



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:11 AM UTC

PDB ID : 8WKQ / pdb\_00008wkq  
EMDB ID : EMD-37605  
Title : Cryo-EM structure of the MS ring (C1) with export apparatus and proximal rod within the flagellar motor-hook complex in the CW state.  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-09-28  
Resolution : 3.80 Å (reported)  
Based on initial models : ., ?

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.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
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) : 2.49

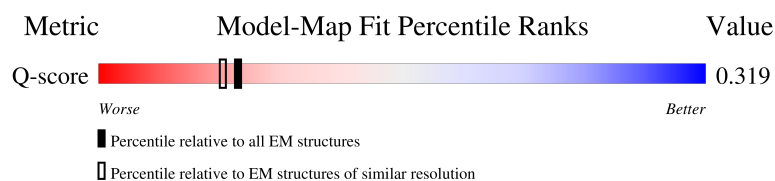
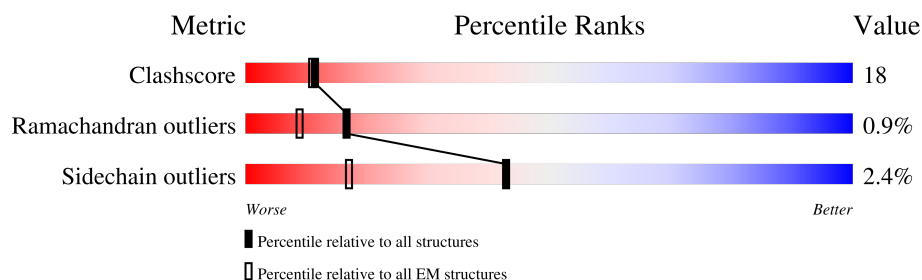
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.



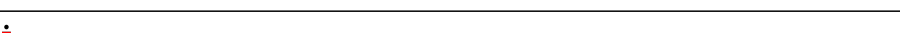
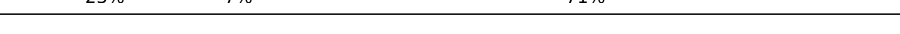
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

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   | 0     | 560    |  |
| 1   | 1     | 560    |  |
| 1   | 2     | 560    |  |
| 1   | 3     | 560    |  |

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| Mol | Chain | Length | Quality of chain                                                                                     |
|-----|-------|--------|------------------------------------------------------------------------------------------------------|
| 1   | 4     | 560    |  22% 7% 71%        |
| 1   | 5     | 560    |  22% 7% 71%        |
| 1   | 6     | 560    |  22% 7% 71%        |
| 1   | 7     | 560    |  22% 7% 71%        |
| 1   | 8     | 560    |  23% 7% 71%        |
| 1   | 9     | 560    |  23% 6% 71%        |
| 1   | AA    | 560    |  23% 6% 71%        |
| 1   | AB    | 560    |  22% 7% 71%        |
| 1   | AC    | 560    |  23% 7% 71%        |
| 1   | AD    | 560    |  22% 7% 71%        |
| 1   | AE    | 560    |  23% 6% 71%        |
| 1   | AF    | 560    |  23% 6% 71%        |
| 1   | AG    | 560    |  23% 7% 71%      |
| 1   | AH    | 560    |  22% 7% 71%      |
| 1   | AI    | 560    |  23% 7% 71%      |
| 1   | AJ    | 560    |  23% 6% 71%      |
| 1   | AK    | 560    |  23% 6% 71%      |
| 1   | AL    | 560    |  23% 6% 71%      |
| 1   | AM    | 560    |  23% 7% 71%      |
| 1   | AN    | 560    |  22% 7% 71%      |
| 1   | AO    | 560    |  22% 7% 71%      |
| 1   | AP    | 560    |  22% 7% 71%      |
| 1   | AQ    | 560    |  23% 6% 71%      |
| 1   | UI    | 560    |  8% 15% 10% 72%  |
| 1   | UJ    | 560    |  10% 14% 11% 72% |

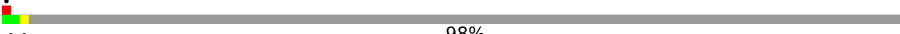
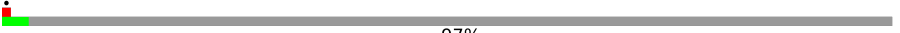
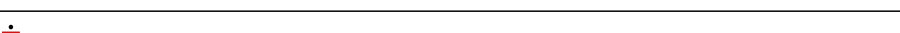
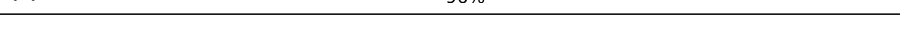
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | UK    | 560    |                  |
| 1   | UL    | 560    |                  |
| 1   | UM    | 560    |                  |
| 1   | UN    | 560    |                  |
| 1   | UO    | 560    |                  |
| 1   | UP    | 560    |                  |
| 1   | WA    | 560    |                  |
| 1   | WB    | 560    |                  |
| 1   | WC    | 560    |                  |
| 1   | WD    | 560    |                  |
| 1   | WE    | 560    |                  |
| 1   | WF    | 560    |                  |
| 1   | WG    | 560    |                  |
| 1   | WH    | 560    |                  |
| 1   | WI    | 560    |                  |
| 1   | WJ    | 560    |                  |
| 1   | WK    | 560    |                  |
| 1   | WL    | 560    |                  |
| 1   | WM    | 560    |                  |
| 1   | WN    | 560    |                  |
| 1   | WO    | 560    |                  |
| 1   | WP    | 560    |                  |
| 1   | WQ    | 560    |                  |
| 1   | WR    | 560    |                  |
| 1   | WS    | 560    |                  |

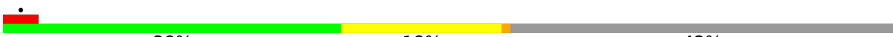
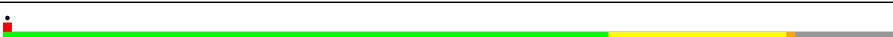
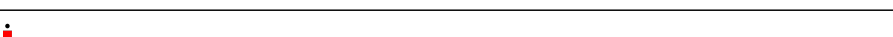
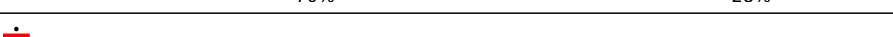
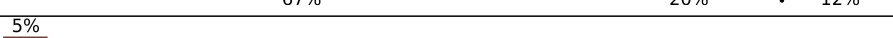
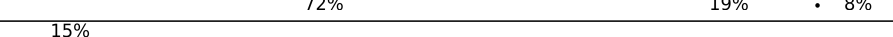
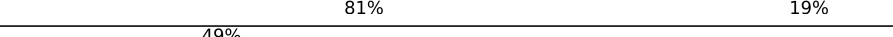
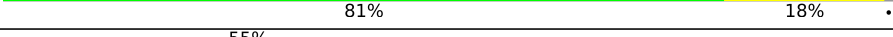
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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1   | WT    | 560    |  10% 8% .. 80% |
| 1   | WU    | 560    |  11% 8% . 80%  |
| 1   | WV    | 560    |  10% 8% . 80%  |
| 1   | WW    | 560    |  9% 9% . 80%   |
| 1   | b     | 560    |  .. 98%        |
| 1   | c     | 560    |  . 97%         |
| 1   | d     | 560    |  .. 96%        |
| 1   | e     | 560    |  .. 97%        |
| 1   | f     | 560    |  . 96%         |
| 1   | g     | 560    |  . 97%         |
| 1   | h     | 560    |  . 96%         |
| 1   | i     | 560    |  . 97%         |
| 1   | j     | 560    |  .. 96%      |
| 1   | k     | 560    |  .. 97%      |
| 1   | l     | 560    |  .. 96%      |
| 1   | t     | 560    |  22% 7% 71%  |
| 1   | u     | 560    |  22% 7% 71%  |
| 1   | v     | 560    |  23% 6% 71%  |
| 1   | w     | 560    |  23% 6% 71%  |
| 1   | x     | 560    |  23% 7% 71%  |
| 1   | y     | 560    |  22% 7% 71%  |
| 1   | z     | 560    |  22% 8% 71%  |
| 2   | A     | 89     |  73% 26% .   |
| 2   | B     | 89     |  66% 34%     |
| 2   | C     | 89     |  66% 34%     |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | D     | 89     |    |
| 3   | E     | 264    |    |
| 4   | F     | 245    |    |
| 4   | G     | 245    |    |
| 4   | H     | 245    |    |
| 4   | I     | 245    |    |
| 4   | J     | 245    |    |
| 5   | K     | 104    |    |
| 5   | L     | 104    |    |
| 5   | M     | 104    |    |
| 5   | N     | 104    |    |
| 5   | O     | 104    |    |
| 5   | P     | 104    |  |
| 6   | Q     | 138    |  |
| 6   | R     | 138    |  |
| 6   | S     | 138    |  |
| 6   | T     | 138    |  |
| 6   | U     | 138    |  |
| 7   | V     | 134    |  |
| 7   | W     | 134    |  |
| 7   | X     | 134    |  |
| 7   | Y     | 134    |  |
| 7   | Z     | 134    |  |
| 7   | a     | 134    |  |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 99073 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 Flagellar M-ring protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | UI    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UJ    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UK    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UL    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UM    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UN    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UO    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | UP    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 1   | WA    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 849   | 534 | 148 | 166 | 1 |         |       |
| 1   | WB    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 836   | 526 | 146 | 163 | 1 |         |       |
| 1   | WC    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 812   | 510 | 142 | 159 | 1 |         |       |
| 1   | WD    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 522 | 144 | 160 | 1 |         |       |
| 1   | WE    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 147 | 164 | 1 |         |       |
| 1   | WF    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 1   | WG    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 147 | 164 | 1 |         |       |
| 1   | WH    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 439 | 126 | 137 | 1 |         |       |
| 1   | WI    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 439 | 126 | 137 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | WJ    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 462 | 131 | 143 | 1 |         |       |
| 1   | WK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 729   | 456 | 130 | 142 | 1 |         |       |
| 1   | WL    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 622   | 389 | 110 | 122 | 1 |         |       |
| 1   | WM    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 596   | 372 | 107 | 116 | 1 |         |       |
| 1   | WN    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 611   | 380 | 109 | 121 | 1 |         |       |
| 1   | WO    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 448 | 127 | 138 | 1 |         |       |
| 1   | WP    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 464 | 132 | 144 | 1 |         |       |
| 1   | WQ    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 1   | WR    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 1   | WS    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 1   | WT    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 1   | WU    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 147 | 164 | 1 |         |       |
| 1   | WV    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 521 | 144 | 161 | 1 |         |       |
| 1   | WW    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 1   | b     | 13       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 81    | 50  | 15  | 16  |   |         |       |
| 1   | c     | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 1   | d     | 20       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 133   | 83  | 23  | 27  |   |         |       |
| 1   | e     | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 1   | f     | 21       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 140   | 88  | 24  | 28  |   |         |       |
| 1   | g     | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 1   | h     | 21       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 140   | 88  | 24  | 28  |   |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | i     | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 1   | j     | 20       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 133   | 83  | 23  | 27  |   |         |       |
| 1   | k     | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 1   | l     | 21       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 140   | 88  | 24  | 28  |   |         |       |
| 1   | t     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | u     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | v     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | w     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | x     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | y     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | z     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 1     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 2     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 3     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 4     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 5     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 6     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 7     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 8     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 9     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | 0     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | AA    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AB    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AC    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AD    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AE    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AF    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AG    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AH    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AI    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AJ    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AK    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AL    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AM    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AN    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AO    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AP    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 1   | AQ    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |

- Molecule 2 is a protein called Flagellar biosynthetic protein FliQ.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | A     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 2   | B     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 2   | D     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |

- Molecule 3 is a protein called Flagellar biosynthetic protein FliR.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | E     | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1945  | 1305 | 307 | 318 | 15 |         |       |

- Molecule 4 is a protein called Flagellar biosynthetic protein FliP.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | F     | 207      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1605  | 1072 | 249 | 272 | 12 |         |       |
| 4   | G     | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1626  | 1086 | 252 | 276 | 12 |         |       |
| 4   | H     | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1614  | 1077 | 251 | 274 | 12 |         |       |
| 4   | I     | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1614  | 1077 | 251 | 274 | 12 |         |       |
| 4   | J     | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | K     | 59       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 429   | 265 | 74  | 83  | 7 |         |       |
| 5   | L     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 672   | 415 | 121 | 129 | 7 |         |       |
| 5   | M     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 686   | 424 | 123 | 132 | 7 |         |       |
| 5   | N     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 686   | 424 | 123 | 132 | 7 |         |       |
| 5   | O     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 686   | 424 | 123 | 132 | 7 |         |       |
| 5   | P     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 679   | 420 | 122 | 130 | 7 |         |       |

- Molecule 6 is a protein called Flagellar basal body rod protein FlgB.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | Q     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1030  | 633 | 189 | 203 | 5 |         |       |
| 6   | R     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 583 | 172 | 182 | 5 |         |       |
| 6   | S     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 598 | 177 | 187 | 5 |         |       |
| 6   | T     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 982   | 606 | 182 | 189 | 5 |         |       |
| 6   | U     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 588 | 172 | 185 | 5 |         |       |

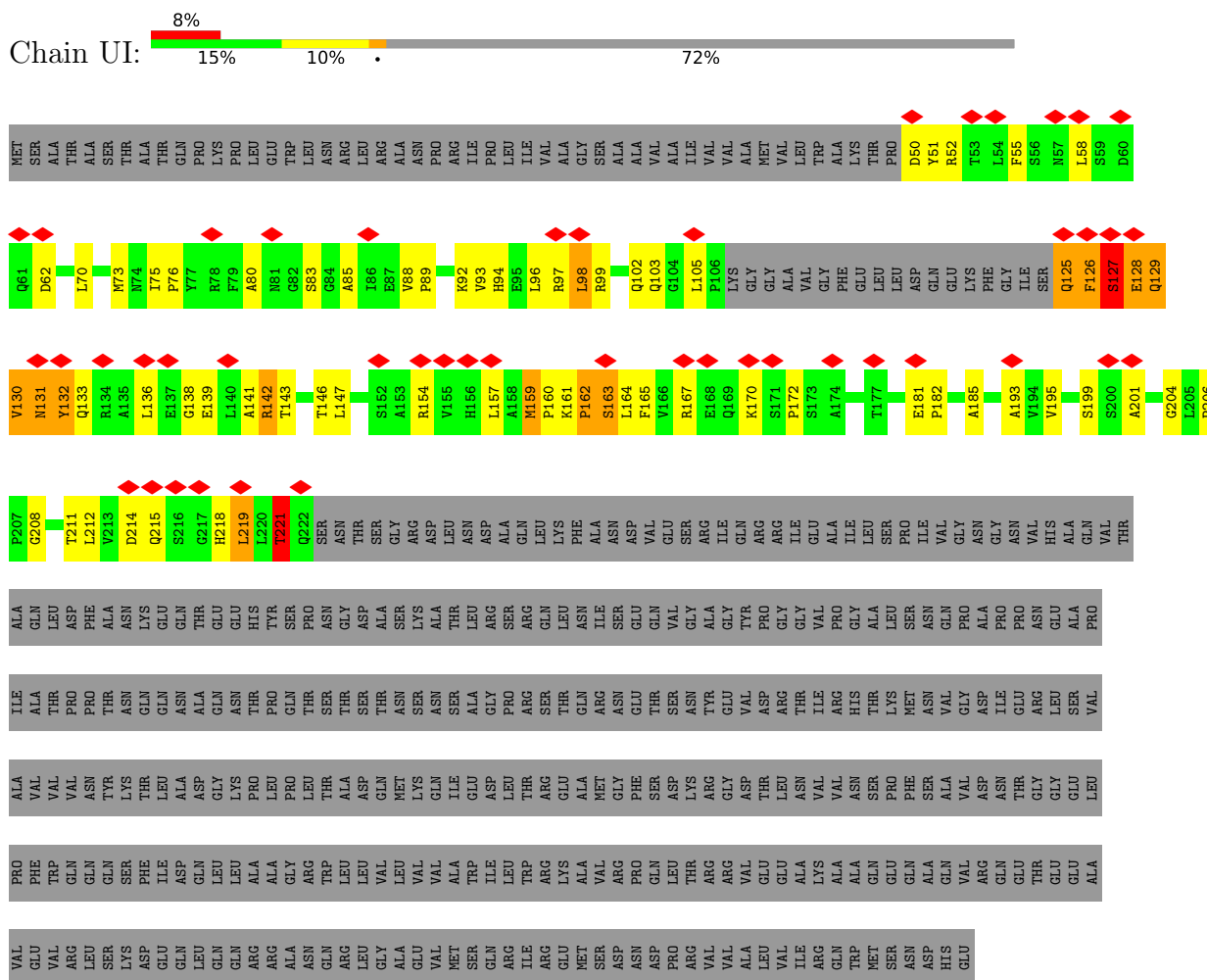
- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | V     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 7   | W     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |
| 7   | X     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 7   | Y     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 7   | Z     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 7   | a     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |

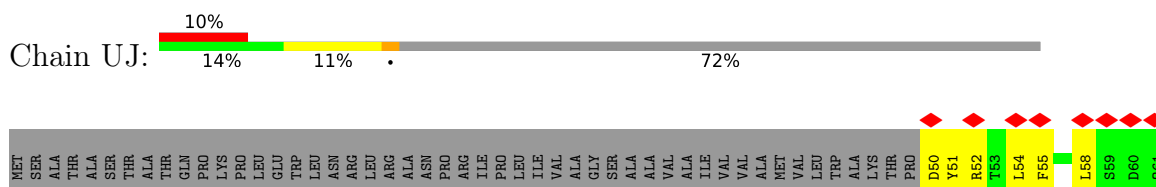
### 3 Residue-property plots

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: Flagellar M-ring protein

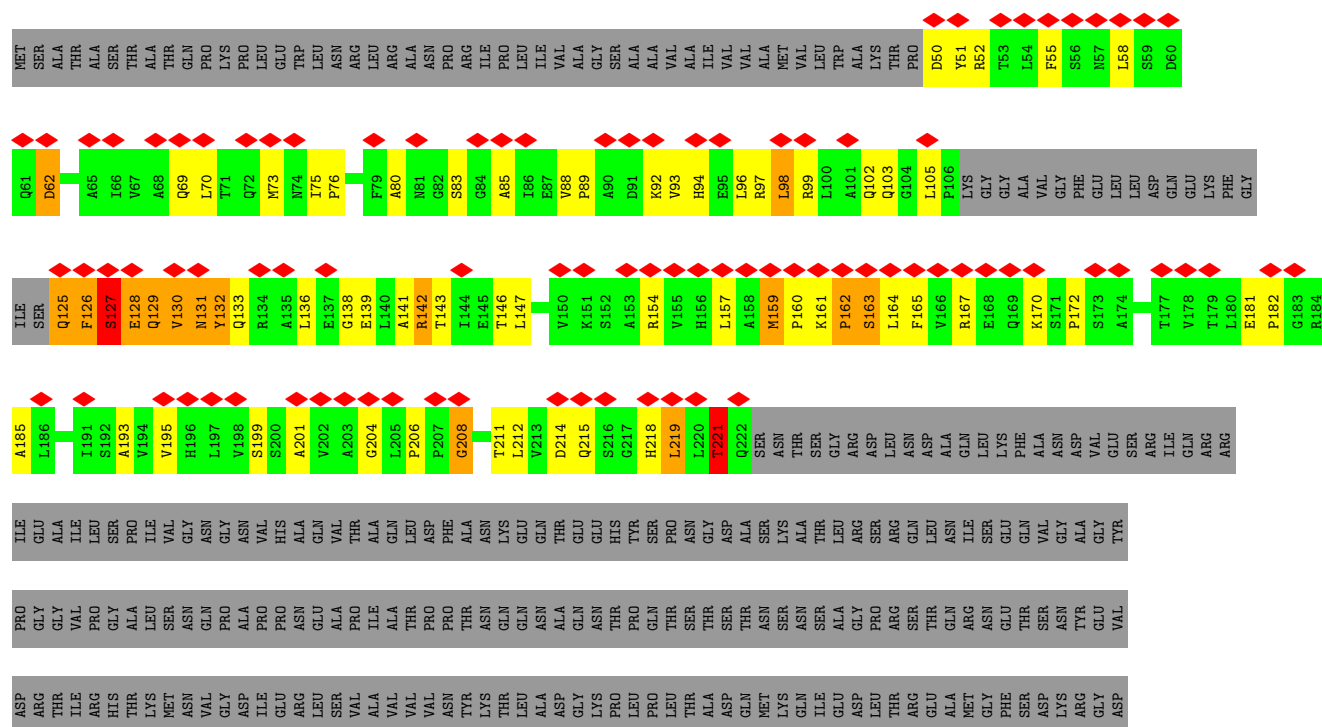


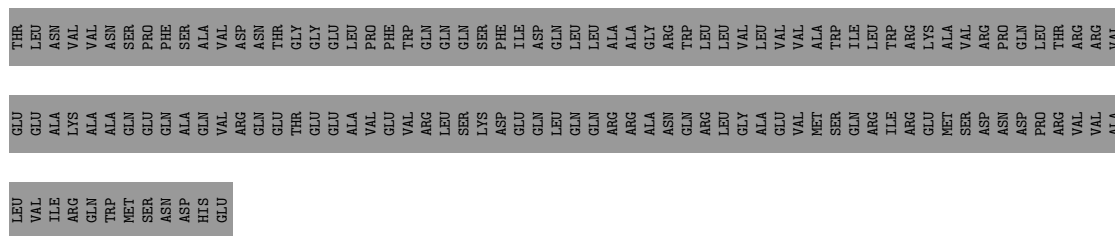
#### • Molecule 1: Flagellar M-ring protein



