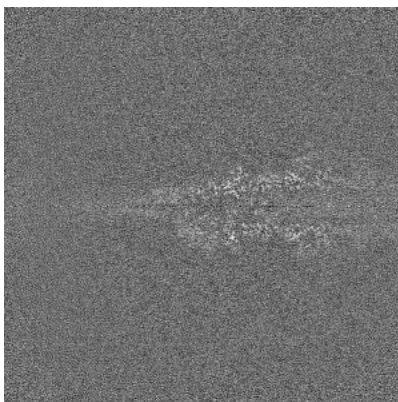


Z Index: 224

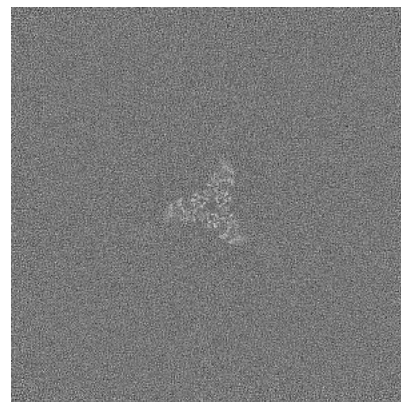
### 6.2.2 Raw map



X Index: 224



Y Index: 224

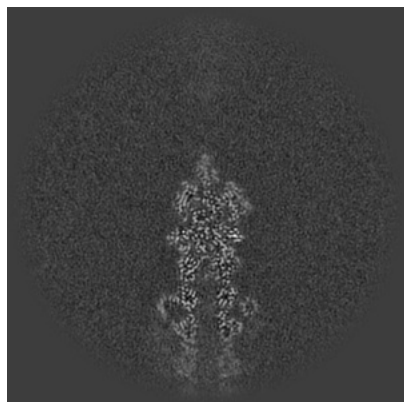


Z Index: 224

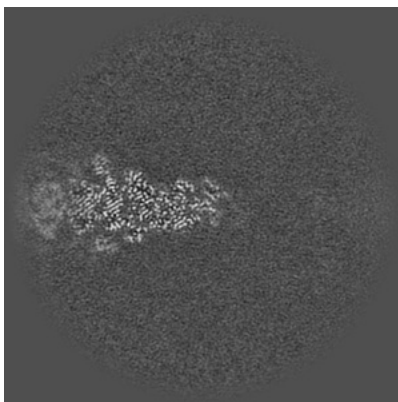
The images above show central slices of the map in three orthogonal directions.

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

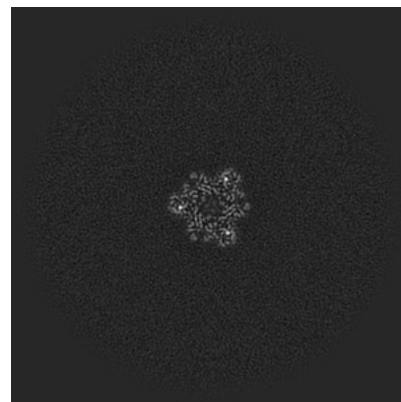
### 6.3.1 Primary map



X Index: 239

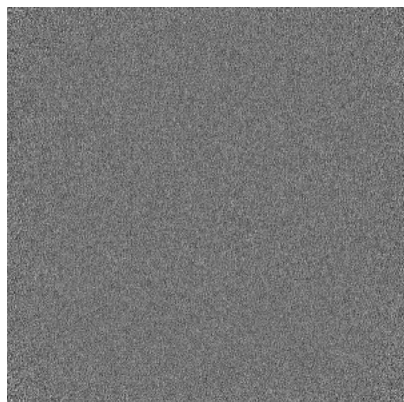


Y Index: 203

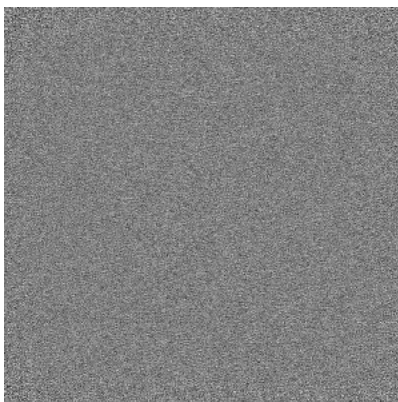


Z Index: 191

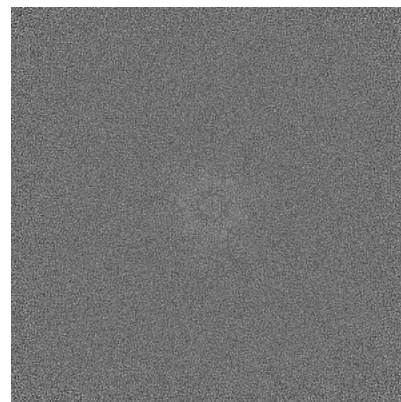
### 6.3.2 Raw map



X Index: 0



Y Index: 0



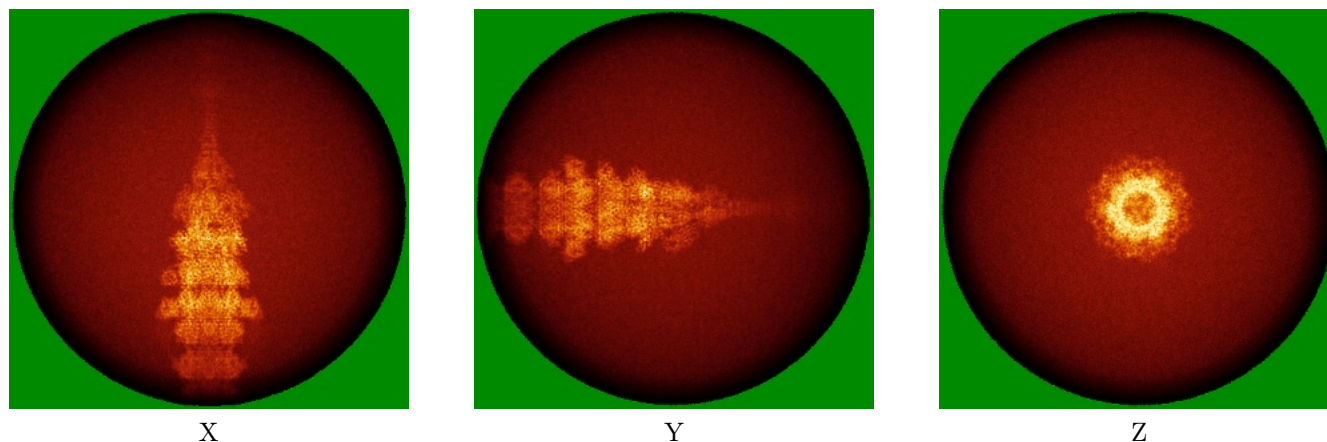
Z Index: 0

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

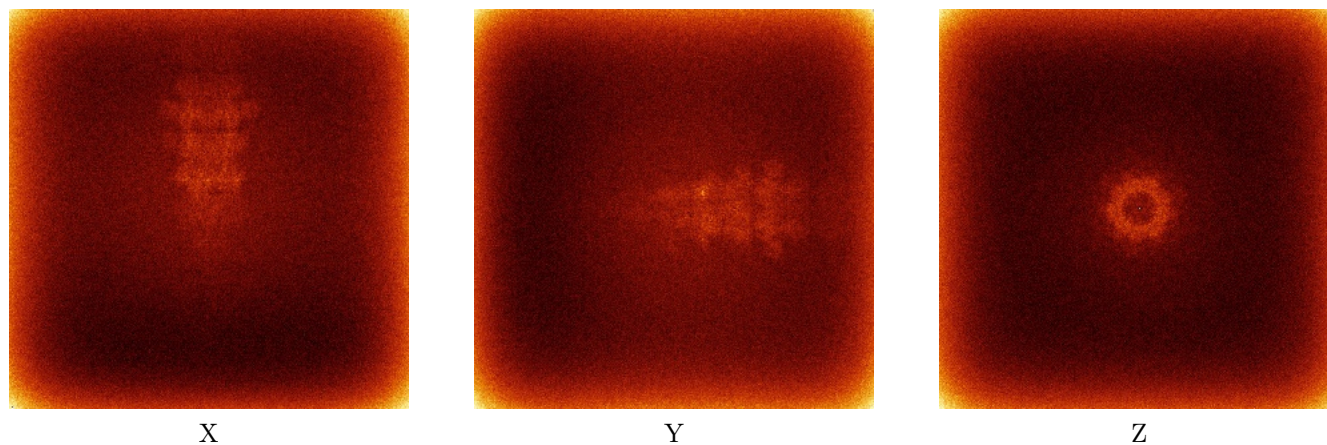


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



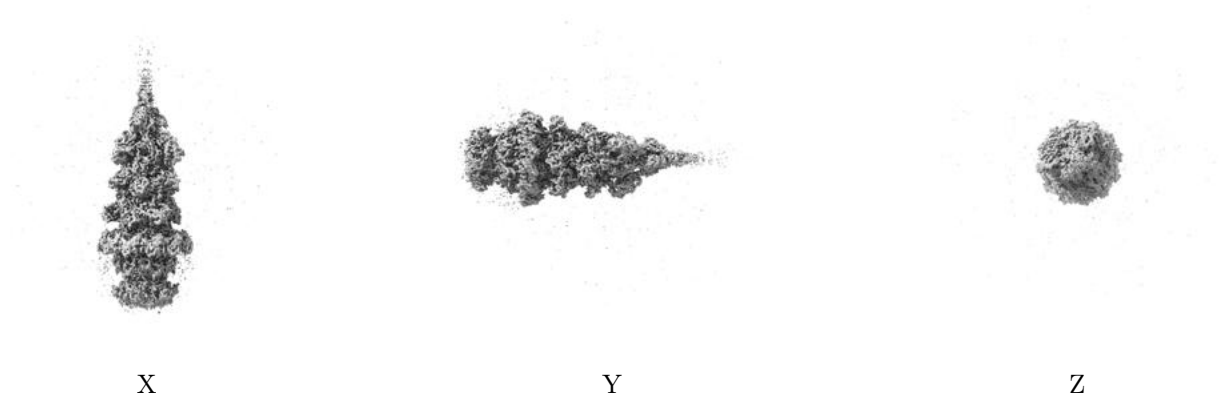
### 6.4.2 Raw map



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.