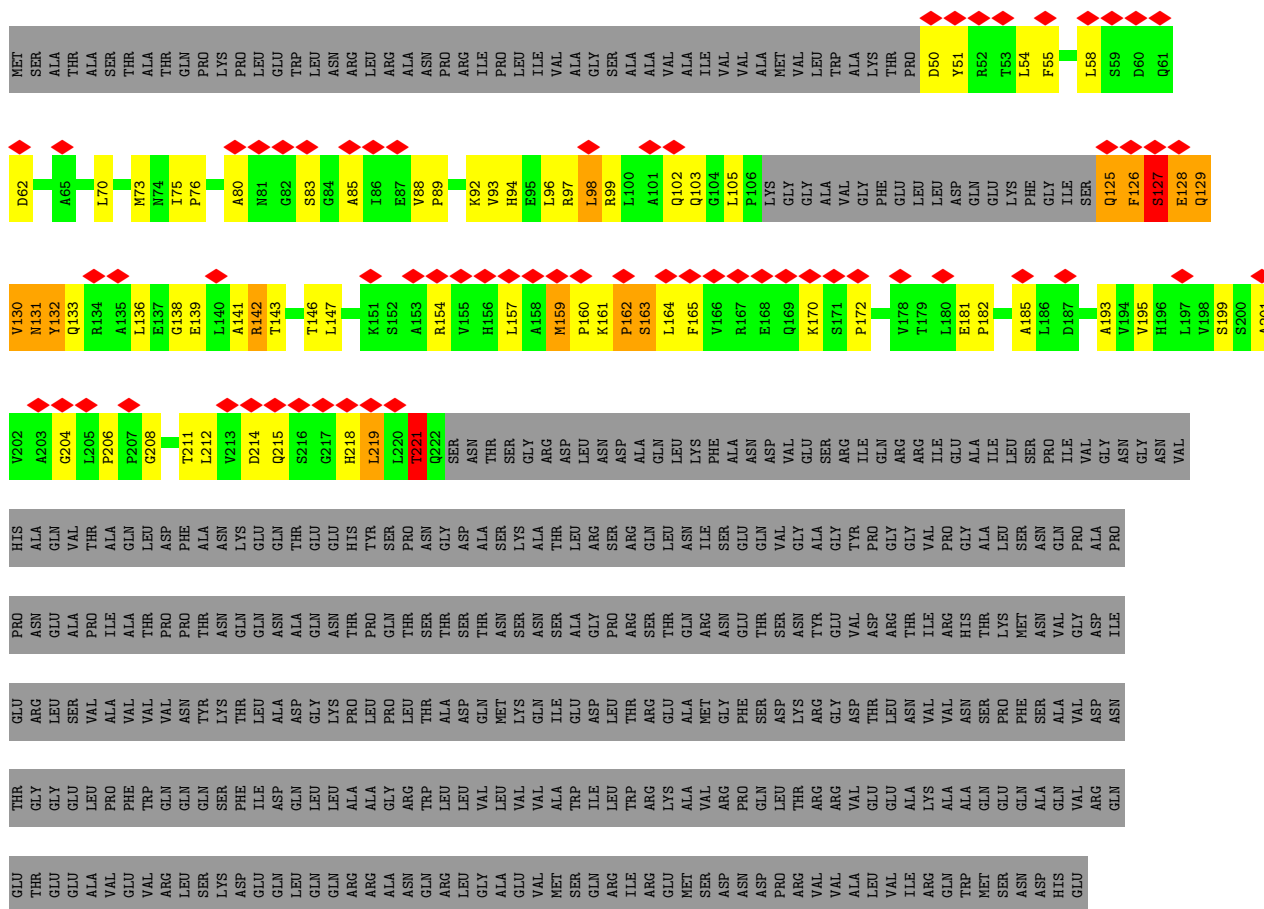




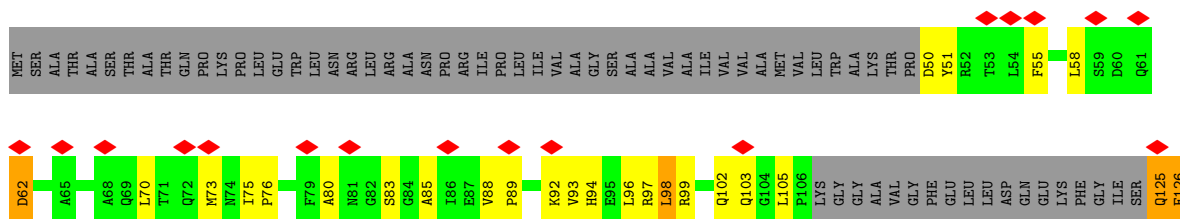




- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein







|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LYS | ASP | GLU | GLN | LEU | GLN | ARG | ARG | ASN | GLN | ARG | LEU | GLY | ALA | GLY | VAL | VAL | VAL | MET | GLN | GLN | ARG | ILE | ARG | GLU | MET | SER | SER | ASP | ASN | PRO | ASP | ARG | VAL | VAL | ALA | ALA | LEU | VAL | ILE | ARG | GLN | TRP | MET | SER | ASN | HIS | GLU |     |     |     |     |     |     |     |     |
| SER | PIE | ILE | GLN | LEU | LEU | ALA | ALA | ARG | TRP | LEU | LEU | VAL | VAL | GLY | VAL | VAL | ALA | ALA | TRP | ILE | LEU | TRP | ARG | LYS | ARG | VAL | VAL | ASP | PRO | GLN | LEU | THR | ARG | VAL | VAL | GLU | GLU | ALA | LYS | ALA | ALA | GLN | GLN | VAL | VAL | ARG | GLN | GLU | THR | GLU | GLU | VAL | ARG | LEU | SER |

- Molecule 1: Flagellar M-ring protein

[illegible]

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |       |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-------|------|------|------|------|------|
| GLN | ASP | GLY | GLY | ALA | ILE | VAL | ALA | ALA | GLN | LEU | THR | GLN | MET | ASN | ILE | TYR | ARG | PHE | ALA | ASN | GLY | SER | GLY | PRO | ALA | ASP | LYS | VAL | GLU | HIS | GLU | VAL | PRO | ALA | ASP | LYS | VAL | GLU | GLY | LEU | ARG | ARG | LEU | ALA | GLN | GLN | GLY | LEU | PRO | GLY | LYS | GLY | GLY | VII1 | GII2 | FIII3 | EII4 | LII6 | DII7 | QII8 | EII9 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| Q129 | Q130 | R134 | R135 | E139 | L140 | A141 | R142 | T143 | L144 | E145 | T146 | L147 | G148 | P149 | S152 | A153 | R154 | V155 | H156 | A158 | M159 | L164 | F165 | V166 | R167 | E168 | Q169 | K170 | S171 | P172 | S175 | E181 | P182 | G183 | R184 | A185 | L186 | L187 | Q190 | L191 | S192 | A193 | V194 | V195 | L196 | L197 | L198 | S199 | S200 | A201 | V202 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

[illegible]

LEU ASP ASP PHE ALA ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER SER ASP ASP ALA SER LYS THR THR ARG SER ARG ARG GLN LEU ASN ILE SER GLU GLN VAL GLY ALA GLY TYR PRO PRO GLY VAL PRO GLY ALA GLY LEU ASN GLN PRO PRO ALA PRO PRO GLU ALA PRO ILE ALA

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |  |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|
| THR | PRO | PRO | THR | ASN | GLN | GLN | ASN | ALA | GLN | THR | THR | PRO | GLN | THR | SER | SER | ASN | SER | ASN | ASN | SER | SER | GLY | ALA | ALA | PRO | ARG | GLU | THR | THR | THR | GLN | ARG | ASN | ASN | TYR | GLU | VAL | ASP | ARG | THR | THR | ILE | ARG | HIS | THR | LYS | MET | ASN | ASN | VAL | GLY | VAL | LEU | SER | VAL | ALA | VAL |  |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| VAL | VAL | ASN | TYR | LYS | THR | LEU | ALA | ASP | LYS | PRO | LEU | LEU | PRO | THR | ASP | GLN | MET | LYS | GLN | ILE | GLU | ASP | LEU | THR | LEU | ARG | GLU | GLU | ALA | ALA | GLY | GLY | ASP | ASP | LYS | ARG | GLY | ASP | THR | THR | LEU | ASN | VAL | VAL | ASN | ASN | PRO | PHE | SER | ALA | VAL | VAL | ASP | ASN | THR | GLY | GLY | GLU | LEU | PRO | PHE |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| TRP | GLN | GLN | GLN | PHE | IIE | ASP | GLN | LEU | LEU | ALA | ALA | GLY | ARG | TRP | LEU | VAL | VAL | VAL | ALA | TRP | IIE | LEU | TRP | PRO | GLN | THR | LEU | ARG | ARG | GLU | GIU | ALA | LYS | ALA | ALA | GLN | GLN | GLN | ALA | ALA | VAL | VAL | VAL | VAL | GLU | GLU | THR | GLU | ALA | ALA | CHG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| VAL | ARG | LEU | SER | LYS | ASP | GLU | GLN | LEU | GLN | ARG | ASN | GLN | ARG | LEU | GLU | VAL | VAL | MET | SER | ASP | ASP | PRO | ARG | VAL | VAL | ALA | LEU | VAL | ILE | ARG | GLU | MET | SER | GLN | ILE | ARG | GLU | MET | SER | ASP | ASN | ASP | PRO | ARG | VAL | VAL | ALA | LEU | VAL | ILE | ARG | GLN | TRP | MET | SER | ASN | ASP | HIS | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 1: Flagellar M-ring protein

[illegible]

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|
| CLN | ASP | GLY | GLY | ALA | ILE | VAL | ALA | VAL | GLN | LEU | THR | GLN | MET | ASN | ILE | Tyr | PRO | ARG | PHE | ALA | ASN | GLY | SER | GLY | ALA | ILE | GLU | VAL | PRO | ALA | ASP | LYS | VAL | HIS | GLU | LEU | ARG | LEU | LEU | ARG | LEU | ALA | GLN | GLN | GLY | PRO | LYS | GLY | GLY | ALA | V111 | F112 | G113 | E114 | L115 | I123 | E128 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|

|      |      |      |      |  |      |      |      |      |      |      |      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |      |  |      |      |      |      |  |      |  |      |      |      |      |      |      |      |  |      |      |      |  |  |      |      |      |  |  |      |      |  |      |      |      |  |
|------|------|------|------|--|------|------|------|------|------|------|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|--|------|------|------|------|--|------|--|------|------|------|------|------|------|------|--|------|------|------|--|--|------|------|------|--|--|------|------|--|------|------|------|--|
| Y132 | Q133 | R134 | A135 |  | E139 | L140 | L141 | R142 | T143 | I144 | F145 | T146 |  | R154 | F155 | H156 | L157 | A158 | M159 | P160 | K161 | P162 | S163 | L164 | F165 | V166 | R167 |  | S175 |  | E181 | P182 | G183 | L184 |  | D187 |  | H196 | L197 | V198 | S199 | S200 | Z201 | V202 |  | L205 | P206 | P207 |  |  | T211 | L212 | V213 |  |  | S216 | G217 |  | T221 | O222 | S223 |  |
|------|------|------|------|--|------|------|------|------|------|------|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|--|------|------|------|------|--|------|--|------|------|------|------|------|------|------|--|------|------|------|--|--|------|------|------|--|--|------|------|--|------|------|------|--|

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|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|
| ASN | THR | SR | GLY | ARG | ASP | LEU | ASN | ASN | ASP | ALA | GLN | LYS | PHE | ALA | ASP | ALA | GLN | LEU | LYS | ASP | VAL | GLU | SR | ARG | ILE | ILE | GLN | ARG | ILE | GLU | ILE | ALA | ALA | LEU | SR | PRO | THR | VAL | VAL | HIS | ASN | GLY | ASN | ASN | VAL | VAL | ASN | ASN | LYS | GLY | GLN | THR | LEU | ASP | PHE | ALA | ASN | ASN | GLN | GLU | GLU | HIS | GLU | THR | TYR | SR |
|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | ASN | GLY | ASP | ALA | SER | LYS | ALA | THR | ARG | SER | ARG | GLN | LEU | ILE | ASN | SER | GLU | GLN | VAL | GLY | ALA | GLY | TYR | PRO | GLY | GLY | GLY | VAL | PRO | GLY | ALA | ALA | ASN | GLN | PRO | PRO | PRO | PRO | ASN | ASN | GLN | GLN | ASN | ALA | ALA | THR | PRO | PRO | THR | THR | ASN | THR | PRO | PRO | GLN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

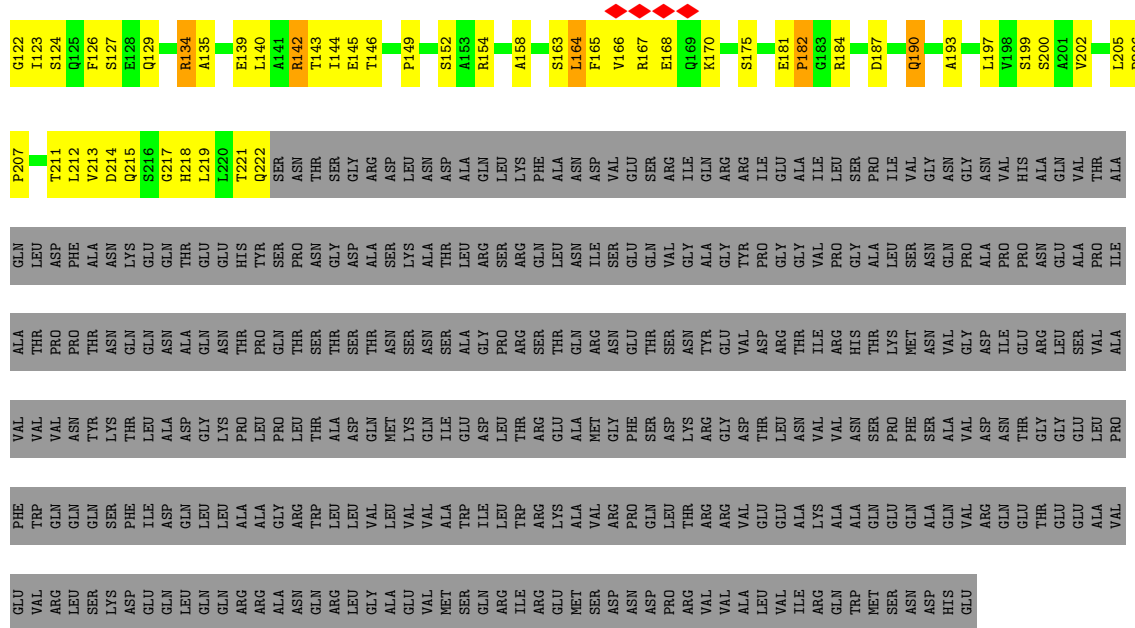
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- Molecule 1: Flagellar M-ring protein

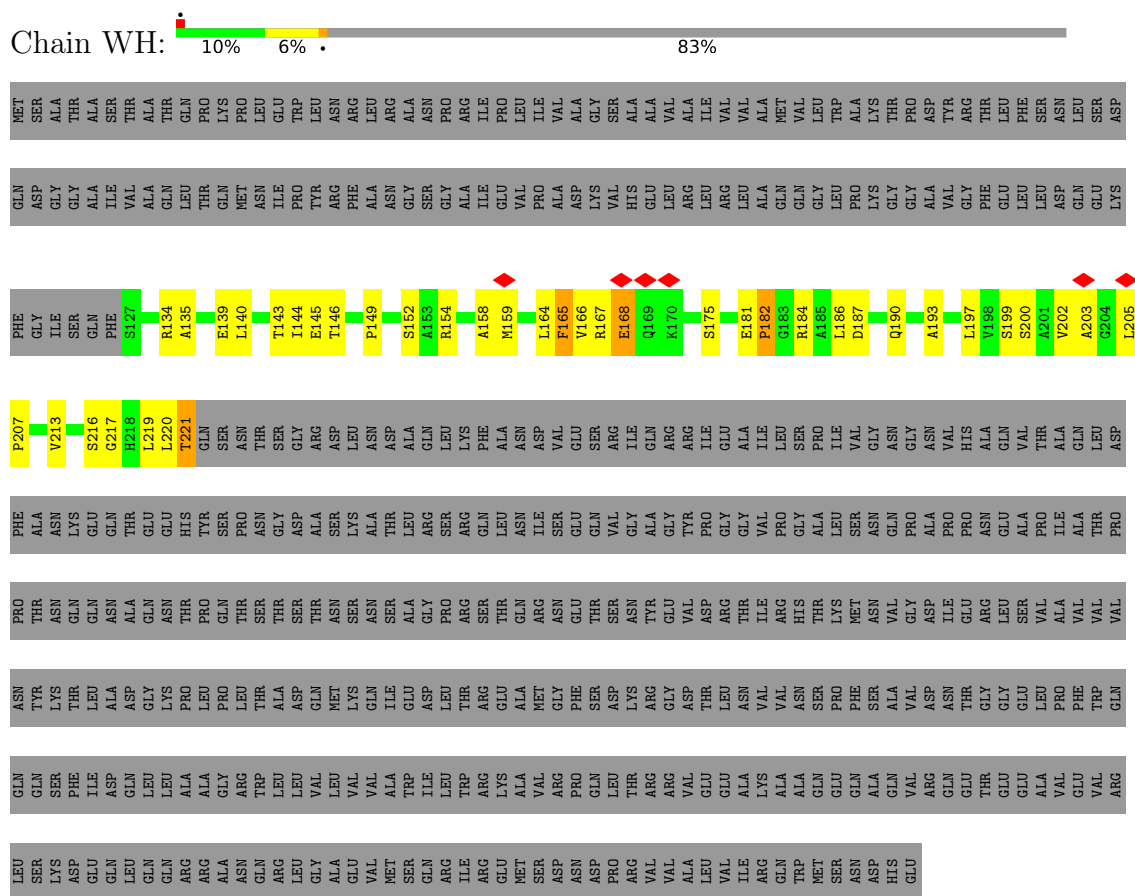
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- Molecule 1: Flagellar M-ring protein

[illegible]



• Molecule 1: Flagellar M-ring protein

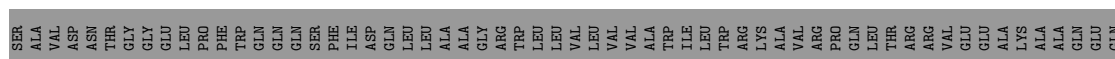
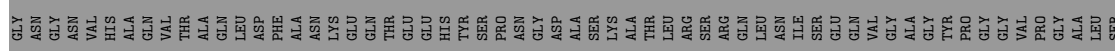
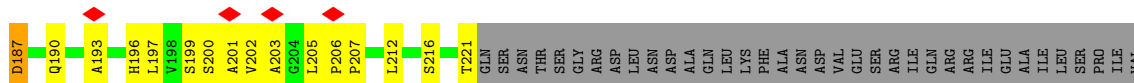
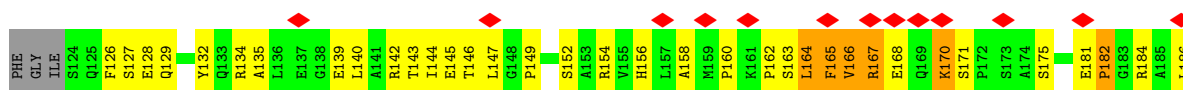
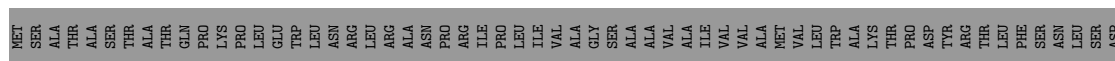


• Molecule 1: Flagellar M-ring protein

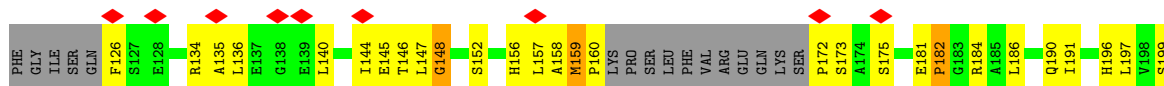
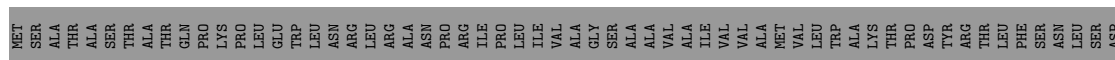