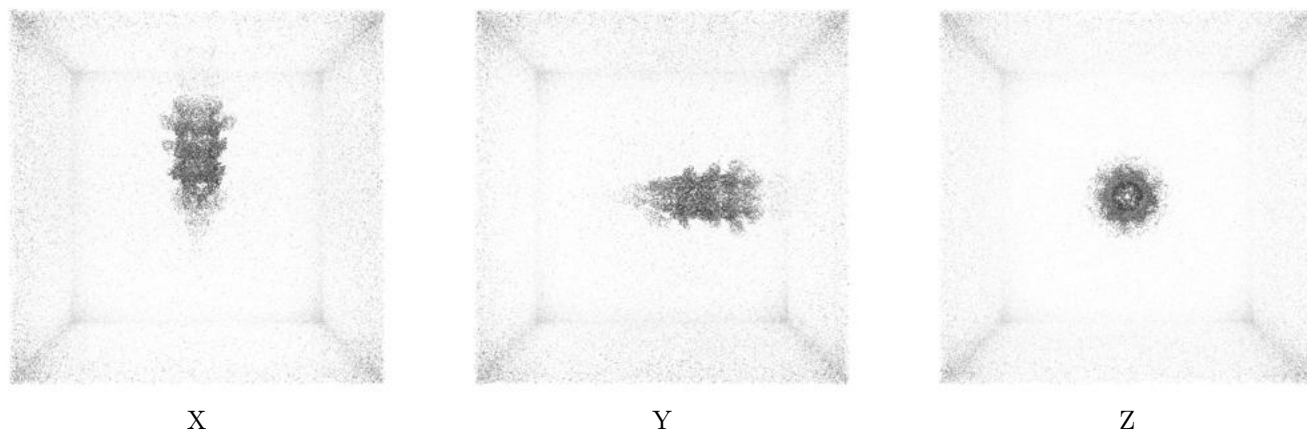
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

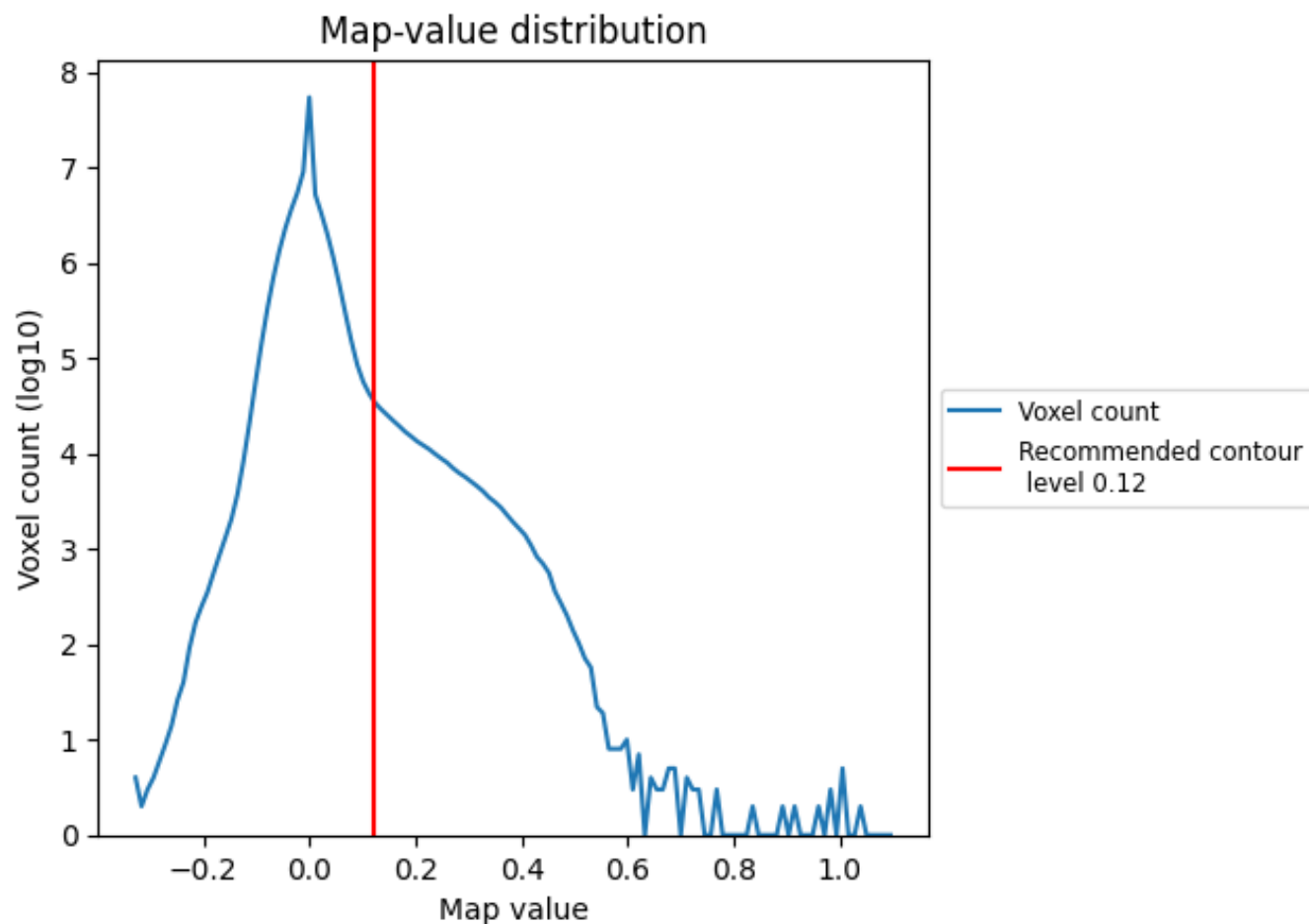
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