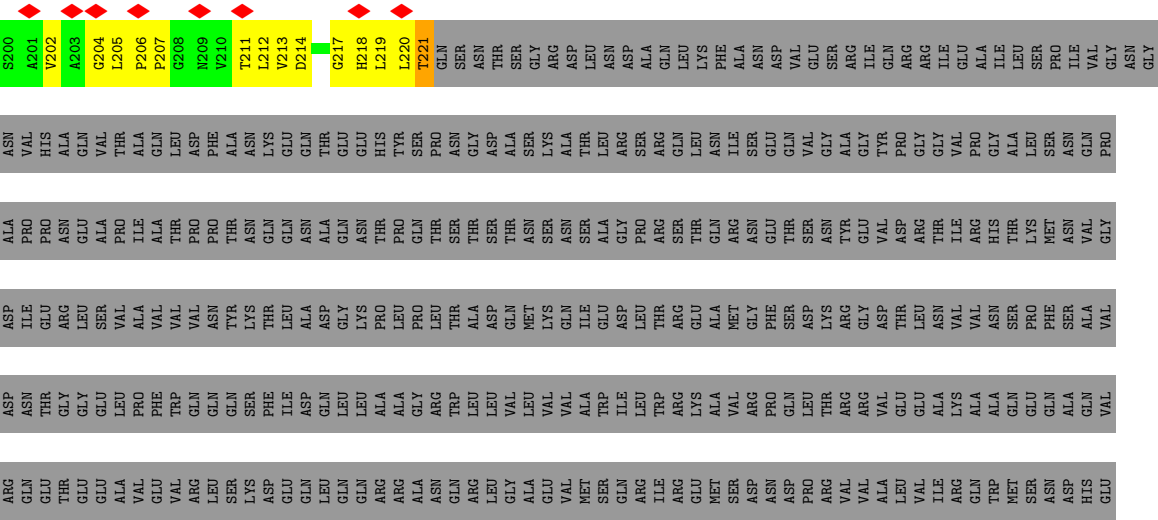


- Molecule 1: Flagellar M-ring protein

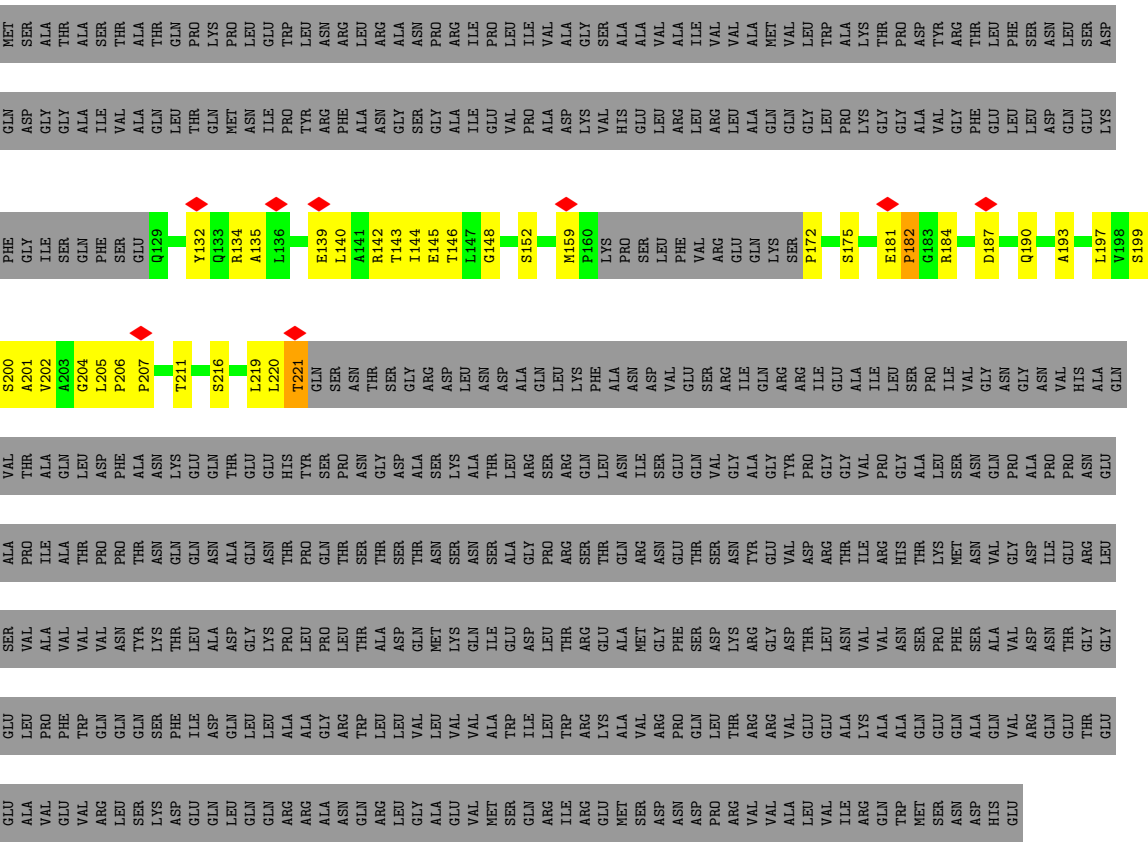


- Molecule 1: Flagellar M-ring protein

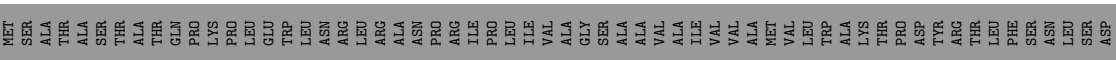




● Molecule 1: Flagellar M-ring protein



● Molecule 1: Flagellar M-ring protein

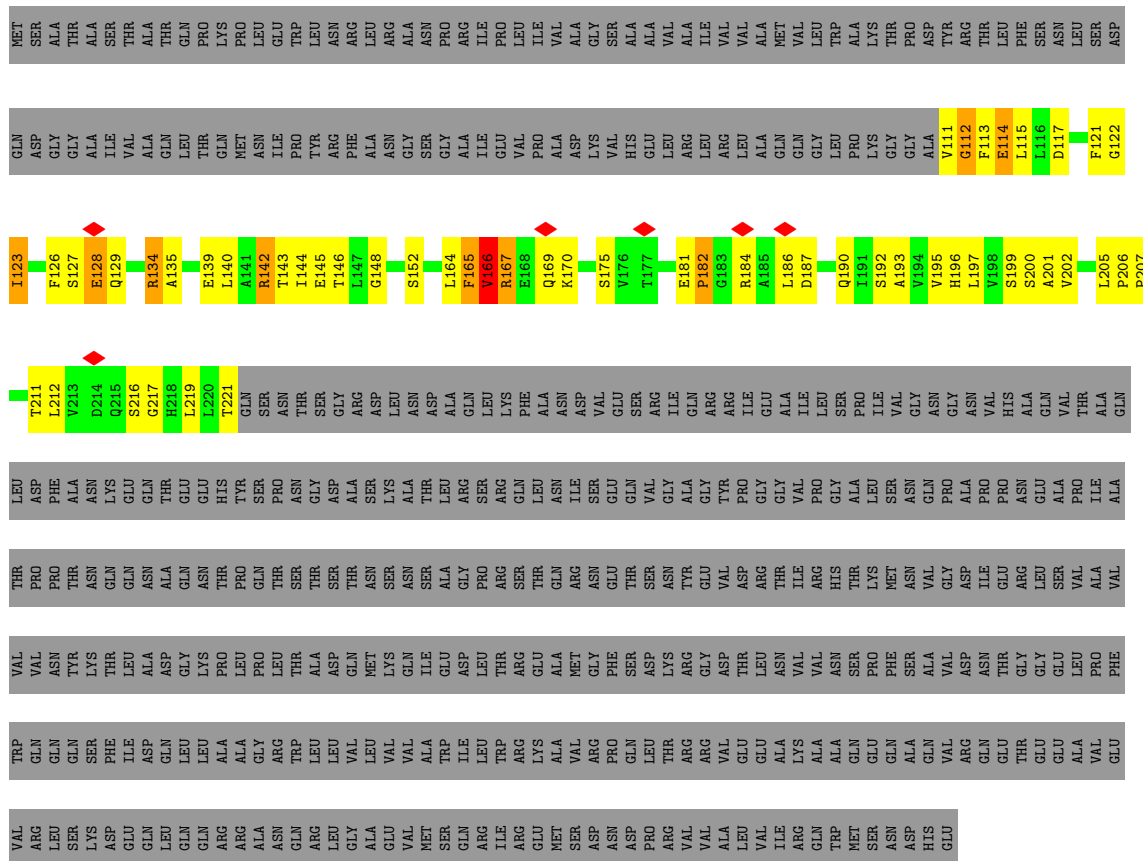




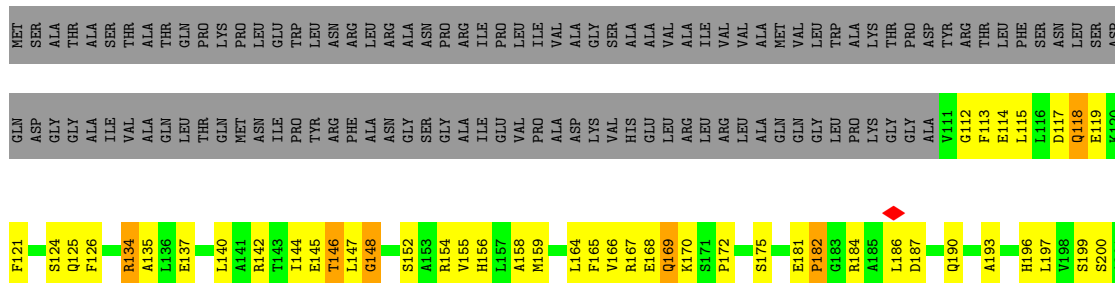


GLU GLU ALA ALA VAL GLU GLU VAL VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN GLN ARG ARG ALA ALA ASN ASN ARG GLU GLU VAL MET SER SER GLN ARG ARG ILE ILE GLU GLU MET SER ASP ASN ASP PRO ARG ARG VAL VAL ALA ALA LEU LEU ILE ILE ARG ARG MET SER ASP ASN HIS GLU

- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein







Chain WW:  9% 9% . 80%



[illegible]

- Molecule 1: Flagellar M-ring protein

[illegible][illegible]

- Molecule 1: Flagellar M-ring protein

[illegible]

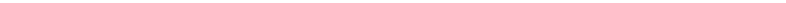


[illegible][illegible][illegible]

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|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | GLU | THR | SER | ASN | TYR | GLU | ASP | ARG  | THR  | ILE  | ARG  | HIS  | THR  | LYS  | MET  | ASN  | VAL  | GLY  | ASP  | ILE | ILE  | GLU  | ARG  | LEU  | SER | VAL | ALA | VAL | VAL | VAL | ASN | TYR | LYS | THR | LEU | ALA | ASP | GLY | LYS | PRO | LEU | PRO | LEU | LEU | THR | THR | ALA | ALA | ASP | GLN | GLN | THR | SER | THR | LYS | ILE | GLU | ASN | ASP | LEU | THR | ARG | GLU | ALA | MET |
| SER | GLU | GLN | VAL | GLY | ALA | GLY | TYR | P309 | G310 | G311 | P312 | P313 | G314 | A315 | L316 | S317 | N318 | Q319 | P320 | ARG | A321 | P322 | P323 | N324 | GLU | ALA | VAL | PRO | ILE | ALA | THR | PRO | PRO | THR | ASN | GLN | GLN | ASN | ALA | GLN | ASN | THR | THR | ASN | PRO | GLN | THR | THR | SER | SER | THR | ASN | GLY | PRO | ARG | SER | THR | GLN |     |     |     |     |     |     |     |

[illegible]

- Molecule 1: Flagellar M-ring protein

Chain h:  96%

[illegible]

- Molecule 1: Flagellar M-ring protein

Chain i:  97%

[illegible]

- Molecule 1: Flagellar M-ring protein

[illegible]

- Molecule 1: Flagellar M-ring protein





- Molecule 1: Flagellar M-ring protein



|     |     |     |
|-----|-----|-----|
| PHE | GLN | MET |
| GLY | ASP | SER |
| ILE | GLY | ALA |
| SER | GLY | THR |
| GLN | ALA | ALA |
| PHE | ILE | SER |
| SER | VAL | THR |
| GLU | ALA | ALA |
| GLN | GLN | THR |
| VAL | LEU | GLN |
| ASN | THR | PRO |
| TYR | GLN | LYS |
| GLN | MET | PRO |
| ARG | ASN | LEU |
| ALA | ILE | GLU |
| LEU | PRO | TRP |
| GLU | TYR | LEU |
| GLY | ARG | ASN |
| GLU | PHE | ARG |
| LEU | ALA | LEU |
| ALA | ASN | ARG |
| ARG | GLY | ALA |
| THR | SER | ASN |
| ILE | GLY | PRO |
| GLU | ALA | ARG |
| THR | ILE | ILE |
| LEU | GLU | PRO |
| GLY | VAL | LEU |
| PRO | PRO | ILE |
| VAL | ALA | VAL |
| LYS | ASP | ALA |
| SER | LYS | GLY |
| ALA | VAL | SER |
| ARG | HIS | ALA |
| VAL | GLU | ALA |
| HIS | LEU | VAL |
| LEU | ARG | ALA |
| ALA | LEU | ILE |
| MET | ARG | VAL |
| PRO | LEU | VAL |
| LYS | ALA | ALA |
| PRO | GLN | MET |
| SER | GLN | VAL |
| LEU | GLY | LEU |
| PHE | LEU | TRP |
| VAL | PRO | ALA |
| ARG | LYS | LYS |
| GLU | GLY | THR |
| GLN | GLY | PRO |
| LYS | ALA | ASP |
| SER | VAL | TYR |
| PRO | GLY | ARG |
| SER | PHE | THR |
| ALA | GLU | LEU |
| SER | LEU | PHE |
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| THR | ASN | ASN |
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| ILE | LYS | SER |

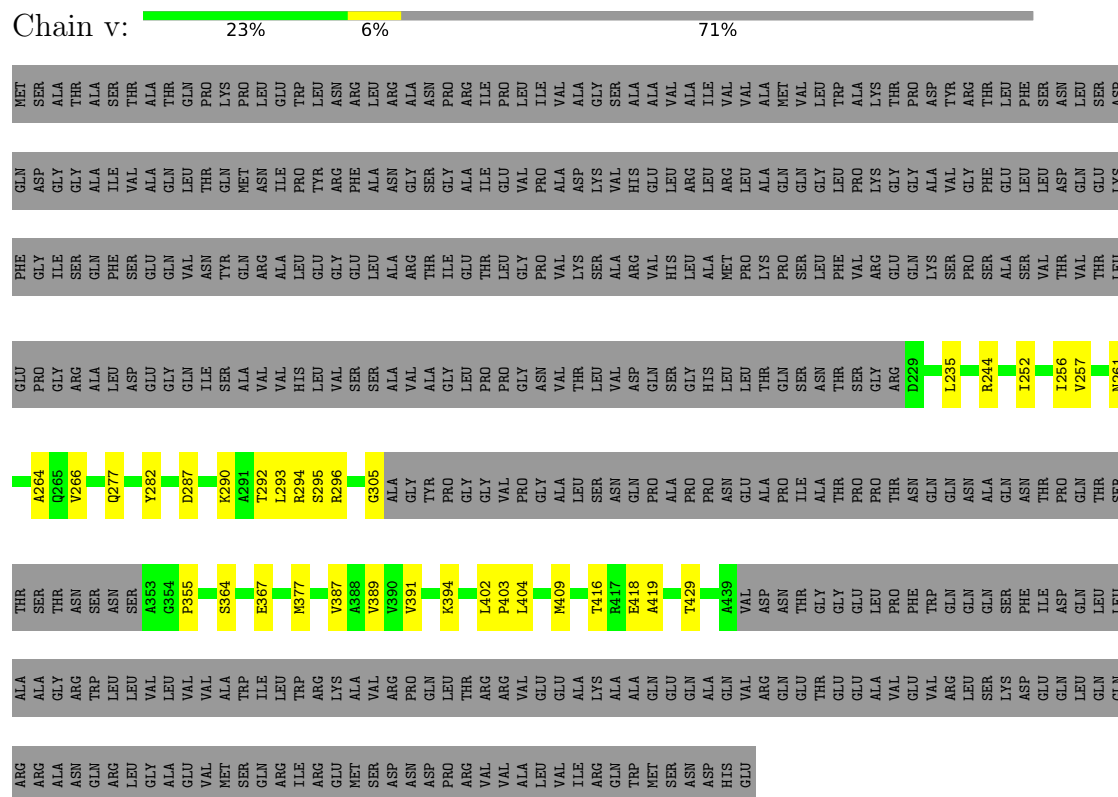
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|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|
|  | GLU  | PRO  | GLY  | ARG  | ALA  | LEU  | ASP  | GLU  | GLN  | ILE  | SER  | ALA  | VAL  | VAL  | HIS  | LEU | VAL | SER | SER | ALA | VAL | ALA | GLY | LEU | PRO | PRO | GLY | ASN | VAL | THR | THR | GLN | SER | GLY | HIS | LEU | LEU | THR | GLN | SER | ASN | THR | SER | GLY | ARG | L229 | L235 | R244 | I252 | T256 | V257 | V261 |     |     |
|  | A264 | Q265 | V266 | Q277 | T278 | Y282 | D287 | K290 | L291 | T292 | L293 | R294 | S295 | R296 | G305 | ALA | GLY | TYR | PRO | GLY | GLY | PRO | VAL | PRO | GLY | ALA | LEU | SER | ASN | GLN | PRO | PRO | PRO | PRO | GLU | ASN | ALA | ALA | GLN | ILE | ALA | THR | PRO | PRO | PRO | GLM  | GLM  | ALA  | GLN  | ASN  | THR  | PRO  | GLM | THR |

[illegible]

- Molecule 1: Flagellar M-ring protein

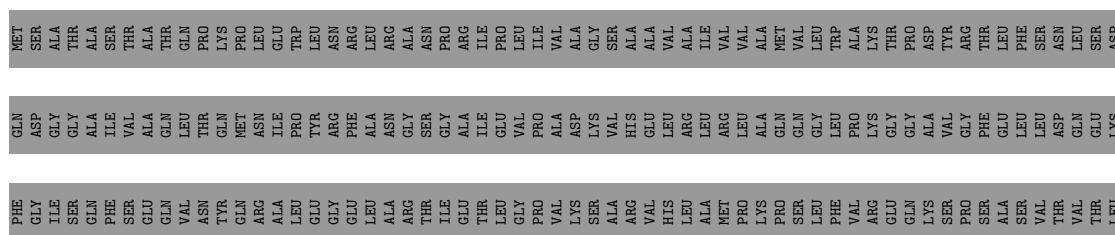
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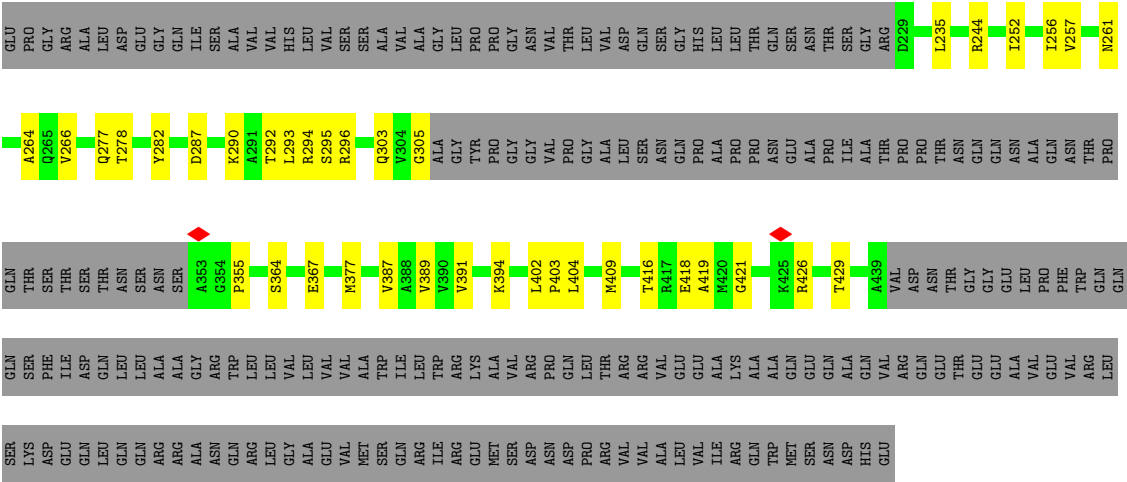
- Molecule 1: Flagellar M-ring protein



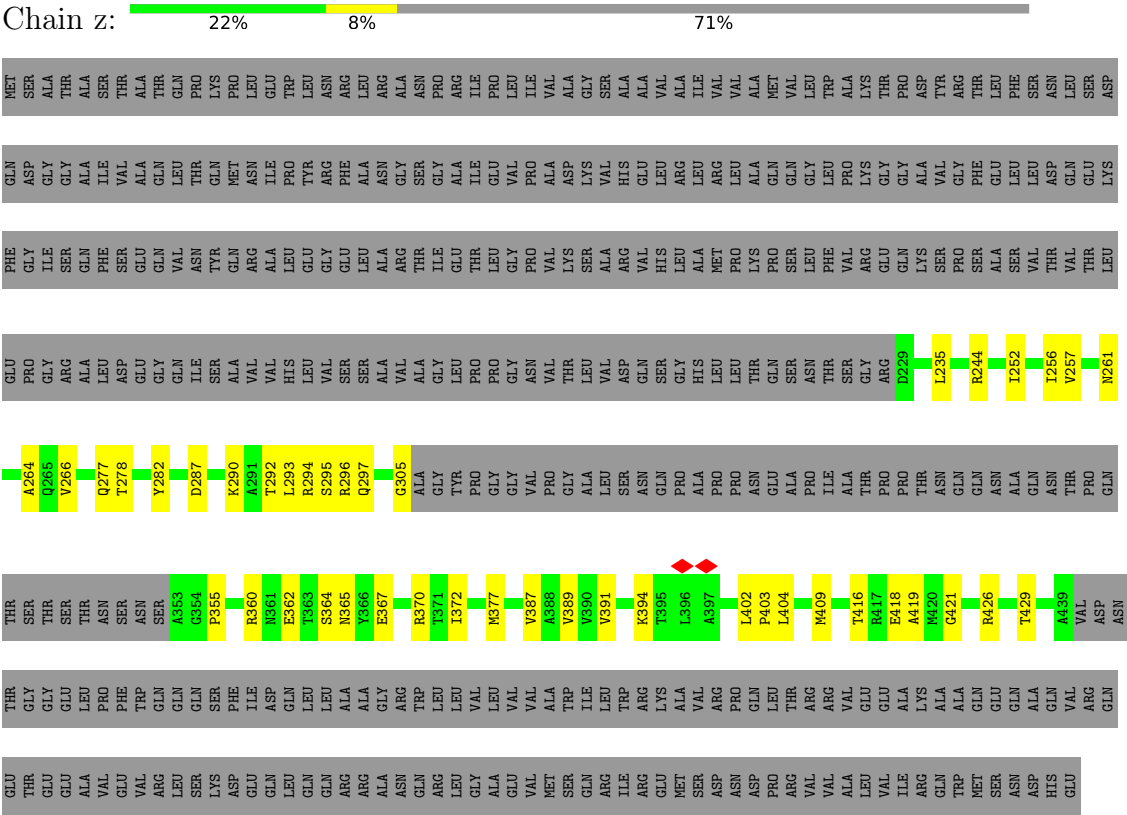
- Molecule 1: Flagellar M-ring protein



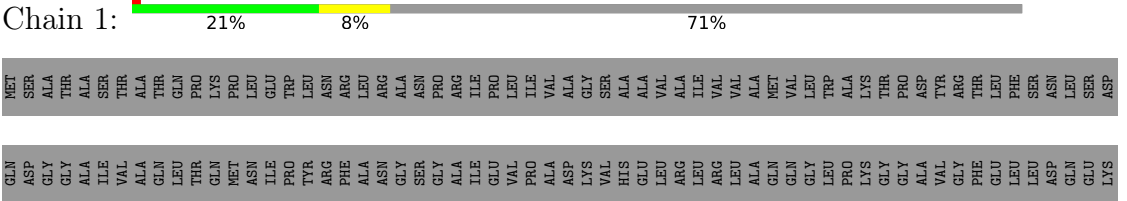




● Molecule 1: Flagellar M-ring protein



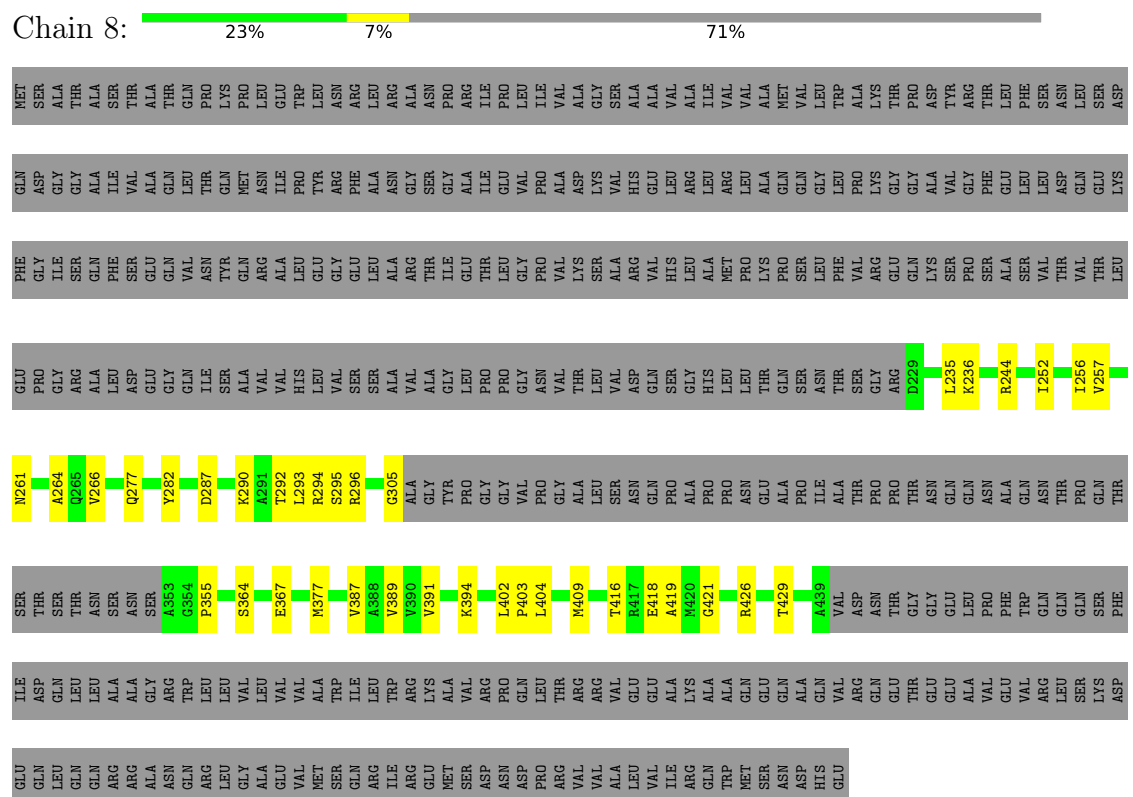
● Molecule 1: Flagellar M-ring protein











Chain 9:  23% 6% 71%

Chain 0:  23% 6% 71%





|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PHE | TRP | GLN | GLN | GLN | SER | PHE | ILE | ASP | GLN | LEU | LEU | ALA | ALA | GLY | ARG | TRP | LEU | LEU | VAL | VAL | VAL | LYS | ALA | VAL | ARG | ARG | GLN | LEU | THR | ARG | VAL | GLU | GLU | ALA | LYS | ALA | ALA | GLN | GLN | GLN | GLN | ARG | GLN | GLU | THR | GLU | GLU | GLU | ALA | VAL | ALA |     |     |     |     |     |     |     |     |
| GLU | VAL | ARG | LEU | SER | LYS | ASP | GLU | GLN | LEU | GLN | GLN | ARG | ARG | ALA | ALA | ASN | GLN | ARG | LEU | GLY | ALA | GLU | VAL | VAL | VAL | MET | SER | GLN | ILE | ARG | GLN | GLN | ILE | THR | PRO | ASP | ASN | ASP | PRO | ARG | VAL | VAL | ALA | LEU | VAL | VAL | ILE | ARG | GLN | GLN | ASP | HIS | THR | GLU | GLU | GLU | ALA | VAL | ALA |

- Molecule 1: Flagellar M-ring protein

Chain AC:  23% 7% 71%

[illegible]

GLN ASP GLY GLY ALA ALA VAL ILE VAL ASP LEU LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ALA GLY SER SER GLY ALA ILE GLU VAL VAL PRO PRO ALA ALA ASP LYS VAL VAL HIS HIS GLU LEU LEU ARG ARG ARG ALA ALA GLN GLN GLY LEU LEU PRO PRO LYS LYS GLY GLY ALA VAL VAL PHE PHE GLU LEU LEU ASP ASP GLN GLN LYS

PHE GLY ILE SER GLN PHE SER GLU GLN GLN VAL VAL ASN TYR GLN ARG ALA ARG ARG THR THR ILE GLU GLU LEU LEU GLY VAL PRO PRO LYS SER SER ALA ALA MET NET PRO PRO LYS PRO SER SER PHE VAL VAL ARG ARG GLU GLN LYS SER SER PRO PRO ALA ALA SER VAL THR THR VAL THR THR

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| GLU | PRO | GLY | ARG | ALA | LEU | ASP | GLU | GLY | GLN | ILE | SER | ALA | VAL | HIS | LEU | VAL | SER | SER | ALA | VAL | ALA | GLY | LEU | PRO | PRO | GLY | ASN | VAL | THR | VAL | ASP | SER | SER | GLY | HIS | LEU | LEU | THR | THR | GLN | SER | ASN | THR | SER | SER | GLY | ARG | D229 | L235 | R244 | I262 | V267 | V261 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|

[illegible]

|     |     |     |     |     |     |     |     |     |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |             |            |            |            |            |            |            |            |            |            |            |            |            |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| THR | SER | THR | THR | ASN | SER | ASN | SER | ASN | <b>A353</b> | <b>G354</b> | <b>P355</b> | <b>S364</b> | <b>E367</b> | <b>R370</b> | <b>T371</b> | <b>I372</b> | <b>R373</b> | <b>H374</b> | <b>M377</b> | <b>V387</b> | <b>A388</b> | <b>V389</b> | <b>V390</b> | <b>V391</b> | <b>K394</b> | <b>G399</b> | <b>L402</b> | <b>P403</b> | <b>L404</b> | <b>M409</b> | <b>T416</b> | <b>R417</b> | <b>E418</b> | <b>A419</b> | <b>T429</b> | <b>A439</b> | <b>V41</b> | <b>ASP</b> | <b>ASN</b> | <b>THR</b> | <b>GLY</b> | <b>GLY</b> | <b>GLY</b> | <b>LEU</b> | <b>PRO</b> | <b>PHE</b> | <b>TRP</b> | <b>GLN</b> |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLN | SER | PHE | ASP | GLN | LEU | LEU | ALA | ALA | GLY | ARG | TRP | LEU | LEU | VAL | VAL | VAL | TRP | ILE | LEU | TRP | ARG | LYS | ALA | VAL | ARG | PRO | GLN | LEU | THR | ARG | ARG | VAL | GLU | GLU | ALA | ALA | LYS | ALA | GLN | VAL | GLN | GLN | THR | GLU | GLU | ALA | VAL | ARG | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | LYS | ASP | GLU | GLN | LEU | GLN | GLN | ARG | ARG | ALA | ASN | GLN | ARG | LEU | GLY | ALA | GLU | VAL | MET | SER | GLN | ARG | ILE | ARG | GLU | MET | SER | ASP | ASN | ASP | PRO | VAL | VAL | ALA | LEU | ILE | ARG | TRP | MET | SER | ASN | ASP | GLN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 1: Flagellar M-ring protein

Chain AD: 

[illegible]

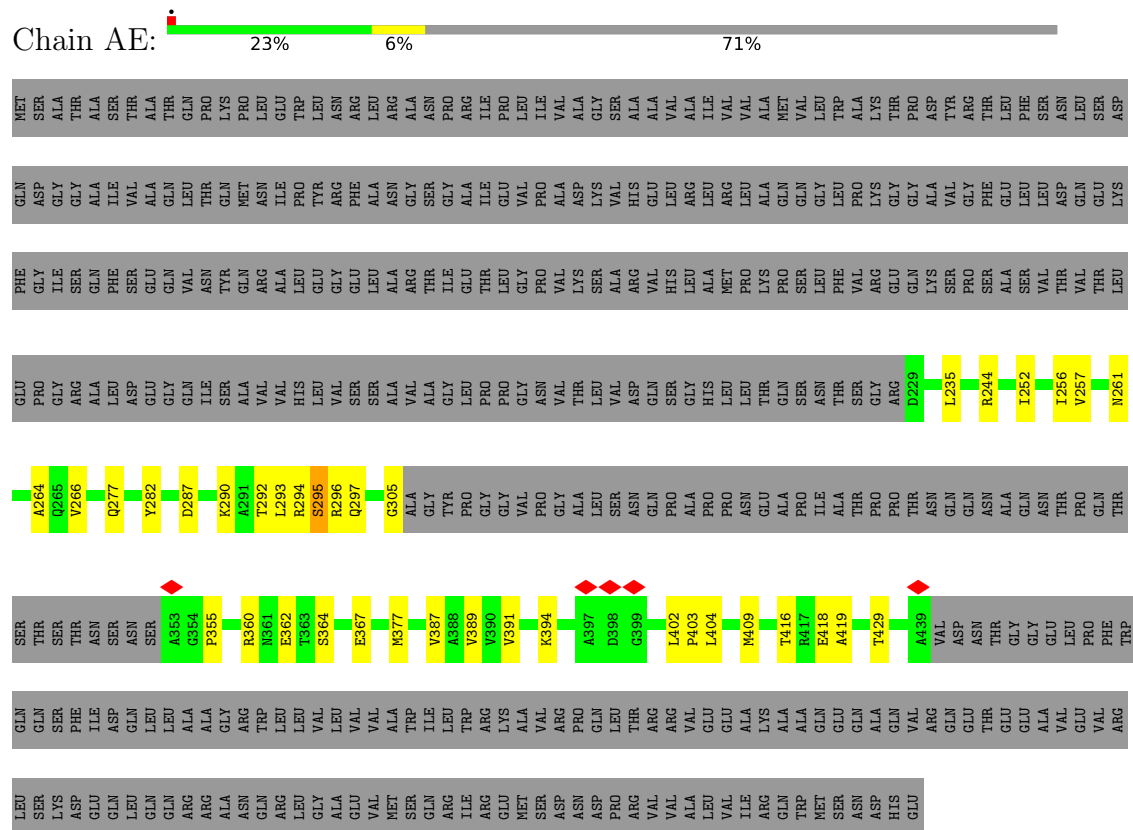
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLN | ASP | GLY | GLY | ALA | ILE | VAL | ALA | ALA | LEU | THR | GLN | MET | ASN | ILE | PRO | TYR | ARG | PHE | ALA | ASN | GLY | SER | GLY | ALA | ILE | GLU | VAL | PRO | ALA | ASP | LYS | HIS | VAL | HIS | GLU | LEU | LEU | ARG | LEU | ALA | GLN | GLN | GLY | LEU | PRO | GLY | LYS | GLY | GLY | VAL | ALA | ALA | PHE | GLY | GLU | LEU | LEU | ASP | GLN | GLN | GLY | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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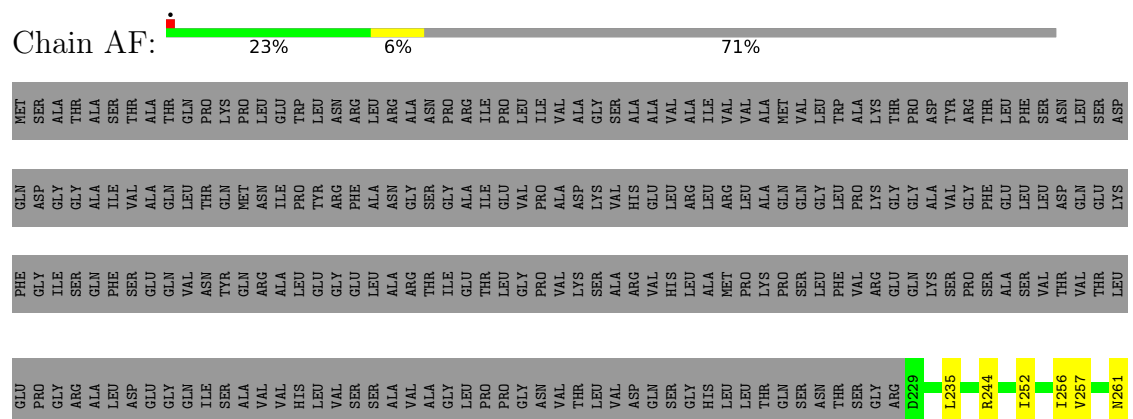
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|--|------|--|------|--|------|--|------|--|------|--|------|
| GLU | PRO | GLY | ARG | ALA | LEU | ASP | GLU | GLY | GLN | ILE | SER | ALA | VAL | VAL | HIS | LEU | VAL | SER | SER | ALA | VAL | VAL | GLY | ASN | VAL | THR | LEU | LEU | LEU | THR | GLN | SER | GLY | HIS | ASN | THR | SER | THR | GLY | ARG | L239 |  | L235 |  | R244 |  | L262 |  | L256 |  | V257 |  | V261 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|--|------|--|------|--|------|--|------|--|------|--|------|

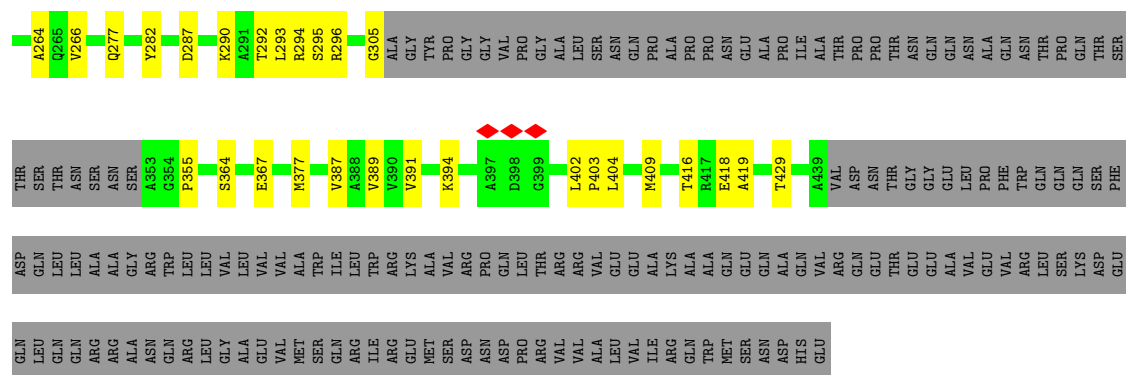
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 Q265  
 V266  
 Q277  
 Y282  
 D287  
 K290  
 A291  
 T292  
 L293  
 R294  
 S295  
 R296  
 Q297  
 G305  
 ALA  
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- Molecule 1: Flagellar M-ring protein

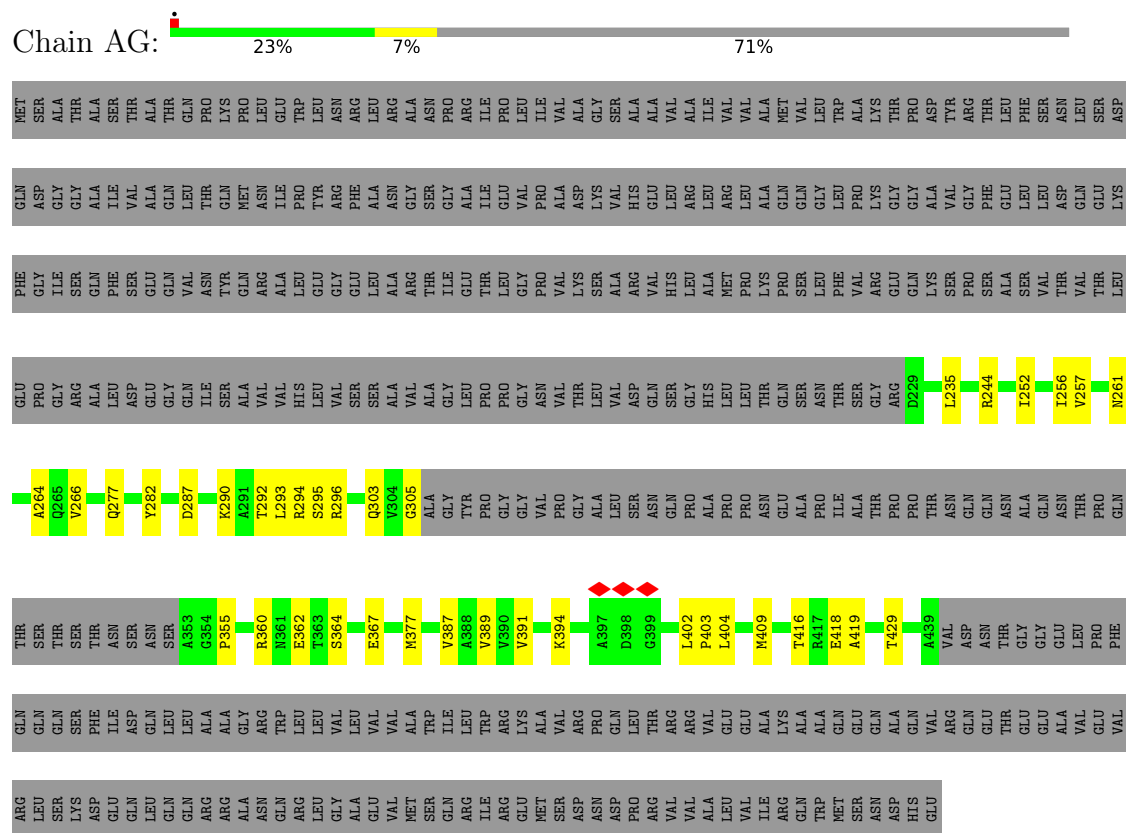


- Molecule 1: Flagellar M-ring protein

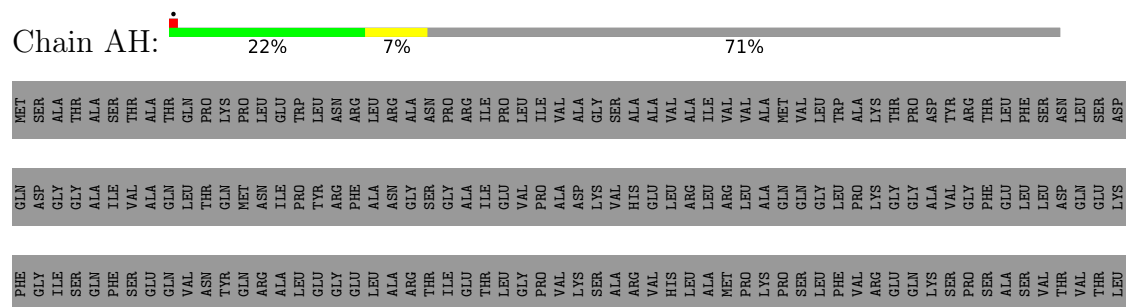




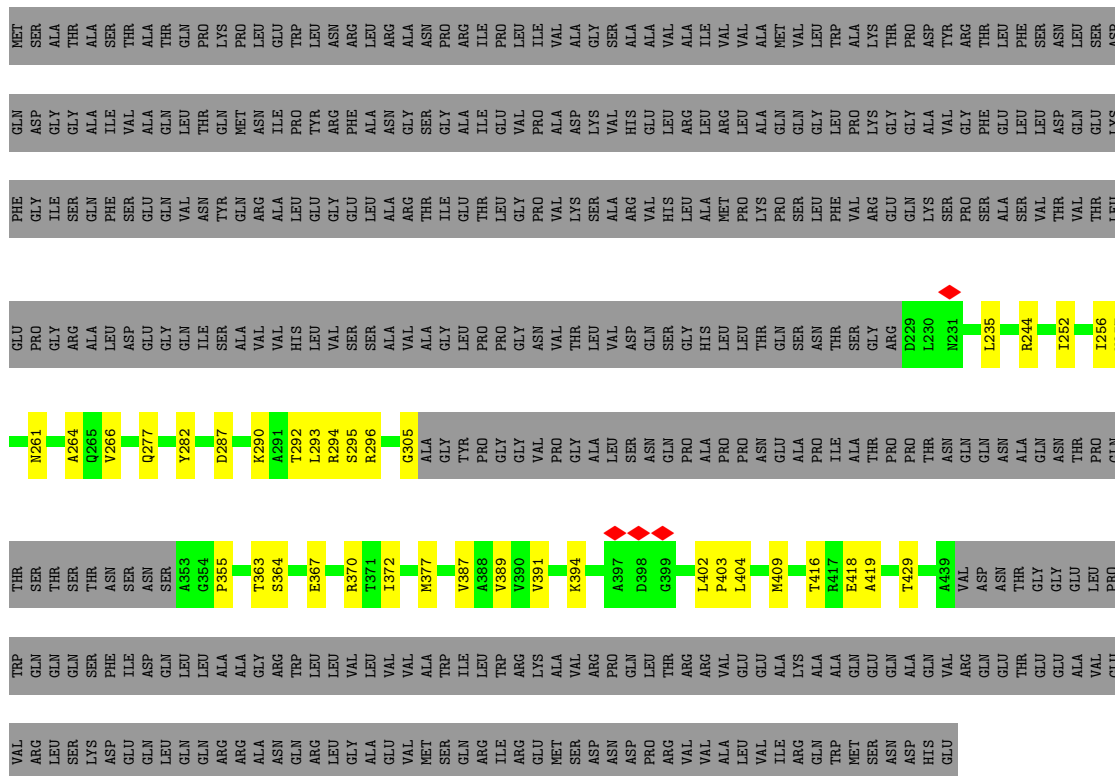
• Molecule 1: Flagellar M-ring protein



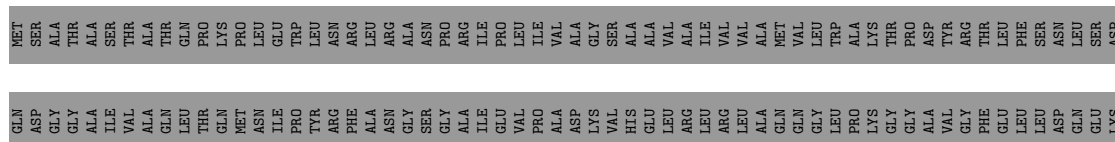
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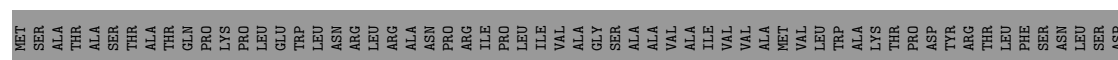


- Molecule 1: Flagellar M-ring protein

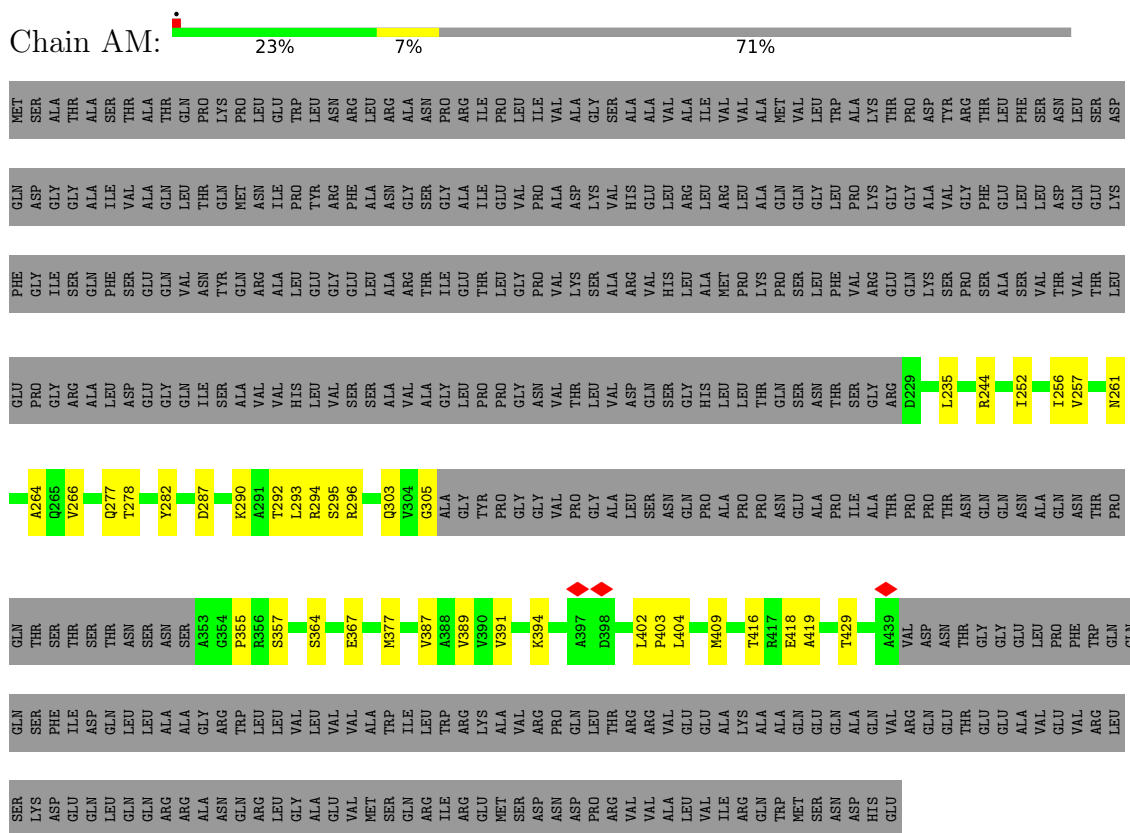


- Molecule 1: Flagellar M-ring protein





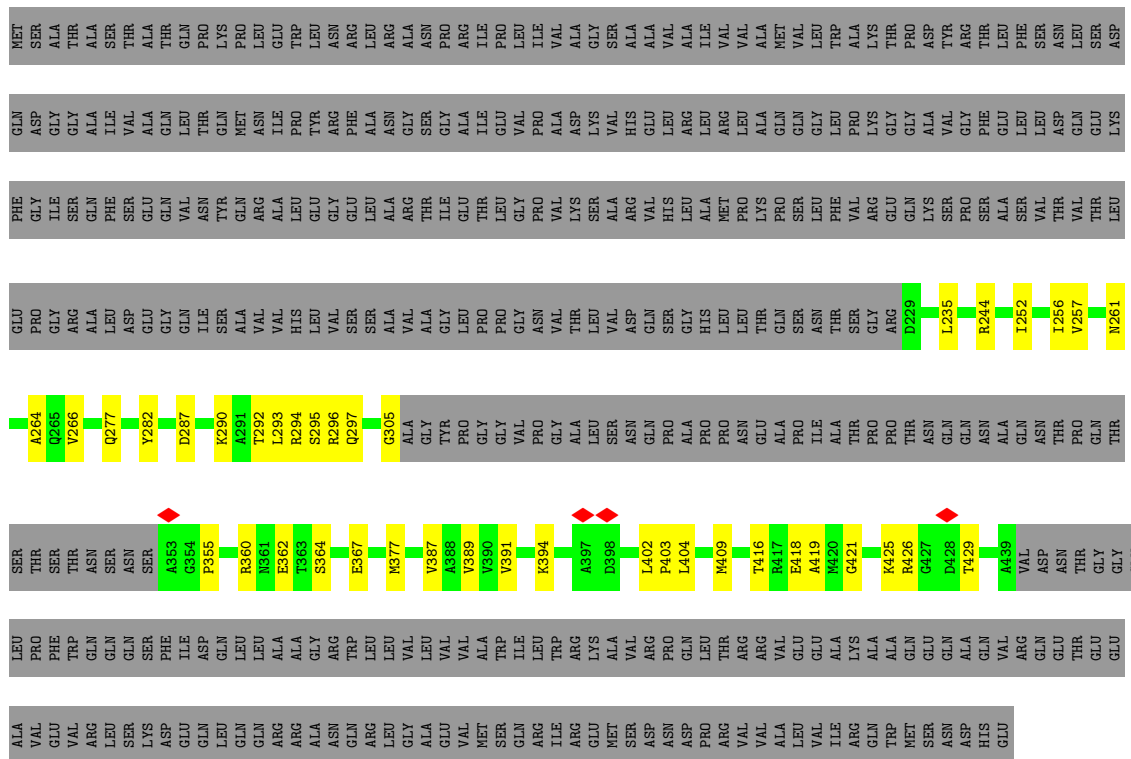
- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein

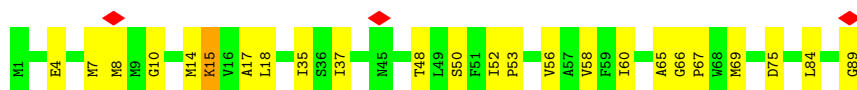
[illegible]

Chain AQ: 

|     |     |      |  |      |     |     |     |     |
|-----|-----|------|--|------|-----|-----|-----|-----|
| ASP | PHE | THR  |  | A264 | GLU | PHE | GLN | MET |
| GLU | ILE | SER  |  | A264 | PRO | ILE | ASP | SER |
| GLN | THR | THR  |  | Q265 | GLY | GLY | GLY | THR |
| GLN | LEU | THR  |  | V266 | ALA | GLN | ALA | THR |
| GLN | LEU | ASN  |  | E276 | LEU | PHE | ILE | SER |
| ARG | ALA | SER  |  | Q277 | ASP | SER | VAL | THR |
| ARG | ALA | ASN  |  | T278 | GLY | GLU | ALA | THR |
| ALA | GLY | SER  |  | Y282 | GLN | GLN | LEU | GLN |
| ASN | ARG | A353 |  | Y282 | GLN | VAL | THR | GLN |
| GLN | TRP | G354 |  | D387 | ILE | ASN | THR | LYS |
| ARG | LEU | P355 |  |      | SER | TYR | MET | PRO |
| LEU | LEU |      |  | K290 | ALA | GLN | GLN | PRO |
| GLY | VAL | S364 |  | A291 | VAL | ARG | ASN | LEU |
| ALA | LEU |      |  | T292 | VAL | ALA | ILE | LEU |
| GLU | VAL | E367 |  | L293 | HIS | GLY | PRO | TRP |
| VAL | VAL |      |  | R294 | LEU | LEU | TYR | LEU |
| MET | ALA | H374 |  | R294 | VAL | GLY | ARG | ASN |
| SER | TRP |      |  | R295 | SER | GLU | PHE | ARG |
| GLN | ILE | M377 |  | R296 | SER | LEU | ALA | ARG |
| ARG | LEU |      |  | G305 | ALA | ALA | ASN | ARG |
| ILE | TRP | V387 |  |      | VAL | ARG | GLY | ALA |
| ARG | ARG | A386 |  | ALA  | VAL | THR | SER | ASN |
| GLU | LYS | V389 |  | GLY  | GLY | ILE | GLY | PRO |
| MET | ALA | V390 |  | TYR  | LEU | GLU | ALA | ARG |
| SER | VAL | V391 |  | PRO  | PRO | THR | ILE | ILE |
| ASP | ARG |      |  | GLY  | PRO | THR | ILE | PRO |
| ASN | GLN | K394 |  | GLY  | GLY | GLY | VAL | LEU |
| ASP | PRO |      |  | VAL  | ASN | PRO | PRO | ILE |
| PRO | LEU | G399 |  | PRO  | VAL | VAL | ALA | VAL |
| ARG | THR |      |  | GLY  | THR | LYS | ASP | ALA |
| VAL | ARG | L402 |  | ALA  | LEU | SER | LYS | GLY |
| VAL | ARG | P403 |  | LEU  | VAL | ALA | VAL | SER |
| ALA | VAL | L404 |  | SER  | ASP | ARG | HIS | ALA |
| LEU | GLU |      |  | ASN  | GLN | VAL | GLU | ALA |
| VAL | GLU | M409 |  | GLN  | SER | HIS | LEU | VAL |
| ILE | ALA |      |  | PRO  | GLY | LEU | ARG | ALA |
| ARG | LYS | T416 |  | ALA  | HIS | ALA | LEU | ILE |
| GLN | ALA | R417 |  | PRO  | LEU | MET | ARG | ILE |
| TRP | ALA | E418 |  | PRO  | LEU | PRO | LEU | VAL |
| MET | GLN | A419 |  | ASN  | THR | LYS | ALA | VAL |
| SER | GLU |      |  | GLU  | GLN | PRO | ALA | VAL |
| ASN | GLN | T429 |  | ALA  | SER | GLN | GLN | MET |
| ASP | ALA |      |  | PRO  | ASN | LEU | GLY | VAL |
| HIS | VAL | A439 |  | ILE  | THR | PHE | LEU | TRP |
| GLU | ARG | VAL  |  | THR  | ARG | VAL | PRO | ALA |
|     | GLN | ASP  |  | PRO  | GLY | ARG | LYS | THR |
|     | GLU | ASN  |  | PRO  | ARG | GLU | GLY | PRO |
|     | THR | THR  |  | THR  | GLN | GLN | GLY | ASP |
|     | GLY | GLY  |  | ASN  | LYS | VAL | ALA | TYR |
|     | GLU | GLU  |  | GLN  | PRO | ARG | GLY | ARG |
|     | ALA | ALA  |  | GLN  | ALA | SER | PHE | THR |
|     | VAL | PRO  |  | ASN  | ASN | ALA | GLU | LEU |
|     | VAL | PHI  |  | ALA  | SER | ALA | LEU | PHE |
|     | VAL | TRP  |  | GLN  | VAL | VAL | LEU | ASN |
|     | ARG | GLN  |  | ASN  | THR | THR | ASP | ASN |
|     | LEU | GLN  |  | THR  | VAL | VAL | GLN | ASN |
|     | SER | GLN  |  | PRO  | GLN | THR | GLN | SER |
|     | YS  | YS   |  | YS   | YS  | YS  | YS  | YS  |

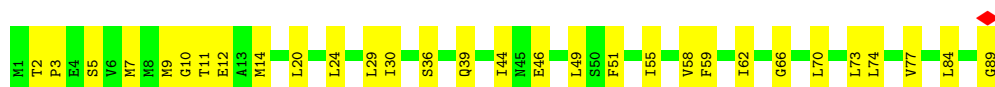
- Molecule 2: Flagellar biosynthetic protein FliQ

Chain A:  73% 26%



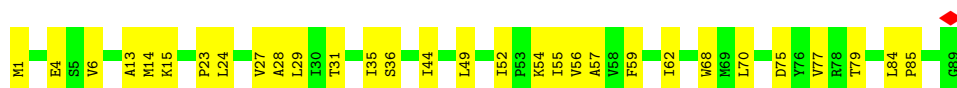
- Molecule 2: Flagellar biosynthetic protein FliQ

Chain B:  66% 34%



- Molecule 2: Flagellar biosynthetic protein FliQ

Chain C:  66% 34%



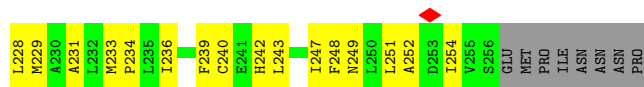
- Molecule 2: Flagellar biosynthetic protein FliQ

Chain D:  63% 35%



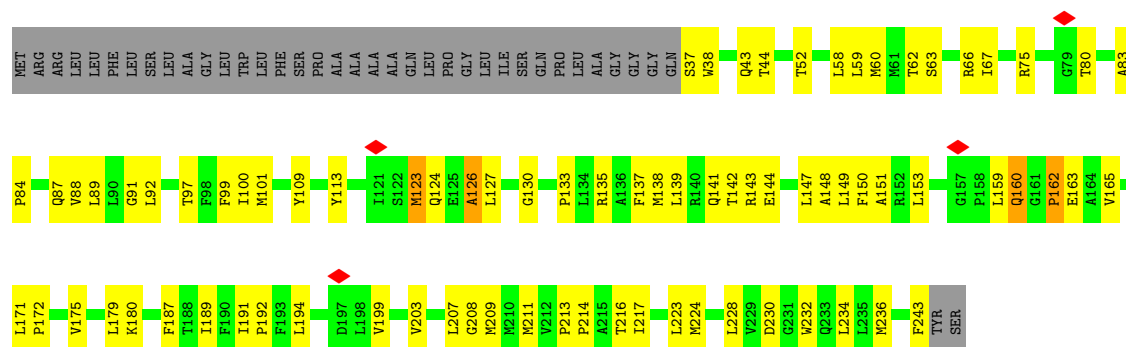
- Molecule 3: Flagellar biosynthetic protein FliR

Chain E:  62% 31%



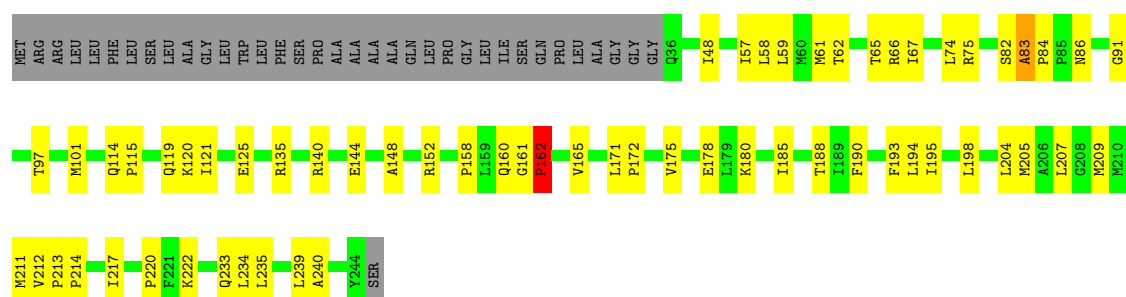
- Molecule 4: Flagellar biosynthetic protein FliP

Chain F:  52% 31% 16%



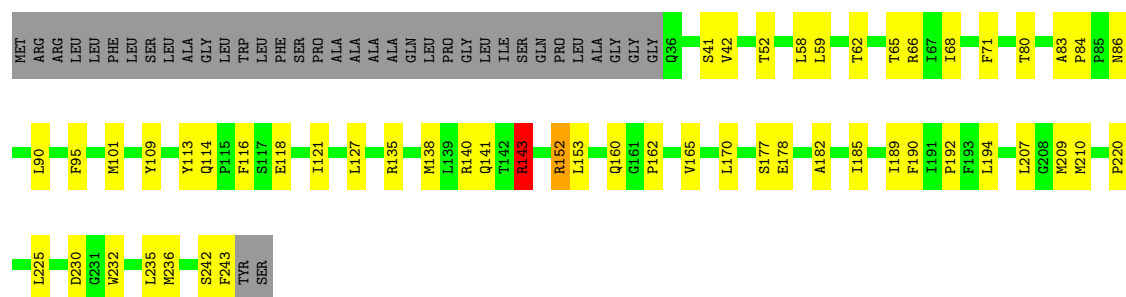
• Molecule 4: Flagellar biosynthetic protein FlpP

Chain G: 60% 24% 15%



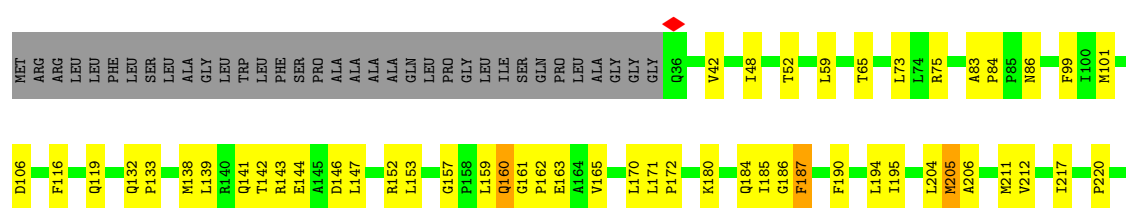
• Molecule 4: Flagellar biosynthetic protein FlpP

Chain H: 63% 21% 15%



• Molecule 4: Flagellar biosynthetic protein FlpP

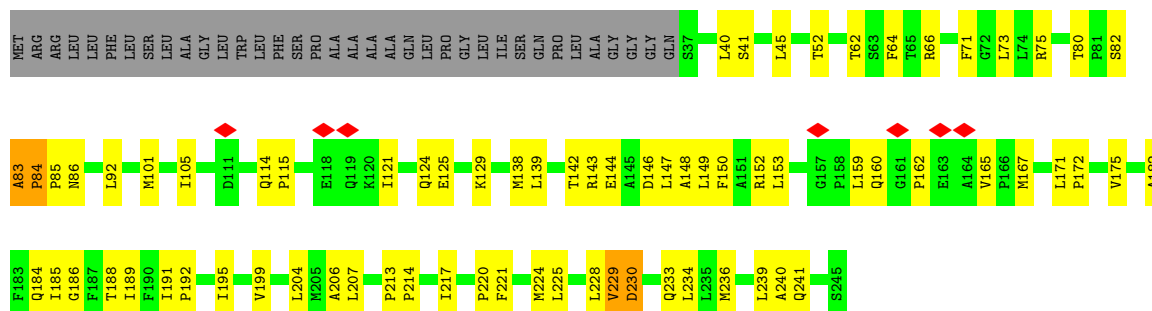
Chain I: 62% 22% 15%





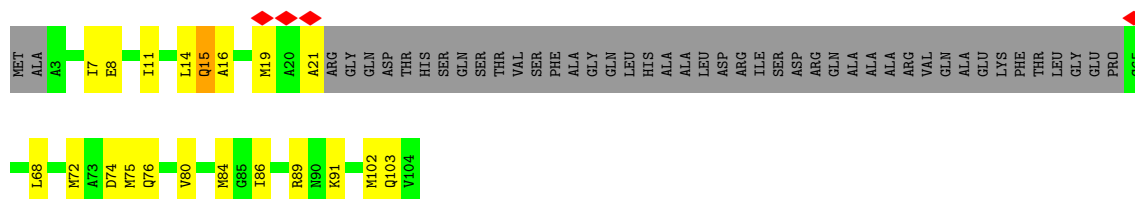
• Molecule 4: Flagellar biosynthetic protein FliP

Chain J: 55% 29% 15%



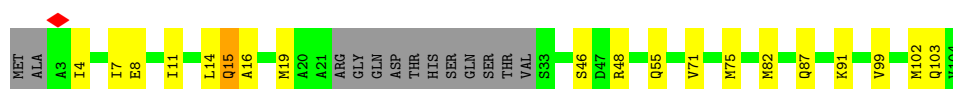
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain K: 38% 18% 43%



• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain L: 69% 17% 12%



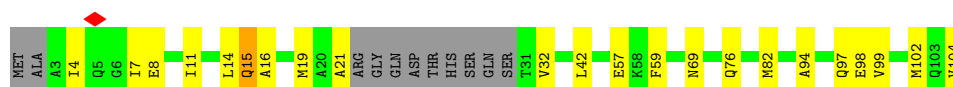
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain M: 69% 15% 5% 11%

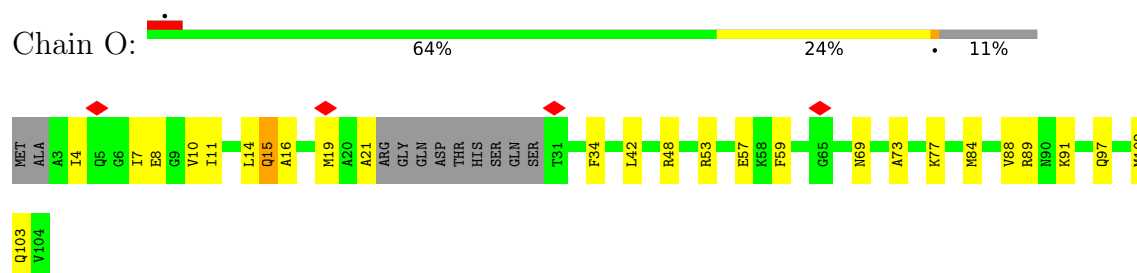


• Molecule 5: Flagellar hook-basal body complex protein FliE

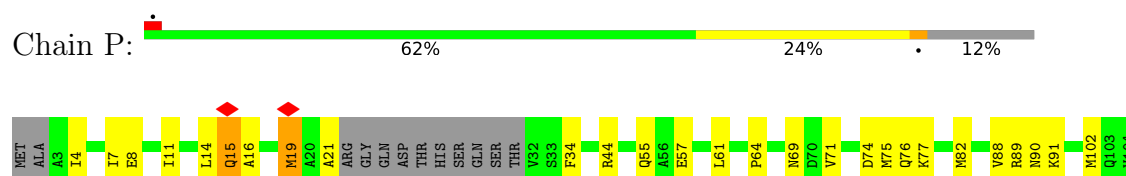
Chain N: 68% 20% 11%



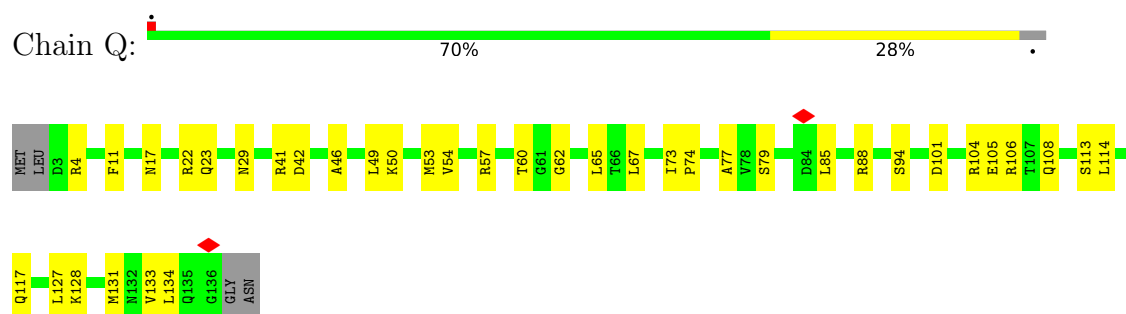
- Molecule 5: Flagellar hook-basal body complex protein FliE



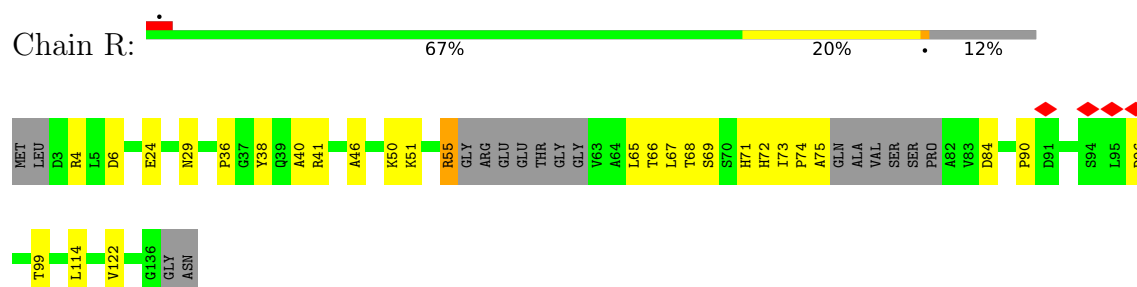
- Molecule 5: Flagellar hook-basal body complex protein FliE



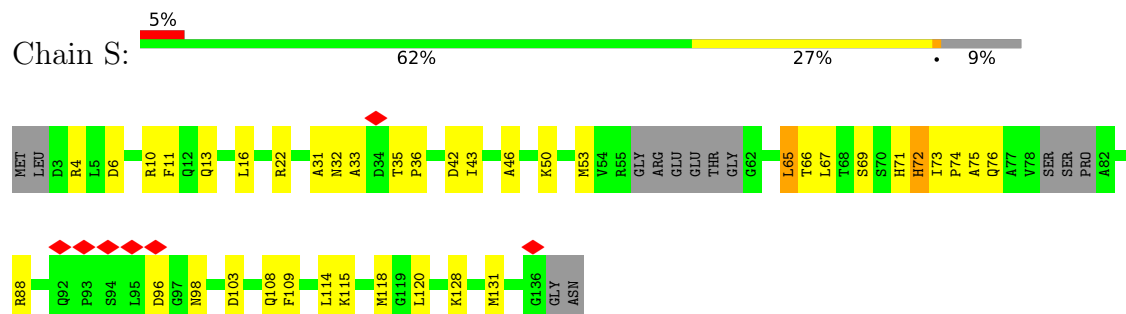
- Molecule 6: Flagellar basal body rod protein FlgB



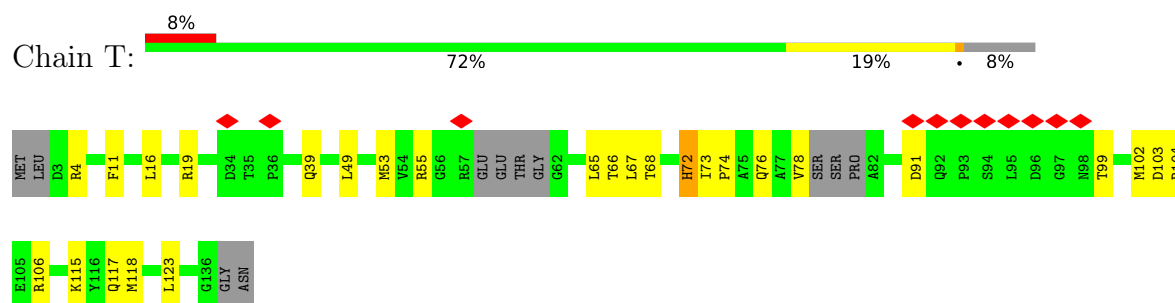
- Molecule 6: Flagellar basal body rod protein FlgB



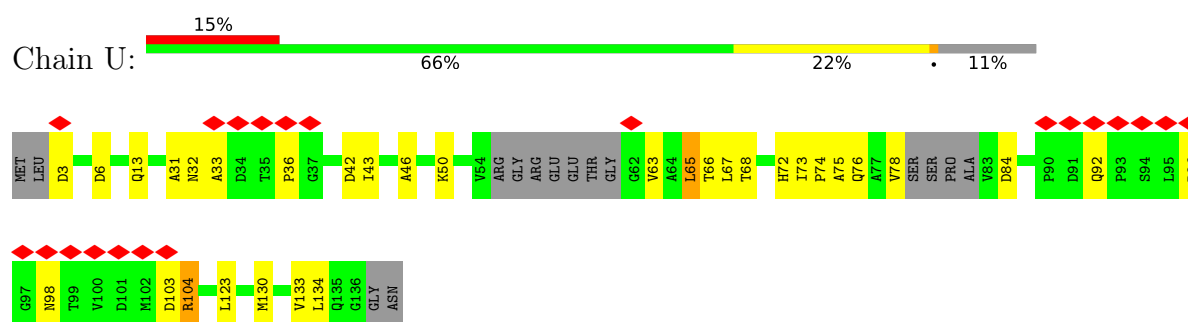
- Molecule 6: Flagellar basal body rod protein FlgB