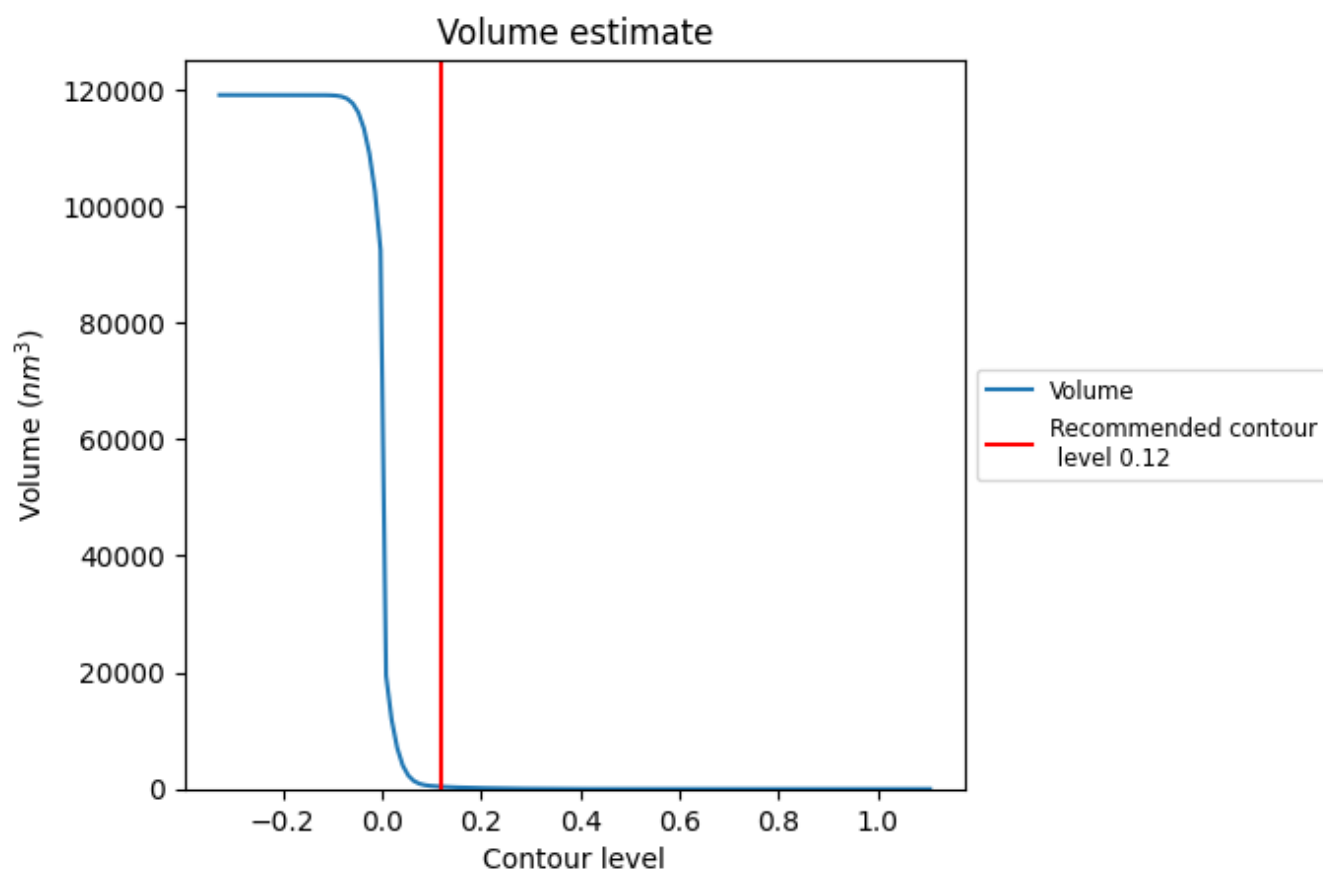
This section contains the results of statistical analysis of the map.