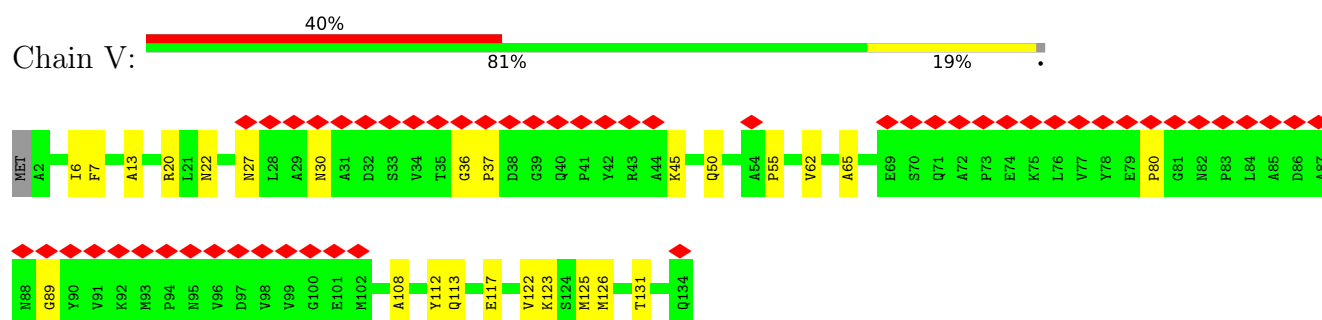
- Molecule 6: Flagellar basal body rod protein FlgB



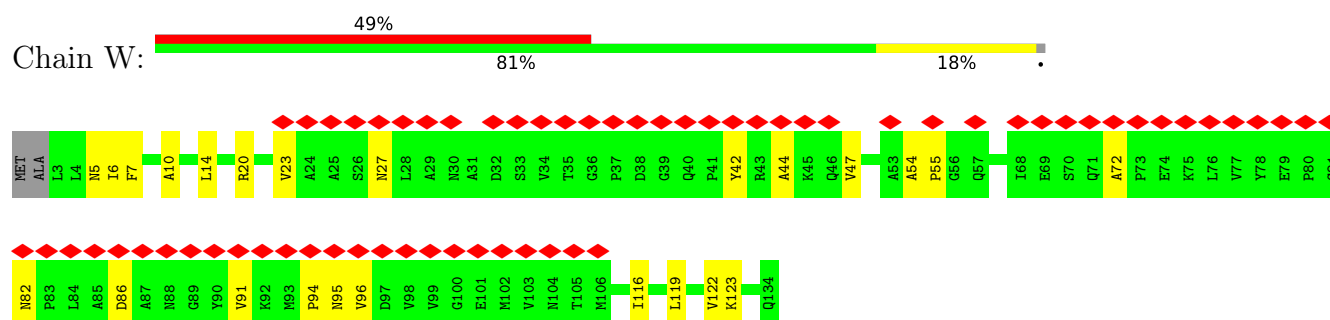
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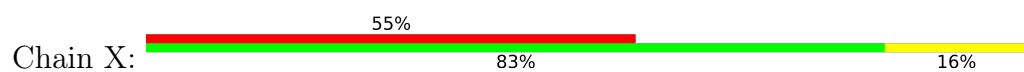
- Molecule 7: Flagellar basal-body rod protein FlgC

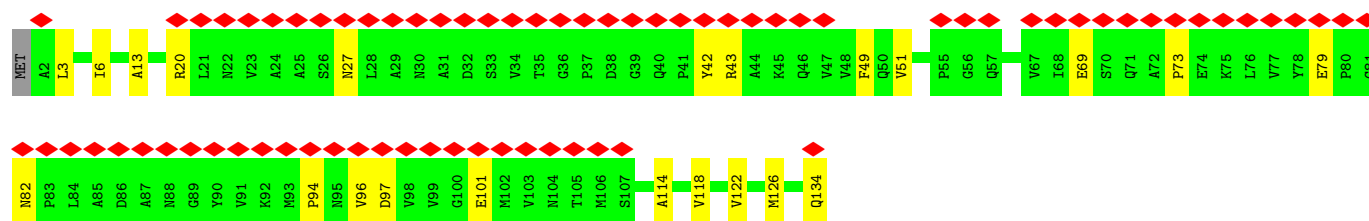


- Molecule 7: Flagellar basal-body rod protein FlgC

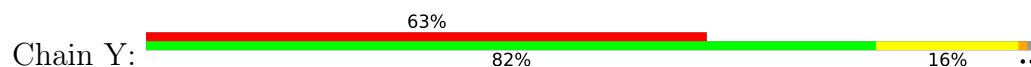


- Molecule 7: Flagellar basal-body rod protein FlgC

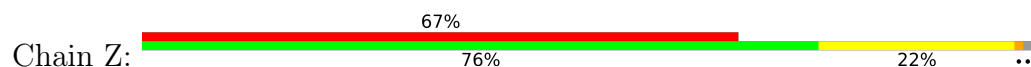




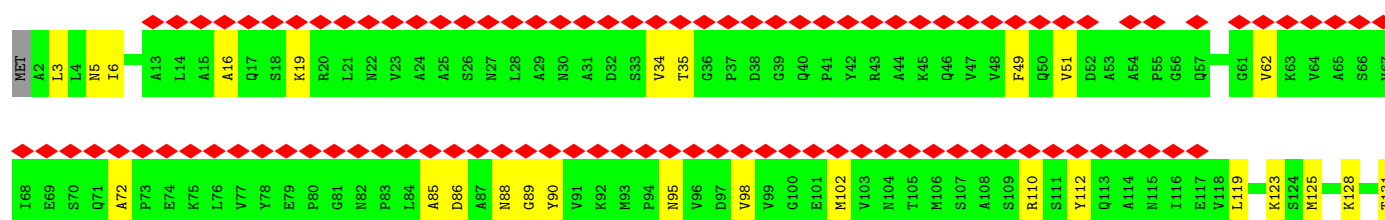
• Molecule 7: Flagellar basal-body rod protein FlgC



• Molecule 7: Flagellar basal-body rod protein FlgC



• Molecule 7: Flagellar basal-body rod protein FlgC



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 24190                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.867                                   | Depositor |
| Minimum map value                    | -0.441                                  | Depositor |
| Average map value                    | -0.001                                  | Depositor |
| Map value standard deviation         | 0.036                                   | Depositor |
| Recommended contour level            | 0.12                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 614.4, 614.4, 614.4                     | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.2, 1.2, 1.2                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$    |
| 1   | 0     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 1     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 2     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 3     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 4     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 5     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 6     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 7     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 8     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | 9     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AA    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AB    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AC    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AD    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AE    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AF    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AG    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AH    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AI    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AJ    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AK    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AL    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AM    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AN    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AO    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AP    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | AQ    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | UI    | 1.26         | 19/1191 (1.6%) | 1.29        | 19/1618 (1.2%) |
| 1   | UJ    | 1.27         | 20/1191 (1.7%) | 1.29        | 19/1618 (1.2%) |
| 1   | UK    | 1.25         | 19/1191 (1.6%) | 1.29        | 19/1618 (1.2%) |
| 1   | UL    | 1.24         | 18/1191 (1.5%) | 1.30        | 19/1618 (1.2%) |
| 1   | UM    | 1.27         | 20/1191 (1.7%) | 1.29        | 19/1618 (1.2%) |
| 1   | UN    | 1.26         | 20/1191 (1.7%) | 1.28        | 18/1618 (1.1%) |
| 1   | UO    | 1.25         | 19/1191 (1.6%) | 1.28        | 19/1618 (1.2%) |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | UP    | 1.27         | 20/1191 (1.7%) | 1.28        | 19/1618 (1.2%) |
| 1   | WA    | 0.89         | 0/863          | 1.20        | 2/1172 (0.2%)  |
| 1   | WB    | 0.91         | 0/850          | 1.21        | 1/1154 (0.1%)  |
| 1   | WC    | 0.89         | 0/825          | 1.15        | 0/1121         |
| 1   | WD    | 0.91         | 0/841          | 1.16        | 0/1142         |
| 1   | WE    | 0.88         | 0/857          | 1.17        | 1/1164 (0.1%)  |
| 1   | WF    | 0.89         | 0/848          | 1.17        | 0/1152         |
| 1   | WG    | 0.88         | 0/857          | 1.16        | 0/1164         |
| 1   | WH    | 0.90         | 0/714          | 1.15        | 1/973 (0.1%)   |
| 1   | WI    | 0.88         | 0/714          | 1.20        | 2/973 (0.2%)   |
| 1   | WJ    | 0.90         | 0/749          | 1.19        | 1/1020 (0.1%)  |
| 1   | WK    | 0.90         | 0/741          | 1.16        | 0/1009         |
| 1   | WL    | 0.89         | 0/631          | 1.16        | 1/860 (0.1%)   |
| 1   | WM    | 0.88         | 0/604          | 1.15        | 1/824 (0.1%)   |
| 1   | WN    | 0.89         | 0/619          | 1.17        | 1/844 (0.1%)   |
| 1   | WO    | 0.89         | 0/726          | 1.19        | 3/989 (0.3%)   |
| 1   | WP    | 0.89         | 0/753          | 1.16        | 0/1025         |
| 1   | WQ    | 0.90         | 0/848          | 1.19        | 0/1152         |
| 1   | WR    | 0.89         | 0/848          | 1.14        | 0/1152         |
| 1   | WS    | 0.91         | 0/848          | 1.19        | 1/1152 (0.1%)  |
| 1   | WT    | 0.89         | 0/848          | 1.18        | 0/1152         |
| 1   | WU    | 0.89         | 0/857          | 1.16        | 1/1164 (0.1%)  |
| 1   | WV    | 0.91         | 0/841          | 1.17        | 0/1142         |
| 1   | WW    | 0.91         | 0/848          | 1.19        | 2/1152 (0.2%)  |
| 1   | b     | 0.71         | 0/83           | 0.97        | 0/114          |
| 1   | c     | 0.17         | 0/107          | 0.37        | 0/148          |
| 1   | d     | 0.27         | 0/137          | 0.52        | 0/191          |
| 1   | e     | 0.20         | 0/107          | 0.45        | 0/148          |
| 1   | f     | 1.32         | 1/145 (0.7%)   | 1.50        | 3/203 (1.5%)   |
| 1   | g     | 0.22         | 0/107          | 0.57        | 0/148          |
| 1   | h     | 0.13         | 0/145          | 0.29        | 0/203          |
| 1   | i     | 0.15         | 0/107          | 0.41        | 0/148          |
| 1   | j     | 0.26         | 0/137          | 0.66        | 0/191          |
| 1   | k     | 0.17         | 0/107          | 0.30        | 0/148          |
| 1   | l     | 0.26         | 0/145          | 0.45        | 0/203          |
| 1   | t     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | u     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | v     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | w     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | x     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | y     | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 1   | z     | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 2   | A     | 0.27         | 0/681          | 0.49        | 0/930          |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 2   | B     | 0.16         | 0/681             | 0.42        | 0/930             |
| 2   | C     | 0.23         | 0/681             | 0.44        | 0/930             |
| 2   | D     | 0.26         | 0/681             | 0.55        | 0/930             |
| 3   | E     | 0.45         | 3/1994 (0.2%)     | 0.61        | 3/2724 (0.1%)     |
| 4   | F     | 0.33         | 0/1643            | 0.61        | 4/2237 (0.2%)     |
| 4   | G     | 0.26         | 0/1665            | 0.46        | 2/2267 (0.1%)     |
| 4   | H     | 0.22         | 0/1652            | 0.42        | 0/2249            |
| 4   | I     | 0.22         | 0/1652            | 0.41        | 1/2249 (0.0%)     |
| 4   | J     | 0.30         | 0/1662            | 0.53        | 1/2263 (0.0%)     |
| 5   | K     | 0.52         | 0/428             | 0.84        | 0/572             |
| 5   | L     | 0.41         | 0/675             | 0.64        | 0/905             |
| 5   | M     | 0.42         | 0/689             | 0.70        | 0/925             |
| 5   | N     | 0.42         | 0/689             | 0.64        | 0/925             |
| 5   | O     | 0.42         | 0/689             | 0.66        | 0/925             |
| 5   | P     | 0.43         | 0/682             | 0.67        | 0/915             |
| 6   | Q     | 0.44         | 0/1042            | 0.59        | 0/1408            |
| 6   | R     | 0.36         | 0/951             | 0.47        | 0/1282            |
| 6   | S     | 0.40         | 0/976             | 0.59        | 0/1316            |
| 6   | T     | 0.39         | 0/991             | 0.64        | 3/1335 (0.2%)     |
| 6   | U     | 0.40         | 0/959             | 0.53        | 0/1293            |
| 7   | V     | 0.16         | 0/981             | 0.31        | 0/1334            |
| 7   | W     | 0.14         | 0/976             | 0.32        | 0/1327            |
| 7   | X     | 0.52         | 2/981 (0.2%)      | 0.98        | 3/1334 (0.2%)     |
| 7   | Y     | 0.16         | 0/981             | 0.37        | 0/1334            |
| 7   | Z     | 0.15         | 0/981             | 0.35        | 0/1334            |
| 7   | a     | 0.19         | 0/981             | 0.37        | 0/1334            |
| All | All   | 0.59         | 161/100455 (0.2%) | 0.76        | 223/136142 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | UI    | 0                   | 2                   |
| 1   | UJ    | 0                   | 2                   |
| 1   | UK    | 0                   | 3                   |
| 1   | UL    | 0                   | 3                   |
| 1   | UM    | 0                   | 2                   |
| 1   | UN    | 0                   | 2                   |
| 1   | UO    | 0                   | 2                   |
| 1   | UP    | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | WA    | 0                   | 3                   |
| 1   | WB    | 0                   | 4                   |
| 1   | WC    | 0                   | 3                   |
| 1   | WD    | 0                   | 1                   |
| 1   | WE    | 0                   | 2                   |
| 1   | WF    | 0                   | 3                   |
| 1   | WG    | 0                   | 3                   |
| 1   | WI    | 0                   | 1                   |
| 1   | WJ    | 0                   | 3                   |
| 1   | WK    | 0                   | 2                   |
| 1   | WL    | 0                   | 2                   |
| 1   | WM    | 0                   | 1                   |
| 1   | WN    | 0                   | 1                   |
| 1   | WO    | 0                   | 1                   |
| 1   | WP    | 0                   | 3                   |
| 1   | WQ    | 0                   | 2                   |
| 1   | WR    | 0                   | 3                   |
| 1   | WS    | 0                   | 1                   |
| 1   | WT    | 0                   | 2                   |
| 1   | WU    | 0                   | 2                   |
| 1   | WV    | 0                   | 3                   |
| 1   | WW    | 0                   | 2                   |
| 4   | H     | 0                   | 1                   |
| 6   | Q     | 0                   | 1                   |
| 6   | U     | 0                   | 1                   |
| 7   | Y     | 0                   | 1                   |
| 7   | a     | 0                   | 1                   |
| All | All   | 0                   | 72                  |