### 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.

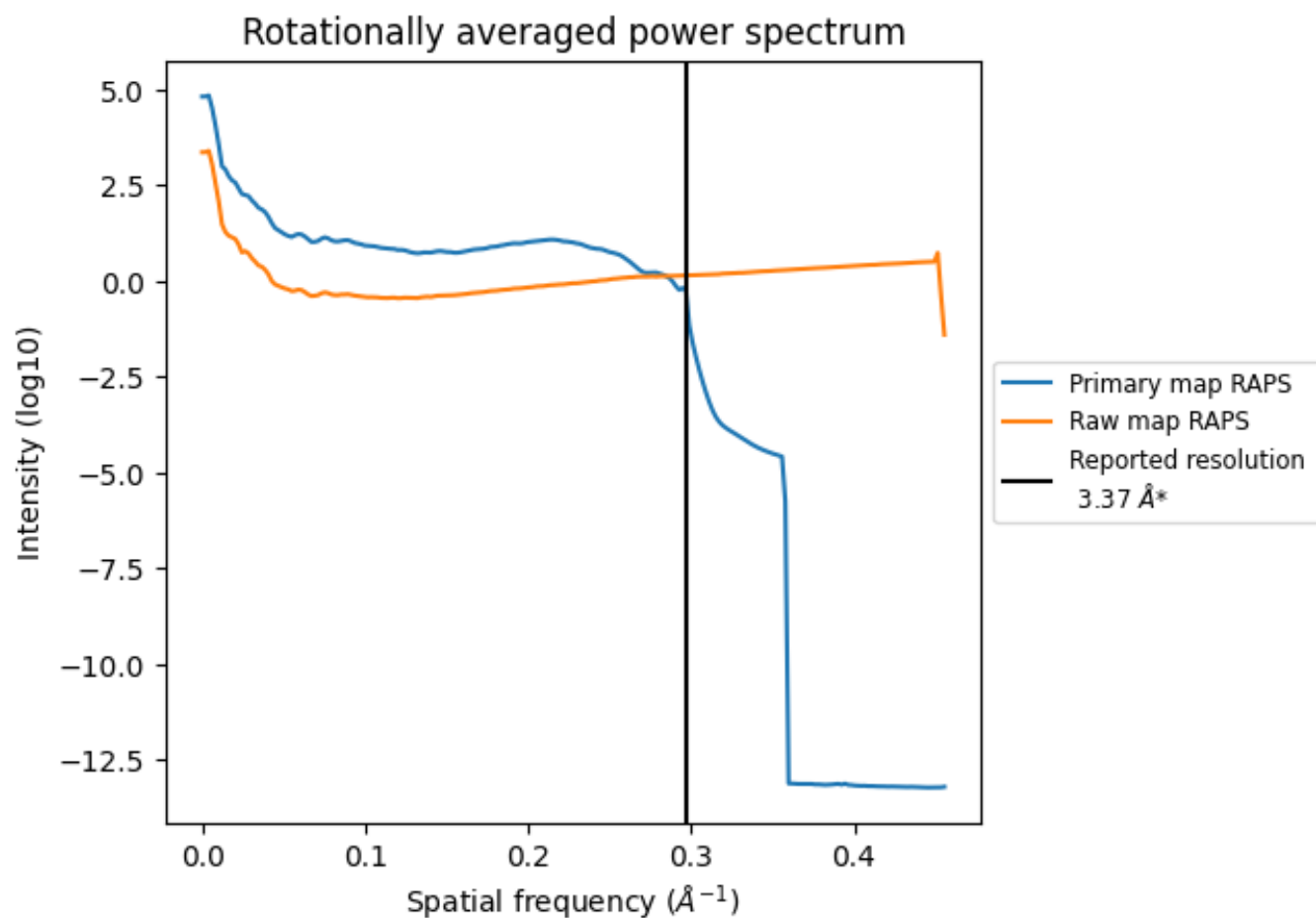
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 385  $\text{nm}^3$ ; this corresponds to an approximate mass of 348 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 ⓘ