All (161) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | f     | 331 | PRO  | CG-CD | -13.84 | 1.03        | 1.50     |
| 1   | UJ    | 125 | GLN  | C-N   | 13.62  | 1.51        | 1.33     |
| 1   | UP    | 125 | GLN  | C-N   | 13.60  | 1.51        | 1.33     |
| 1   | UK    | 125 | GLN  | C-N   | 13.59  | 1.51        | 1.33     |
| 1   | UO    | 125 | GLN  | C-N   | 13.55  | 1.51        | 1.33     |
| 1   | UI    | 125 | GLN  | C-N   | 13.53  | 1.51        | 1.33     |
| 1   | UM    | 125 | GLN  | C-N   | 13.52  | 1.51        | 1.33     |
| 1   | UL    | 125 | GLN  | C-N   | 13.51  | 1.51        | 1.33     |
| 1   | UN    | 125 | GLN  | C-N   | 13.45  | 1.51        | 1.33     |
| 7   | X     | 73  | PRO  | CG-CD | -12.40 | 1.08        | 1.50     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | E     | 185 | MET  | C-O   | 9.83  | 1.35        | 1.24     |
| 1   | UL    | 172 | PRO  | N-CD  | -9.46 | 1.34        | 1.47     |
| 1   | UM    | 172 | PRO  | N-CD  | -9.45 | 1.34        | 1.47     |
| 1   | UP    | 172 | PRO  | N-CD  | -9.43 | 1.34        | 1.47     |
| 1   | UN    | 172 | PRO  | N-CD  | -9.40 | 1.34        | 1.47     |
| 1   | UJ    | 172 | PRO  | N-CD  | -9.40 | 1.34        | 1.47     |
| 1   | UI    | 172 | PRO  | N-CD  | -9.38 | 1.34        | 1.47     |
| 1   | UO    | 172 | PRO  | N-CD  | -9.37 | 1.34        | 1.47     |
| 1   | UK    | 172 | PRO  | N-CD  | -9.35 | 1.34        | 1.47     |
| 7   | X     | 73  | PRO  | CB-CG | -7.58 | 1.11        | 1.49     |
| 1   | UM    | 93  | VAL  | C-N   | -7.36 | 1.24        | 1.33     |
| 1   | UN    | 93  | VAL  | C-N   | -7.30 | 1.24        | 1.33     |
| 1   | UP    | 93  | VAL  | C-N   | -7.28 | 1.24        | 1.33     |
| 1   | UL    | 93  | VAL  | C-N   | -7.26 | 1.24        | 1.33     |
| 1   | UI    | 93  | VAL  | C-N   | -7.23 | 1.24        | 1.33     |
| 1   | UJ    | 93  | VAL  | C-N   | -7.23 | 1.24        | 1.33     |
| 1   | UK    | 93  | VAL  | C-N   | -7.19 | 1.24        | 1.33     |
| 1   | UO    | 93  | VAL  | C-N   | -7.18 | 1.24        | 1.33     |
| 1   | UI    | 172 | PRO  | C-N   | -6.98 | 1.23        | 1.33     |
| 1   | UO    | 172 | PRO  | C-N   | -6.97 | 1.23        | 1.33     |
| 1   | UL    | 172 | PRO  | C-N   | -6.94 | 1.23        | 1.33     |
| 1   | UM    | 172 | PRO  | C-N   | -6.92 | 1.23        | 1.33     |
| 1   | UP    | 172 | PRO  | C-N   | -6.92 | 1.23        | 1.33     |
| 1   | UN    | 172 | PRO  | C-N   | -6.91 | 1.23        | 1.33     |
| 1   | UK    | 172 | PRO  | C-N   | -6.90 | 1.23        | 1.33     |
| 1   | UJ    | 172 | PRO  | C-N   | -6.89 | 1.23        | 1.33     |
| 1   | UO    | 141 | ALA  | C-N   | -6.86 | 1.25        | 1.33     |
| 1   | UP    | 141 | ALA  | C-N   | -6.84 | 1.25        | 1.33     |
| 1   | UJ    | 138 | GLY  | C-N   | -6.80 | 1.25        | 1.33     |
| 1   | UI    | 141 | ALA  | C-N   | -6.80 | 1.25        | 1.33     |
| 1   | UN    | 138 | GLY  | C-N   | -6.78 | 1.25        | 1.33     |
| 1   | UK    | 138 | GLY  | C-N   | -6.76 | 1.25        | 1.33     |
| 1   | UO    | 138 | GLY  | C-N   | -6.76 | 1.25        | 1.33     |
| 1   | UI    | 138 | GLY  | C-N   | -6.76 | 1.25        | 1.33     |
| 1   | UK    | 141 | ALA  | C-N   | -6.75 | 1.25        | 1.33     |
| 1   | UM    | 138 | GLY  | C-N   | -6.75 | 1.25        | 1.33     |
| 1   | UM    | 141 | ALA  | C-N   | -6.75 | 1.25        | 1.33     |
| 1   | UN    | 141 | ALA  | C-N   | -6.75 | 1.25        | 1.33     |
| 1   | UP    | 138 | GLY  | C-N   | -6.73 | 1.25        | 1.33     |
| 1   | UL    | 141 | ALA  | C-N   | -6.72 | 1.25        | 1.33     |
| 1   | UJ    | 141 | ALA  | C-N   | -6.72 | 1.25        | 1.33     |
| 1   | UL    | 138 | GLY  | C-N   | -6.68 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | E     | 182 | ASN  | C-O   | 6.60  | 1.32        | 1.24     |
| 1   | UP    | 92  | LYS  | C-N   | -6.47 | 1.25        | 1.33     |
| 1   | UJ    | 92  | LYS  | C-N   | -6.42 | 1.25        | 1.33     |
| 1   | UI    | 92  | LYS  | C-N   | -6.41 | 1.25        | 1.33     |
| 1   | UO    | 92  | LYS  | C-N   | -6.41 | 1.25        | 1.33     |
| 1   | UK    | 92  | LYS  | C-N   | -6.40 | 1.25        | 1.33     |
| 1   | UM    | 92  | LYS  | C-N   | -6.38 | 1.25        | 1.33     |
| 1   | UL    | 92  | LYS  | C-N   | -6.38 | 1.25        | 1.33     |
| 1   | UN    | 92  | LYS  | C-N   | -6.36 | 1.25        | 1.33     |
| 1   | UL    | 201 | ALA  | C-N   | -6.19 | 1.25        | 1.33     |
| 1   | UJ    | 195 | VAL  | C-N   | -6.17 | 1.25        | 1.33     |
| 1   | UK    | 195 | VAL  | C-N   | -6.16 | 1.25        | 1.33     |
| 1   | UL    | 195 | VAL  | C-N   | -6.16 | 1.25        | 1.33     |
| 1   | UM    | 201 | ALA  | C-N   | -6.15 | 1.25        | 1.33     |
| 1   | UO    | 195 | VAL  | C-N   | -6.13 | 1.25        | 1.33     |
| 1   | UP    | 195 | VAL  | C-N   | -6.11 | 1.25        | 1.33     |
| 1   | UI    | 195 | VAL  | C-N   | -6.09 | 1.25        | 1.33     |
| 1   | UM    | 105 | LEU  | C-N   | -6.09 | 1.24        | 1.34     |
| 1   | UO    | 201 | ALA  | C-N   | -6.09 | 1.25        | 1.33     |
| 1   | UI    | 201 | ALA  | C-N   | -6.08 | 1.25        | 1.33     |
| 1   | UK    | 201 | ALA  | C-N   | -6.08 | 1.25        | 1.33     |
| 1   | UM    | 195 | VAL  | C-N   | -6.07 | 1.25        | 1.33     |
| 1   | UJ    | 105 | LEU  | C-N   | -6.07 | 1.24        | 1.34     |
| 1   | UJ    | 182 | PRO  | C-N   | -6.07 | 1.24        | 1.33     |
| 1   | UP    | 201 | ALA  | C-N   | -6.07 | 1.25        | 1.33     |
| 1   | UN    | 201 | ALA  | C-N   | -6.06 | 1.25        | 1.33     |
| 1   | UN    | 195 | VAL  | C-N   | -6.04 | 1.25        | 1.33     |
| 1   | UP    | 105 | LEU  | C-N   | -6.04 | 1.24        | 1.34     |
| 1   | UJ    | 250 | ALA  | C-N   | -6.03 | 1.25        | 1.33     |
| 1   | UN    | 105 | LEU  | C-N   | -6.02 | 1.25        | 1.34     |
| 1   | UM    | 182 | PRO  | C-N   | -6.02 | 1.24        | 1.33     |
| 1   | UI    | 182 | PRO  | C-N   | -6.01 | 1.24        | 1.33     |
| 1   | UO    | 105 | LEU  | C-N   | -6.01 | 1.25        | 1.34     |
| 1   | UN    | 182 | PRO  | C-N   | -5.99 | 1.24        | 1.33     |
| 1   | UL    | 105 | LEU  | C-N   | -5.99 | 1.25        | 1.34     |
| 1   | UN    | 199 | SER  | C-N   | -5.99 | 1.25        | 1.33     |
| 1   | UI    | 105 | LEU  | C-N   | -5.97 | 1.25        | 1.34     |
| 1   | UK    | 182 | PRO  | C-N   | -5.97 | 1.24        | 1.33     |
| 1   | UK    | 105 | LEU  | C-N   | -5.96 | 1.25        | 1.34     |
| 1   | UL    | 182 | PRO  | C-N   | -5.96 | 1.24        | 1.33     |
| 1   | UO    | 182 | PRO  | C-N   | -5.95 | 1.25        | 1.33     |
| 1   | UP    | 182 | PRO  | C-N   | -5.91 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | UL    | 199 | SER  | C-N   | -5.88 | 1.25        | 1.33     |
| 1   | UJ    | 248 | SER  | C-N   | -5.88 | 1.25        | 1.33     |
| 1   | UK    | 199 | SER  | C-N   | -5.88 | 1.25        | 1.33     |
| 1   | UP    | 62  | ASP  | C-N   | -5.87 | 1.26        | 1.33     |
| 1   | UI    | 199 | SER  | C-N   | -5.85 | 1.25        | 1.33     |
| 1   | UM    | 199 | SER  | C-N   | -5.84 | 1.25        | 1.33     |
| 1   | UP    | 199 | SER  | C-N   | -5.83 | 1.25        | 1.33     |
| 1   | UO    | 199 | SER  | C-N   | -5.79 | 1.25        | 1.33     |
| 1   | UM    | 62  | ASP  | C-N   | -5.79 | 1.26        | 1.33     |
| 1   | UP    | 97  | ARG  | C-N   | -5.78 | 1.26        | 1.33     |
| 1   | UK    | 97  | ARG  | C-N   | -5.78 | 1.26        | 1.33     |
| 1   | UI    | 97  | ARG  | C-N   | -5.77 | 1.26        | 1.33     |
| 1   | UL    | 97  | ARG  | C-N   | -5.76 | 1.26        | 1.33     |
| 1   | UM    | 97  | ARG  | C-N   | -5.75 | 1.26        | 1.33     |
| 1   | UN    | 97  | ARG  | C-N   | -5.74 | 1.26        | 1.33     |
| 1   | UJ    | 62  | ASP  | C-N   | -5.74 | 1.26        | 1.33     |
| 1   | UN    | 62  | ASP  | C-N   | -5.73 | 1.26        | 1.33     |
| 1   | UJ    | 97  | ARG  | C-N   | -5.73 | 1.26        | 1.33     |
| 1   | UP    | 142 | ARG  | C-N   | -5.72 | 1.26        | 1.33     |
| 1   | UL    | 142 | ARG  | C-N   | -5.71 | 1.26        | 1.33     |
| 1   | UM    | 142 | ARG  | C-N   | -5.69 | 1.26        | 1.33     |
| 1   | UK    | 142 | ARG  | C-N   | -5.68 | 1.26        | 1.33     |
| 1   | UI    | 142 | ARG  | C-N   | -5.67 | 1.26        | 1.33     |
| 1   | UJ    | 142 | ARG  | C-N   | -5.66 | 1.26        | 1.33     |
| 1   | UN    | 185 | ALA  | C-N   | -5.66 | 1.25        | 1.33     |
| 1   | UL    | 131 | ASN  | C-N   | -5.66 | 1.26        | 1.33     |
| 1   | UO    | 185 | ALA  | C-N   | -5.63 | 1.25        | 1.33     |
| 1   | UO    | 131 | ASN  | C-N   | -5.63 | 1.26        | 1.33     |
| 1   | UN    | 142 | ARG  | C-N   | -5.63 | 1.26        | 1.33     |
| 1   | UK    | 131 | ASN  | C-N   | -5.62 | 1.26        | 1.33     |
| 1   | UI    | 185 | ALA  | C-N   | -5.61 | 1.25        | 1.33     |
| 1   | UN    | 131 | ASN  | C-N   | -5.61 | 1.26        | 1.33     |
| 1   | UP    | 131 | ASN  | C-N   | -5.61 | 1.26        | 1.33     |
| 1   | UO    | 142 | ARG  | C-N   | -5.60 | 1.26        | 1.33     |
| 1   | UJ    | 131 | ASN  | C-N   | -5.60 | 1.26        | 1.33     |
| 1   | UK    | 215 | GLN  | C-N   | -5.59 | 1.25        | 1.33     |
| 1   | UI    | 131 | ASN  | C-N   | -5.59 | 1.26        | 1.33     |
| 1   | UP    | 185 | ALA  | C-N   | -5.58 | 1.25        | 1.33     |
| 1   | UK    | 185 | ALA  | C-N   | -5.58 | 1.25        | 1.33     |
| 1   | UM    | 131 | ASN  | C-N   | -5.57 | 1.26        | 1.33     |
| 1   | UO    | 97  | ARG  | C-N   | -5.56 | 1.26        | 1.33     |
| 1   | UJ    | 257 | GLY  | C-N   | -5.56 | 1.26        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | UL    | 185 | ALA  | C-N   | -5.56 | 1.25        | 1.33     |
| 1   | UM    | 208 | GLY  | C-N   | -5.56 | 1.26        | 1.33     |
| 1   | UM    | 185 | ALA  | C-N   | -5.56 | 1.25        | 1.33     |
| 1   | UO    | 215 | GLN  | C-N   | -5.55 | 1.25        | 1.33     |
| 1   | UK    | 208 | GLY  | C-N   | -5.55 | 1.26        | 1.33     |
| 1   | UJ    | 185 | ALA  | C-N   | -5.54 | 1.25        | 1.33     |
| 1   | UI    | 208 | GLY  | C-N   | -5.54 | 1.26        | 1.33     |
| 1   | UN    | 215 | GLN  | C-N   | -5.53 | 1.25        | 1.33     |
| 1   | UJ    | 264 | GLN  | C-N   | -5.52 | 1.25        | 1.33     |
| 1   | UP    | 208 | GLY  | C-N   | -5.52 | 1.26        | 1.33     |
| 1   | UI    | 215 | GLN  | C-N   | -5.51 | 1.25        | 1.33     |
| 1   | UP    | 215 | GLN  | C-N   | -5.51 | 1.25        | 1.33     |
| 1   | UN    | 208 | GLY  | C-N   | -5.51 | 1.26        | 1.33     |
| 1   | UL    | 208 | GLY  | C-N   | -5.50 | 1.26        | 1.33     |
| 1   | UM    | 215 | GLN  | C-N   | -5.49 | 1.25        | 1.33     |
| 3   | E     | 184 | LEU  | C-O   | -5.49 | 1.17        | 1.24     |
| 1   | UO    | 208 | GLY  | C-N   | -5.49 | 1.26        | 1.33     |
| 1   | UK    | 70  | LEU  | C-N   | -5.47 | 1.26        | 1.33     |
| 1   | UN    | 70  | LEU  | C-N   | -5.45 | 1.26        | 1.33     |
| 1   | UO    | 70  | LEU  | C-N   | -5.45 | 1.26        | 1.33     |
| 1   | UL    | 70  | LEU  | C-N   | -5.42 | 1.26        | 1.33     |
| 1   | UP    | 70  | LEU  | C-N   | -5.40 | 1.26        | 1.33     |
| 1   | UM    | 70  | LEU  | C-N   | -5.40 | 1.26        | 1.33     |
| 1   | UI    | 70  | LEU  | C-N   | -5.39 | 1.26        | 1.33     |
| 1   | UJ    | 70  | LEU  | C-N   | -5.39 | 1.26        | 1.33     |

All (223) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 7   | X     | 73  | PRO  | CB-CG-CD | 23.05  | 179.86      | 106.10   |
| 7   | X     | 73  | PRO  | N-CD-CG  | -18.80 | 75.00       | 103.20   |
| 1   | f     | 331 | PRO  | N-CD-CG  | -16.10 | 79.05       | 103.20   |
| 7   | X     | 73  | PRO  | CA-CB-CG | -14.26 | 77.40       | 104.50   |
| 1   | UO    | 126 | PHE  | O-C-N    | 13.87  | 136.82      | 122.12   |
| 1   | UL    | 126 | PHE  | O-C-N    | 13.87  | 136.82      | 122.12   |
| 1   | UK    | 126 | PHE  | O-C-N    | 13.84  | 136.79      | 122.12   |
| 1   | UI    | 126 | PHE  | O-C-N    | 13.83  | 136.78      | 122.12   |
| 1   | UN    | 126 | PHE  | O-C-N    | 13.82  | 136.77      | 122.12   |
| 1   | UJ    | 126 | PHE  | O-C-N    | 13.81  | 136.76      | 122.12   |
| 1   | UM    | 126 | PHE  | O-C-N    | 13.79  | 136.74      | 122.12   |
| 1   | UP    | 126 | PHE  | O-C-N    | 13.77  | 136.72      | 122.12   |
| 4   | F     | 162 | PRO  | CA-N-CD  | -12.41 | 94.62       | 112.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | UK    | 129 | GLN  | O-C-N    | 10.52 | 132.90      | 122.07   |
| 1   | UP    | 129 | GLN  | O-C-N    | 10.50 | 132.89      | 122.07   |
| 1   | UO    | 129 | GLN  | O-C-N    | 10.45 | 132.83      | 122.07   |
| 1   | UJ    | 129 | GLN  | O-C-N    | 10.41 | 132.79      | 122.07   |
| 1   | UM    | 129 | GLN  | O-C-N    | 10.39 | 132.78      | 122.07   |
| 1   | UI    | 129 | GLN  | O-C-N    | 10.38 | 132.76      | 122.07   |
| 1   | UN    | 129 | GLN  | O-C-N    | 10.38 | 132.76      | 122.07   |
| 1   | UL    | 129 | GLN  | O-C-N    | 10.37 | 132.75      | 122.07   |
| 1   | f     | 331 | PRO  | CA-CB-CG | -9.26 | 86.91       | 104.50   |
| 1   | UL    | 126 | PHE  | CA-C-N   | -9.13 | 107.33      | 120.29   |
| 1   | UL    | 126 | PHE  | C-N-CA   | -9.13 | 107.33      | 120.29   |
| 1   | UO    | 126 | PHE  | CA-C-N   | -9.11 | 107.36      | 120.29   |
| 1   | UO    | 126 | PHE  | C-N-CA   | -9.11 | 107.36      | 120.29   |
| 1   | UK    | 126 | PHE  | CA-C-N   | -9.10 | 107.37      | 120.29   |
| 1   | UK    | 126 | PHE  | C-N-CA   | -9.10 | 107.37      | 120.29   |
| 1   | UM    | 126 | PHE  | CA-C-N   | -9.10 | 107.37      | 120.29   |
| 1   | UM    | 126 | PHE  | C-N-CA   | -9.10 | 107.37      | 120.29   |
| 1   | UI    | 126 | PHE  | CA-C-N   | -9.09 | 107.39      | 120.29   |
| 1   | UI    | 126 | PHE  | C-N-CA   | -9.09 | 107.39      | 120.29   |
| 1   | UP    | 126 | PHE  | CA-C-N   | -9.09 | 107.39      | 120.29   |
| 1   | UP    | 126 | PHE  | C-N-CA   | -9.09 | 107.39      | 120.29   |
| 1   | UN    | 126 | PHE  | CA-C-N   | -9.08 | 107.39      | 120.29   |
| 1   | UN    | 126 | PHE  | C-N-CA   | -9.08 | 107.39      | 120.29   |
| 1   | UJ    | 126 | PHE  | CA-C-N   | -9.08 | 107.40      | 120.29   |
| 1   | UJ    | 126 | PHE  | C-N-CA   | -9.08 | 107.40      | 120.29   |
| 1   | UJ    | 130 | VAL  | O-C-N    | 8.64  | 130.25      | 121.87   |
| 1   | UK    | 130 | VAL  | O-C-N    | 8.63  | 130.25      | 121.87   |
| 1   | UI    | 130 | VAL  | O-C-N    | 8.63  | 130.24      | 121.87   |
| 1   | UL    | 130 | VAL  | O-C-N    | 8.63  | 130.24      | 121.87   |
| 1   | UN    | 130 | VAL  | O-C-N    | 8.62  | 130.23      | 121.87   |
| 1   | UP    | 130 | VAL  | O-C-N    | 8.60  | 130.21      | 121.87   |
| 1   | UM    | 130 | VAL  | O-C-N    | 8.58  | 130.19      | 121.87   |
| 1   | UO    | 130 | VAL  | O-C-N    | 8.51  | 130.12      | 121.87   |
| 1   | WA    | 162 | PRO  | N-CA-C   | 7.76  | 128.46      | 112.47   |
| 4   | J     | 84  | PRO  | N-CA-C   | -7.73 | 101.26      | 110.70   |
| 6   | T     | 72  | HIS  | CA-C-N   | -7.43 | 116.21      | 123.04   |
| 6   | T     | 72  | HIS  | C-N-CA   | -7.43 | 116.21      | 123.04   |
| 1   | f     | 331 | PRO  | N-CA-CB  | -7.40 | 94.86       | 103.00   |
| 6   | T     | 72  | HIS  | CA-CB-CG | -7.28 | 106.52      | 113.80   |
| 1   | UO    | 129 | GLN  | CA-C-N   | -6.72 | 111.25      | 120.46   |
| 1   | UO    | 129 | GLN  | C-N-CA   | -6.72 | 111.25      | 120.46   |
| 1   | UK    | 129 | GLN  | CA-C-N   | -6.72 | 111.26      | 120.46   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | UK    | 129 | GLN  | C-N-CA  | -6.72 | 111.26      | 120.46   |
| 1   | UP    | 129 | GLN  | CA-C-N  | -6.71 | 111.27      | 120.46   |
| 1   | UP    | 129 | GLN  | C-N-CA  | -6.71 | 111.27      | 120.46   |
| 1   | UJ    | 129 | GLN  | CA-C-N  | -6.71 | 111.27      | 120.46   |
| 1   | UJ    | 129 | GLN  | C-N-CA  | -6.71 | 111.27      | 120.46   |
| 1   | UI    | 129 | GLN  | CA-C-N  | -6.70 | 111.28      | 120.46   |
| 1   | UI    | 129 | GLN  | C-N-CA  | -6.70 | 111.28      | 120.46   |
| 1   | UL    | 129 | GLN  | CA-C-N  | -6.68 | 111.31      | 120.46   |
| 1   | UL    | 129 | GLN  | C-N-CA  | -6.68 | 111.31      | 120.46   |
| 1   | UN    | 129 | GLN  | CA-C-N  | -6.67 | 111.33      | 120.46   |
| 1   | UN    | 129 | GLN  | C-N-CA  | -6.67 | 111.33      | 120.46   |
| 1   | UM    | 129 | GLN  | CA-C-N  | -6.66 | 111.34      | 120.46   |
| 1   | UM    | 129 | GLN  | C-N-CA  | -6.66 | 111.34      | 120.46   |
| 1   | WA    | 162 | PRO  | CB-CA-C | -6.64 | 100.60      | 111.56   |
| 4   | F     | 162 | PRO  | N-CD-CG | -6.53 | 93.41       | 103.20   |
| 1   | UI    | 181 | GLU  | O-C-N   | 6.39  | 127.89      | 121.30   |
| 1   | UN    | 181 | GLU  | O-C-N   | 6.39  | 127.88      | 121.30   |
| 1   | UJ    | 181 | GLU  | O-C-N   | 6.39  | 127.88      | 121.30   |
| 1   | UL    | 131 | ASN  | O-C-N   | 6.33  | 129.37      | 122.15   |
| 1   | UP    | 131 | ASN  | O-C-N   | 6.32  | 129.35      | 122.15   |
| 1   | UK    | 181 | GLU  | O-C-N   | 6.32  | 127.81      | 121.30   |
| 1   | UK    | 131 | ASN  | O-C-N   | 6.31  | 129.34      | 122.15   |
| 1   | UO    | 131 | ASN  | O-C-N   | 6.31  | 129.34      | 122.15   |
| 1   | UL    | 181 | GLU  | O-C-N   | 6.31  | 127.80      | 121.30   |
| 1   | UN    | 131 | ASN  | O-C-N   | 6.29  | 129.32      | 122.15   |
| 1   | UL    | 221 | THR  | O-C-N   | -6.28 | 115.69      | 123.04   |
| 1   | UO    | 181 | GLU  | O-C-N   | 6.27  | 127.76      | 121.30   |
| 1   | UJ    | 131 | ASN  | O-C-N   | 6.27  | 129.30      | 122.15   |
| 1   | UK    | 221 | THR  | O-C-N   | -6.25 | 115.72      | 123.04   |
| 1   | UP    | 181 | GLU  | O-C-N   | 6.25  | 127.74      | 121.30   |
| 1   | UM    | 181 | GLU  | O-C-N   | 6.24  | 127.73      | 121.30   |
| 1   | UN    | 221 | THR  | O-C-N   | -6.24 | 115.74      | 123.04   |
| 1   | UJ    | 270 | THR  | O-C-N   | -6.22 | 115.77      | 123.04   |
| 1   | UM    | 131 | ASN  | O-C-N   | 6.21  | 129.23      | 122.15   |
| 1   | UI    | 221 | THR  | O-C-N   | -6.20 | 115.79      | 123.04   |
| 1   | UI    | 131 | ASN  | O-C-N   | 6.18  | 129.20      | 122.15   |
| 1   | UP    | 221 | THR  | O-C-N   | -6.18 | 115.81      | 123.04   |
| 1   | UM    | 221 | THR  | O-C-N   | -6.17 | 115.82      | 123.04   |
| 1   | UL    | 127 | SER  | O-C-N   | 6.17  | 129.19      | 122.15   |
| 1   | UO    | 221 | THR  | O-C-N   | -6.17 | 115.83      | 123.04   |
| 1   | UJ    | 127 | SER  | O-C-N   | 6.15  | 129.16      | 122.15   |
| 4   | G     | 162 | PRO  | N-CA-CB | -6.15 | 96.80       | 103.25   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | UN    | 127 | SER  | O-C-N   | 6.13  | 129.14      | 122.15   |
| 1   | UK    | 127 | SER  | O-C-N   | 6.13  | 129.14      | 122.15   |
| 1   | UM    | 127 | SER  | O-C-N   | 6.12  | 129.13      | 122.15   |
| 3   | E     | 185 | MET  | CA-C-N  | -6.11 | 112.29      | 120.54   |
| 3   | E     | 185 | MET  | C-N-CA  | -6.11 | 112.29      | 120.54   |
| 1   | UO    | 127 | SER  | O-C-N   | 6.11  | 129.12      | 122.15   |
| 1   | UI    | 127 | SER  | O-C-N   | 6.08  | 129.07      | 122.15   |
| 1   | UP    | 127 | SER  | O-C-N   | 6.00  | 128.99      | 122.15   |
| 3   | E     | 189 | PRO  | CA-N-CD | -5.86 | 103.80      | 112.00   |
| 1   | UP    | 132 | TYR  | O-C-N   | 5.78  | 128.02      | 122.07   |
| 1   | UI    | 132 | TYR  | O-C-N   | 5.75  | 127.99      | 122.07   |
| 1   | UK    | 132 | TYR  | O-C-N   | 5.74  | 127.98      | 122.07   |
| 1   | UL    | 132 | TYR  | O-C-N   | 5.74  | 127.98      | 122.07   |
| 1   | UN    | 132 | TYR  | O-C-N   | 5.72  | 127.96      | 122.07   |
| 1   | UO    | 132 | TYR  | O-C-N   | 5.71  | 127.95      | 122.07   |
| 1   | UM    | 132 | TYR  | O-C-N   | 5.70  | 127.94      | 122.07   |
| 1   | UJ    | 132 | TYR  | O-C-N   | 5.69  | 127.93      | 122.07   |
| 1   | WB    | 221 | THR  | CB-CA-C | -5.61 | 109.00      | 117.07   |
| 4   | G     | 120 | LYS  | N-CA-C  | -5.58 | 104.30      | 113.50   |
| 1   | WI    | 167 | ARG  | CB-CA-C | -5.57 | 109.66      | 117.23   |
| 1   | WJ    | 214 | ASP  | CB-CA-C | -5.53 | 99.99       | 113.15   |
| 1   | UP    | 125 | GLN  | CA-C-N  | -5.48 | 112.88      | 120.38   |
| 1   | UP    | 125 | GLN  | C-N-CA  | -5.48 | 112.88      | 120.38   |
| 1   | UL    | 125 | GLN  | CA-C-N  | -5.47 | 112.89      | 120.38   |
| 1   | UL    | 125 | GLN  | C-N-CA  | -5.47 | 112.89      | 120.38   |
| 1   | UN    | 125 | GLN  | CA-C-N  | -5.47 | 112.89      | 120.38   |
| 1   | UN    | 125 | GLN  | C-N-CA  | -5.47 | 112.89      | 120.38   |
| 1   | UK    | 125 | GLN  | CA-C-N  | -5.46 | 112.89      | 120.38   |
| 1   | UK    | 125 | GLN  | C-N-CA  | -5.46 | 112.89      | 120.38   |
| 1   | UI    | 125 | GLN  | CA-C-N  | -5.46 | 112.90      | 120.38   |
| 1   | UI    | 125 | GLN  | C-N-CA  | -5.46 | 112.90      | 120.38   |
| 1   | UJ    | 125 | GLN  | CA-C-N  | -5.46 | 112.90      | 120.38   |
| 1   | UJ    | 125 | GLN  | C-N-CA  | -5.46 | 112.90      | 120.38   |
| 1   | UO    | 125 | GLN  | CA-C-N  | -5.46 | 112.90      | 120.38   |
| 1   | UO    | 125 | GLN  | C-N-CA  | -5.46 | 112.90      | 120.38   |
| 1   | x     | 261 | ASN  | N-CA-C  | -5.41 | 106.53      | 113.02   |
| 1   | UM    | 125 | GLN  | CA-C-N  | -5.41 | 112.97      | 120.38   |
| 1   | UM    | 125 | GLN  | C-N-CA  | -5.41 | 112.97      | 120.38   |
| 1   | 4     | 261 | ASN  | N-CA-C  | -5.41 | 106.53      | 113.02   |
| 1   | AP    | 261 | ASN  | N-CA-C  | -5.40 | 106.53      | 113.02   |
| 1   | AI    | 261 | ASN  | N-CA-C  | -5.40 | 106.54      | 113.02   |
| 1   | 0     | 261 | ASN  | N-CA-C  | -5.39 | 106.55      | 113.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | WM    | 220 | LEU  | N-CA-C  | -5.39 | 106.68      | 113.20   |
| 1   | AH    | 261 | ASN  | N-CA-C  | -5.39 | 106.56      | 113.02   |
| 1   | AK    | 261 | ASN  | N-CA-C  | -5.39 | 106.56      | 113.02   |
| 1   | z     | 261 | ASN  | N-CA-C  | -5.38 | 106.56      | 113.02   |
| 4   | F     | 126 | ALA  | CA-C-N  | -5.38 | 113.01      | 120.38   |
| 4   | F     | 126 | ALA  | C-N-CA  | -5.38 | 113.01      | 120.38   |
| 1   | 8     | 261 | ASN  | N-CA-C  | -5.38 | 106.56      | 113.02   |
| 1   | AQ    | 261 | ASN  | N-CA-C  | -5.38 | 106.56      | 113.02   |
| 1   | WW    | 220 | LEU  | N-CA-C  | -5.38 | 106.69      | 113.20   |
| 1   | WH    | 220 | LEU  | N-CA-C  | -5.37 | 106.70      | 113.20   |
| 1   | 2     | 261 | ASN  | N-CA-C  | -5.37 | 106.58      | 113.02   |
| 1   | AM    | 261 | ASN  | N-CA-C  | -5.37 | 106.58      | 113.02   |
| 1   | AB    | 261 | ASN  | N-CA-C  | -5.36 | 106.58      | 113.02   |
| 1   | 6     | 261 | ASN  | N-CA-C  | -5.36 | 106.59      | 113.02   |
| 1   | 7     | 261 | ASN  | N-CA-C  | -5.36 | 106.59      | 113.02   |
| 1   | AO    | 261 | ASN  | N-CA-C  | -5.35 | 106.60      | 113.02   |
| 1   | AF    | 261 | ASN  | N-CA-C  | -5.35 | 106.60      | 113.02   |
| 1   | WS    | 220 | LEU  | N-CA-C  | -5.34 | 106.73      | 113.20   |
| 1   | AG    | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | AL    | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | y     | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | AA    | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | AC    | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | AE    | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | u     | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | 3     | 261 | ASN  | N-CA-C  | -5.34 | 106.62      | 113.02   |
| 1   | AD    | 261 | ASN  | N-CA-C  | -5.34 | 106.61      | 113.02   |
| 1   | WE    | 160 | PRO  | N-CA-CB | -5.33 | 97.65       | 103.25   |
| 1   | v     | 261 | ASN  | N-CA-C  | -5.33 | 106.62      | 113.02   |
| 1   | AN    | 261 | ASN  | N-CA-C  | -5.33 | 106.62      | 113.02   |
| 1   | WO    | 220 | LEU  | N-CA-C  | -5.33 | 106.75      | 113.20   |
| 1   | 1     | 261 | ASN  | N-CA-C  | -5.33 | 106.63      | 113.02   |
| 1   | WL    | 220 | LEU  | N-CA-C  | -5.32 | 106.76      | 113.20   |
| 1   | 5     | 261 | ASN  | N-CA-C  | -5.32 | 106.64      | 113.02   |
| 1   | AJ    | 261 | ASN  | N-CA-C  | -5.32 | 106.64      | 113.02   |
| 1   | 9     | 261 | ASN  | N-CA-C  | -5.32 | 106.64      | 113.02   |
| 1   | w     | 261 | ASN  | N-CA-C  | -5.31 | 106.64      | 113.02   |
| 1   | UK    | 130 | VAL  | CA-C-N  | -5.31 | 112.75      | 120.29   |
| 1   | UK    | 130 | VAL  | C-N-CA  | -5.31 | 112.75      | 120.29   |
| 1   | UN    | 130 | VAL  | CA-C-N  | -5.31 | 112.75      | 120.29   |
| 1   | UN    | 130 | VAL  | C-N-CA  | -5.31 | 112.75      | 120.29   |
| 1   | UI    | 130 | VAL  | CA-C-N  | -5.29 | 112.78      | 120.29   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | UI    | 130 | VAL  | C-N-CA  | -5.29 | 112.78      | 120.29   |
| 1   | t     | 261 | ASN  | N-CA-C  | -5.29 | 106.67      | 113.02   |
| 1   | UL    | 130 | VAL  | CA-C-N  | -5.28 | 112.80      | 120.29   |
| 1   | UL    | 130 | VAL  | C-N-CA  | -5.28 | 112.80      | 120.29   |
| 1   | UP    | 130 | VAL  | CA-C-N  | -5.27 | 112.80      | 120.29   |
| 1   | UP    | 130 | VAL  | C-N-CA  | -5.27 | 112.80      | 120.29   |
| 1   | UM    | 130 | VAL  | CA-C-N  | -5.26 | 112.81      | 120.29   |
| 1   | UM    | 130 | VAL  | C-N-CA  | -5.26 | 112.81      | 120.29   |
| 1   | WN    | 220 | LEU  | N-CA-C  | -5.26 | 106.83      | 113.20   |
| 1   | UO    | 130 | VAL  | CA-C-N  | -5.26 | 112.82      | 120.29   |
| 1   | UO    | 130 | VAL  | C-N-CA  | -5.26 | 112.82      | 120.29   |
| 1   | UJ    | 130 | VAL  | CA-C-N  | -5.25 | 112.83      | 120.29   |
| 1   | UJ    | 130 | VAL  | C-N-CA  | -5.25 | 112.83      | 120.29   |
| 1   | WI    | 165 | PHE  | CB-CA-C | 5.17  | 119.68      | 111.51   |
| 1   | UM    | 128 | GLU  | CA-C-N  | -5.13 | 113.76      | 120.44   |
| 1   | UM    | 128 | GLU  | C-N-CA  | -5.13 | 113.76      | 120.44   |
| 1   | UL    | 128 | GLU  | O-C-N   | 5.13  | 127.63      | 122.09   |
| 1   | UJ    | 128 | GLU  | CA-C-N  | -5.13 | 113.77      | 120.44   |
| 1   | UJ    | 128 | GLU  | C-N-CA  | -5.13 | 113.77      | 120.44   |
| 1   | UL    | 128 | GLU  | CA-C-N  | -5.12 | 113.78      | 120.44   |
| 1   | UL    | 128 | GLU  | C-N-CA  | -5.12 | 113.78      | 120.44   |
| 1   | UI    | 128 | GLU  | CA-C-N  | -5.12 | 113.78      | 120.44   |
| 1   | UI    | 128 | GLU  | C-N-CA  | -5.12 | 113.78      | 120.44   |
| 1   | WU    | 164 | LEU  | N-CA-C  | -5.11 | 107.00      | 113.18   |
| 1   | UP    | 128 | GLU  | CA-C-N  | -5.10 | 113.81      | 120.44   |
| 1   | UP    | 128 | GLU  | C-N-CA  | -5.10 | 113.81      | 120.44   |
| 1   | WO    | 167 | ARG  | CA-C-O  | -5.10 | 114.94      | 120.09   |
| 1   | WO    | 168 | GLU  | CB-CA-C | -5.10 | 100.28      | 110.42   |
| 1   | UO    | 128 | GLU  | CA-C-N  | -5.09 | 113.82      | 120.44   |
| 1   | UO    | 128 | GLU  | C-N-CA  | -5.09 | 113.82      | 120.44   |
| 1   | UK    | 128 | GLU  | CA-C-N  | -5.09 | 113.83      | 120.44   |
| 1   | UK    | 128 | GLU  | C-N-CA  | -5.09 | 113.83      | 120.44   |
| 1   | UK    | 128 | GLU  | O-C-N   | 5.09  | 127.58      | 122.09   |
| 1   | UM    | 128 | GLU  | O-C-N   | 5.08  | 127.58      | 122.09   |
| 1   | UN    | 128 | GLU  | CA-C-N  | -5.05 | 113.87      | 120.44   |
| 1   | UN    | 128 | GLU  | C-N-CA  | -5.05 | 113.87      | 120.44   |
| 1   | UP    | 128 | GLU  | O-C-N   | 5.02  | 127.52      | 122.09   |
| 1   | UI    | 128 | GLU  | O-C-N   | 5.02  | 127.51      | 122.09   |
| 1   | UJ    | 128 | GLU  | O-C-N   | 5.01  | 127.50      | 122.09   |
| 1   | UO    | 128 | GLU  | O-C-N   | 5.01  | 127.51      | 122.09   |
| 4   | I     | 157 | GLY  | O-C-N   | -5.01 | 116.76      | 121.77   |
| 1   | WW    | 164 | LEU  | N-CA-C  | -5.01 | 106.42      | 112.88   |