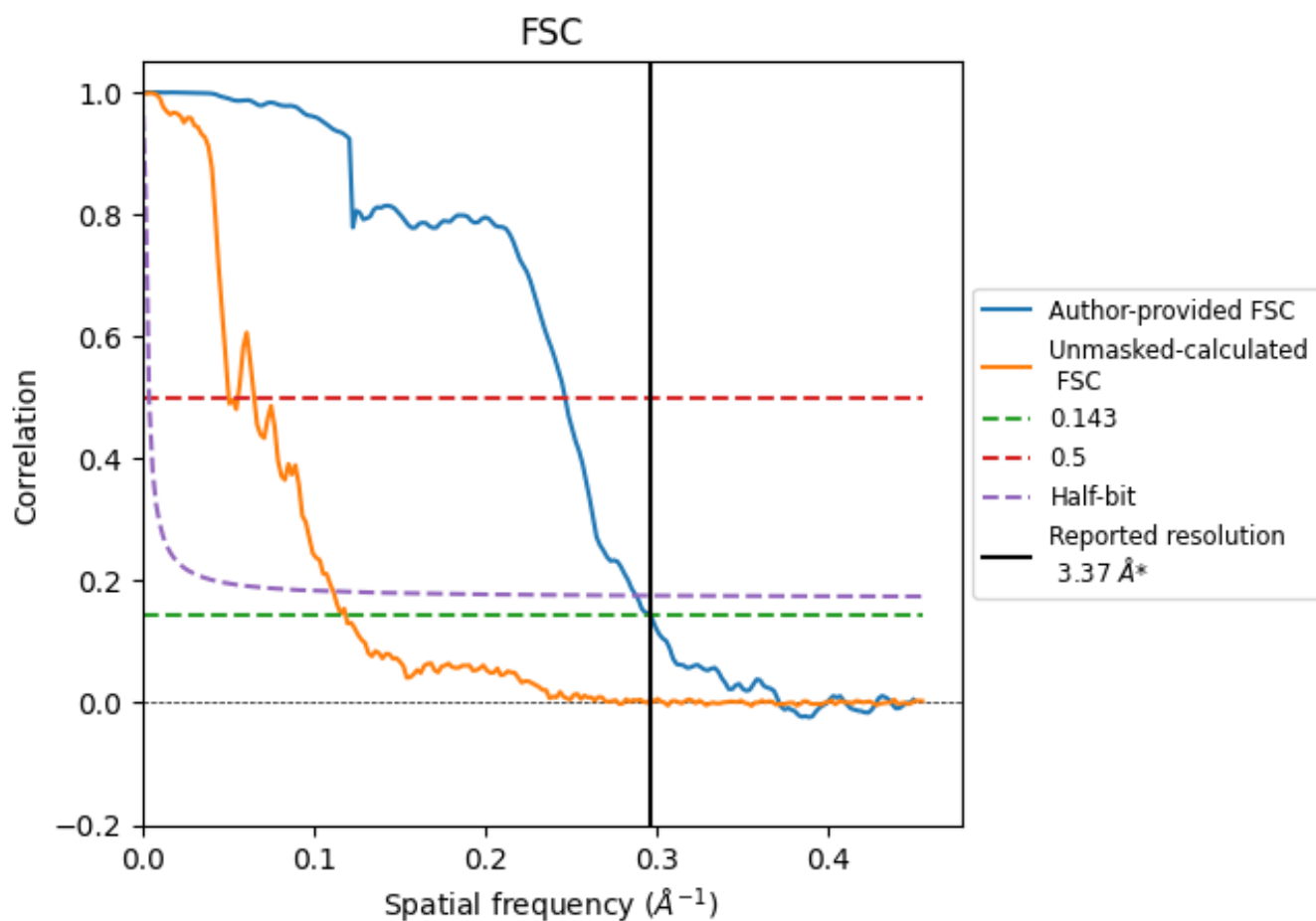
\*Reported resolution corresponds to spatial frequency of 0.297 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.297 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

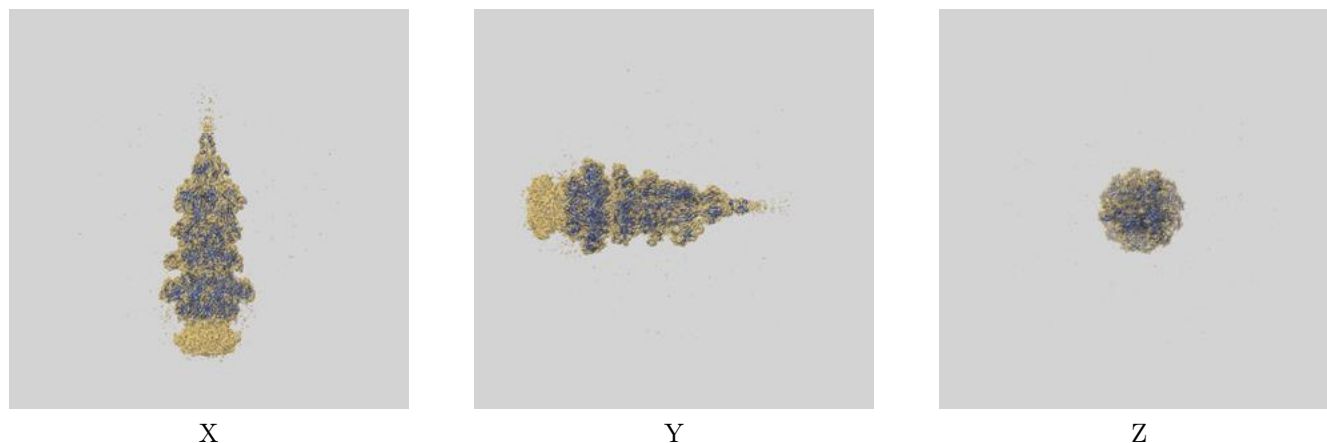
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.37                               | -     | -        |
| Author-provided FSC curve | 3.37                               | 4.05  | 3.47     |
| Unmasked-calculated*      | 8.42                               | 19.80 | 8.96     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.42 differs from the reported value 3.37 by more than 10 %

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

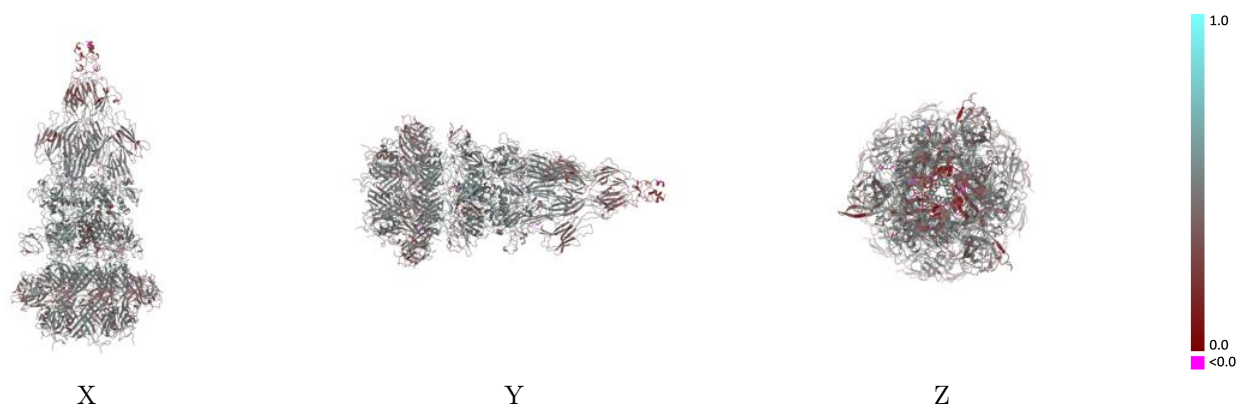
This section contains information regarding the fit between EMDB map EMD-47685 and PDB model 9E7M. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



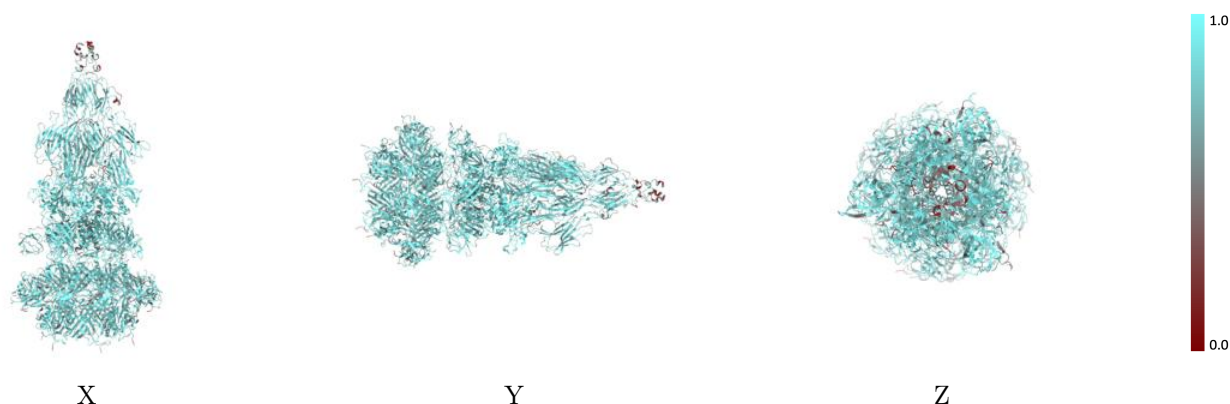
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



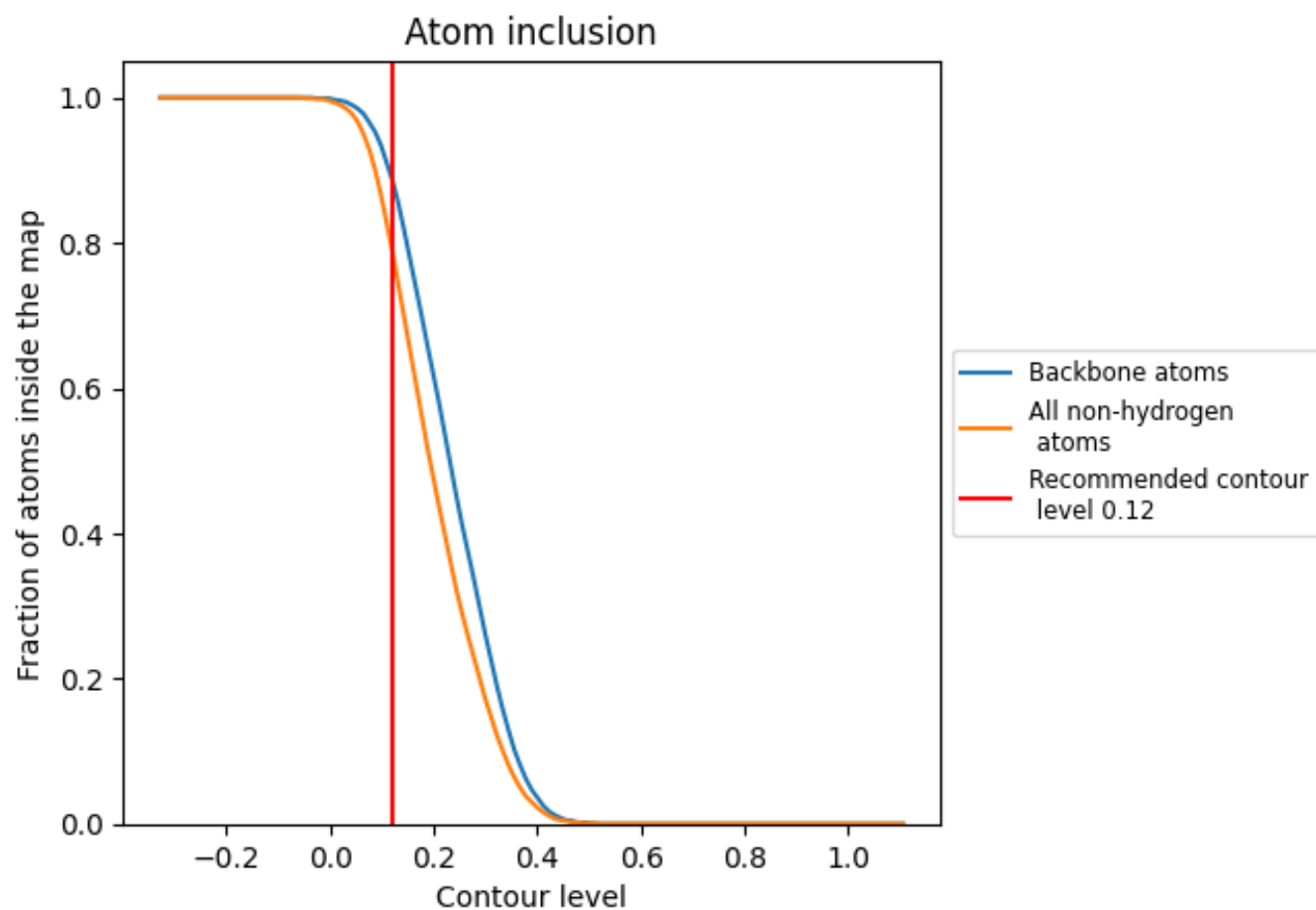
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7890   |  0.4460   |
| Ha    |  0.7650   |  0.4530   |
| Hb    |  0.7520   |  0.4470   |
| Hc    |  0.7610   |  0.4410   |
| Ia    |  0.7530   |  0.4380   |
| Ib    |  0.7120   |  0.4250   |
| Ic    |  0.7620   |  0.4750   |
| Ja    |  0.7860   |  0.4320   |
| Jb    |  0.7900   |  0.4390   |
| Jc    |  0.7840   |  0.4330   |
| La    |  0.8590   |  0.4930   |
| Lb    |  0.8600   |  0.4910   |
| Lc    |  0.8540   |  0.4870   |
| Ma    |  0.8150   |  0.4630   |
| Mb    |  0.8540  |  0.4900  |
| Mc    |  0.8140 |  0.4630 |
| Md    |  0.8420 |  0.4900 |
| Me    |  0.8210 |  0.4610 |
| Mf    |  0.8430 |  0.4870 |
| Ta    |  0.7450 |  0.4270 |
| Tb    |  0.7380 |  0.4390 |
| Tc    |  0.7050 |  0.3890 |
| Td    |  0.7150 |  0.3990 |
| Te    |  0.7310 |  0.4260 |
| Tf    |  0.7090 |  0.3980 |
| Tg    |  0.7360 |  0.4260 |
| Th    |  0.7330 |  0.4270 |
| Ti    |  0.6970 |  0.3990 |
| Tj    |  0.7350 |  0.4160 |
| Tk    |  0.6970 |  0.3880 |
| Tl    |  0.7100 |  0.3910 |
| Va    |  0.8170 |  0.4690 |
| Vb    |  0.8020 |  0.4670 |
| Vc    |  0.8200 |  0.4710 |
| Vd    |  0.8040 |  0.4670 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Ve    |  0.8140 |  0.4670 |
| Vf    |  0.7960 |  0.4600 |