There are no chirality outliers.

All (72) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | H     | 143 | ARG  | Sidechain |
| 6   | Q     | 106 | ARG  | Sidechain |
| 6   | U     | 104 | ARG  | Sidechain |
| 1   | UI    | 221 | THR  | Mainchain |
| 1   | UI    | 50  | ASP  | Mainchain |
| 1   | UJ    | 270 | THR  | Mainchain |
| 1   | UJ    | 50  | ASP  | Mainchain |
| 1   | UK    | 167 | ARG  | Sidechain |
| 1   | UK    | 221 | THR  | Mainchain |
| 1   | UK    | 50  | ASP  | Mainchain |
| 1   | UL    | 167 | ARG  | Sidechain |
| 1   | UL    | 221 | THR  | Mainchain |
| 1   | UL    | 50  | ASP  | Mainchain |
| 1   | UM    | 221 | THR  | Mainchain |
| 1   | UM    | 50  | ASP  | Mainchain |
| 1   | UN    | 221 | THR  | Mainchain |
| 1   | UN    | 50  | ASP  | Mainchain |
| 1   | UO    | 221 | THR  | Mainchain |
| 1   | UO    | 50  | ASP  | Mainchain |
| 1   | UP    | 167 | ARG  | Sidechain |
| 1   | UP    | 221 | THR  | Mainchain |
| 1   | UP    | 50  | ASP  | Mainchain |
| 1   | WA    | 134 | ARG  | Sidechain |
| 1   | WA    | 142 | ARG  | Sidechain |
| 1   | WA    | 167 | ARG  | Sidechain |
| 1   | WB    | 134 | ARG  | Sidechain |
| 1   | WB    | 142 | ARG  | Sidechain |
| 1   | WB    | 154 | ARG  | Sidechain |
| 1   | WB    | 167 | ARG  | Sidechain |
| 1   | WC    | 134 | ARG  | Sidechain |
| 1   | WC    | 142 | ARG  | Sidechain |
| 1   | WC    | 167 | ARG  | Sidechain |
| 1   | WD    | 134 | ARG  | Sidechain |
| 1   | WE    | 134 | ARG  | Sidechain |
| 1   | WE    | 142 | ARG  | Sidechain |
| 1   | WF    | 134 | ARG  | Sidechain |
| 1   | WF    | 142 | ARG  | Sidechain |
| 1   | WF    | 167 | ARG  | Sidechain |
| 1   | WG    | 134 | ARG  | Sidechain |
| 1   | WG    | 142 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | WG    | 167 | ARG  | Sidechain |
| 1   | WI    | 142 | ARG  | Sidechain |
| 1   | WJ    | 134 | ARG  | Sidechain |
| 1   | WJ    | 142 | ARG  | Sidechain |
| 1   | WJ    | 167 | ARG  | Sidechain |
| 1   | WK    | 134 | ARG  | Sidechain |
| 1   | WK    | 142 | ARG  | Sidechain |
| 1   | WL    | 134 | ARG  | Sidechain |
| 1   | WL    | 157 | LEU  | Mainchain |
| 1   | WM    | 134 | ARG  | Sidechain |
| 1   | WN    | 134 | ARG  | Sidechain |
| 1   | WO    | 134 | ARG  | Sidechain |
| 1   | WP    | 134 | ARG  | Sidechain |
| 1   | WP    | 142 | ARG  | Sidechain |
| 1   | WP    | 154 | ARG  | Sidechain |
| 1   | WQ    | 134 | ARG  | Sidechain |
| 1   | WQ    | 142 | ARG  | Sidechain |
| 1   | WR    | 134 | ARG  | Sidechain |
| 1   | WR    | 142 | ARG  | Sidechain |
| 1   | WR    | 167 | ARG  | Sidechain |
| 1   | WS    | 167 | ARG  | Sidechain |
| 1   | WT    | 134 | ARG  | Sidechain |
| 1   | WT    | 142 | ARG  | Sidechain |
| 1   | WU    | 134 | ARG  | Sidechain |
| 1   | WU    | 142 | ARG  | Sidechain |
| 1   | WV    | 134 | ARG  | Sidechain |
| 1   | WV    | 142 | ARG  | Sidechain |
| 1   | WV    | 167 | ARG  | Sidechain |
| 1   | WW    | 134 | ARG  | Sidechain |
| 1   | WW    | 167 | ARG  | Sidechain |
| 7   | Y     | 110 | ARG  | Sidechain |
| 7   | a     | 110 | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1275  | 0        | 1254     | 34      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 1275  | 0        | 1254     | 59      | 0            |
| 1   | 2     | 1275  | 0        | 1254     | 40      | 0            |
| 1   | 3     | 1275  | 0        | 1254     | 31      | 0            |
| 1   | 4     | 1275  | 0        | 1254     | 45      | 0            |
| 1   | 5     | 1275  | 0        | 1254     | 39      | 0            |
| 1   | 6     | 1275  | 0        | 1254     | 50      | 0            |
| 1   | 7     | 1275  | 0        | 1254     | 54      | 0            |
| 1   | 8     | 1275  | 0        | 1254     | 34      | 0            |
| 1   | 9     | 1275  | 0        | 1254     | 32      | 0            |
| 1   | AA    | 1275  | 0        | 1254     | 30      | 0            |
| 1   | AB    | 1275  | 0        | 1254     | 44      | 0            |
| 1   | AC    | 1275  | 0        | 1254     | 47      | 0            |
| 1   | AD    | 1275  | 0        | 1254     | 47      | 0            |
| 1   | AE    | 1275  | 0        | 1254     | 46      | 0            |
| 1   | AF    | 1275  | 0        | 1254     | 29      | 0            |
| 1   | AG    | 1275  | 0        | 1254     | 33      | 0            |
| 1   | AH    | 1275  | 0        | 1254     | 52      | 0            |
| 1   | AI    | 1275  | 0        | 1254     | 48      | 0            |
| 1   | AJ    | 1275  | 0        | 1254     | 42      | 0            |
| 1   | AK    | 1275  | 0        | 1254     | 41      | 0            |
| 1   | AL    | 1275  | 0        | 1254     | 39      | 0            |
| 1   | AM    | 1275  | 0        | 1254     | 39      | 0            |
| 1   | AN    | 1275  | 0        | 1254     | 31      | 0            |
| 1   | AO    | 1275  | 0        | 1254     | 34      | 0            |
| 1   | AP    | 1275  | 0        | 1254     | 39      | 0            |
| 1   | AQ    | 1275  | 0        | 1254     | 33      | 0            |
| 1   | UI    | 1172  | 0        | 1181     | 64      | 0            |
| 1   | UJ    | 1172  | 0        | 1181     | 81      | 0            |
| 1   | UK    | 1172  | 0        | 1181     | 75      | 0            |
| 1   | UL    | 1172  | 0        | 1181     | 74      | 0            |
| 1   | UM    | 1172  | 0        | 1181     | 70      | 0            |
| 1   | UN    | 1172  | 0        | 1181     | 71      | 0            |
| 1   | UO    | 1172  | 0        | 1181     | 64      | 0            |
| 1   | UP    | 1172  | 0        | 1181     | 68      | 0            |
| 1   | WA    | 849   | 0        | 860      | 82      | 0            |
| 1   | WB    | 836   | 0        | 846      | 82      | 0            |
| 1   | WC    | 812   | 0        | 826      | 72      | 0            |
| 1   | WD    | 827   | 0        | 840      | 98      | 0            |
| 1   | WE    | 843   | 0        | 855      | 90      | 0            |
| 1   | WF    | 834   | 0        | 847      | 64      | 0            |
| 1   | WG    | 843   | 0        | 855      | 72      | 0            |
| 1   | WH    | 703   | 0        | 722      | 69      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | WI    | 703   | 0        | 722      | 78      | 0            |
| 1   | WJ    | 737   | 0        | 755      | 93      | 0            |
| 1   | WK    | 729   | 0        | 744      | 86      | 0            |
| 1   | WL    | 622   | 0        | 632      | 61      | 0            |
| 1   | WM    | 596   | 0        | 612      | 49      | 0            |
| 1   | WN    | 611   | 0        | 623      | 59      | 0            |
| 1   | WO    | 714   | 0        | 731      | 54      | 0            |
| 1   | WP    | 741   | 0        | 758      | 75      | 0            |
| 1   | WQ    | 834   | 0        | 847      | 75      | 0            |
| 1   | WR    | 834   | 0        | 847      | 64      | 0            |
| 1   | WS    | 834   | 0        | 847      | 83      | 0            |
| 1   | WT    | 834   | 0        | 847      | 77      | 0            |
| 1   | WU    | 843   | 0        | 855      | 68      | 0            |
| 1   | WV    | 827   | 0        | 838      | 67      | 0            |
| 1   | WW    | 834   | 0        | 847      | 89      | 0            |
| 1   | b     | 81    | 0        | 78       | 6       | 0            |
| 1   | c     | 103   | 0        | 99       | 0       | 0            |
| 1   | d     | 133   | 0        | 129      | 7       | 0            |
| 1   | e     | 103   | 0        | 99       | 4       | 0            |
| 1   | f     | 140   | 0        | 136      | 4       | 0            |
| 1   | g     | 103   | 0        | 99       | 3       | 0            |
| 1   | h     | 140   | 0        | 136      | 0       | 0            |
| 1   | i     | 103   | 0        | 99       | 1       | 0            |
| 1   | j     | 133   | 0        | 129      | 10      | 0            |
| 1   | k     | 103   | 0        | 99       | 3       | 0            |
| 1   | l     | 140   | 0        | 136      | 2       | 0            |
| 1   | t     | 1275  | 0        | 1254     | 45      | 0            |
| 1   | u     | 1275  | 0        | 1254     | 34      | 0            |
| 1   | v     | 1275  | 0        | 1254     | 28      | 0            |
| 1   | w     | 1275  | 0        | 1254     | 30      | 0            |
| 1   | x     | 1275  | 0        | 1254     | 33      | 0            |
| 1   | y     | 1275  | 0        | 1254     | 37      | 0            |
| 1   | z     | 1275  | 0        | 1254     | 51      | 0            |
| 2   | A     | 670   | 0        | 739      | 35      | 0            |
| 2   | B     | 670   | 0        | 739      | 38      | 0            |
| 2   | C     | 670   | 0        | 739      | 35      | 0            |
| 2   | D     | 670   | 0        | 739      | 42      | 0            |
| 3   | E     | 1945  | 0        | 2063     | 124     | 0            |
| 4   | F     | 1605  | 0        | 1701     | 87      | 0            |
| 4   | G     | 1626  | 0        | 1718     | 63      | 0            |
| 4   | H     | 1614  | 0        | 1709     | 57      | 0            |
| 4   | I     | 1614  | 0        | 1709     | 77      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | J     | 1623  | 0        | 1715     | 93      | 0            |
| 5   | K     | 429   | 0        | 445      | 40      | 0            |
| 5   | L     | 672   | 0        | 684      | 53      | 0            |
| 5   | M     | 686   | 0        | 700      | 54      | 0            |
| 5   | N     | 686   | 0        | 700      | 47      | 0            |
| 5   | O     | 686   | 0        | 700      | 53      | 0            |
| 5   | P     | 679   | 0        | 693      | 51      | 0            |
| 6   | Q     | 1030  | 0        | 1025     | 29      | 0            |
| 6   | R     | 942   | 0        | 943      | 37      | 0            |
| 6   | S     | 967   | 0        | 968      | 61      | 0            |
| 6   | T     | 982   | 0        | 984      | 46      | 0            |
| 6   | U     | 950   | 0        | 946      | 60      | 0            |
| 7   | V     | 969   | 0        | 981      | 23      | 0            |
| 7   | W     | 964   | 0        | 976      | 16      | 0            |
| 7   | X     | 969   | 0        | 981      | 16      | 0            |
| 7   | Y     | 969   | 0        | 981      | 18      | 0            |
| 7   | Z     | 969   | 0        | 981      | 22      | 0            |
| 7   | a     | 969   | 0        | 981      | 21      | 0            |
| All | All   | 99073 | 0        | 99719    | 3548    | 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 18.

All (3548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:WD:168:GLU:CD   | 1:WD:170:LYS:HE3 | 1.40                     | 1.43              |
| 1:WC:121:PHE:HZ   | 2:C:15:LYS:NZ    | 1.21                     | 1.35              |
| 1:UP:103:GLN:HG2  | 1:WW:182:PRO:CB  | 1.58                     | 1.33              |
| 1:UP:103:GLN:CG   | 1:WW:182:PRO:HB3 | 1.56                     | 1.32              |
| 5:L:11:ILE:HG22   | 1:AH:372:ILE:CD1 | 1.58                     | 1.32              |
| 6:U:72:HIS:CD2    | 1:1:365:ASN:HB3  | 1.64                     | 1.32              |
| 5:O:7:ILE:HG21    | 1:z:278:THR:CG2  | 1.56                     | 1.31              |
| 6:S:73:ILE:CD1    | 1:AE:297:GLN:HB2 | 1.61                     | 1.31              |
| 1:WJ:164:LEU:HD13 | 3:E:145:TRP:CD1  | 1.65                     | 1.29              |
| 1:WD:168:GLU:CG   | 1:WD:170:LYS:HE3 | 1.64                     | 1.28              |
| 1:WP:166:VAL:CG2  | 4:F:160:GLN:HB3  | 1.63                     | 1.28              |
| 5:O:7:ILE:CG2     | 1:z:278:THR:HG21 | 1.65                     | 1.25              |
| 6:R:72:HIS:ND1    | 1:AJ:365:ASN:HB3 | 1.47                     | 1.25              |
| 5:L:7:ILE:HD11    | 1:AI:370:ARG:NH2 | 1.54                     | 1.23              |
| 1:WQ:197:LEU:HD12 | 1:WR:175:SER:OG  | 1.39                     | 1.23              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WF:197:LEU:HD12 | 1:WG:175:SER:OG   | 1.34                     | 1.23              |
| 1:WR:197:LEU:HD12 | 1:WS:175:SER:OG   | 1.36                     | 1.22              |
| 5:K:7:ILE:HG21    | 1:AM:278:THR:CG2  | 1.69                     | 1.22              |
| 1:WA:128:GLU:HG2  | 1:WB:126:PHE:CD2  | 1.74                     | 1.22              |
| 1:WA:128:GLU:CG   | 1:WB:126:PHE:CD2  | 2.23                     | 1.21              |
| 5:L:11:ILE:CG2    | 1:AH:372:ILE:HG21 | 1.68                     | 1.21              |
| 1:WD:165:PHE:HB2  | 4:I:142:THR:O     | 1.35                     | 1.21              |
| 1:WK:167:ARG:HG2  | 3:E:156:THR:HG22  | 1.22                     | 1.21              |
| 5:P:7:ILE:CG2     | 1:t:278:THR:HG21  | 1.70                     | 1.20              |
| 1:WA:128:GLU:CG   | 1:WB:126:PHE:HD2  | 1.56                     | 1.19              |
| 1:WI:197:LEU:HD12 | 1:WJ:175:SER:CB   | 1.74                     | 1.18              |
| 6:U:78:VAL:CG1    | 1:1:299:ASN:HD22  | 1.58                     | 1.17              |
| 6:T:72:HIS:CD2    | 1:7:365:ASN:HB3   | 1.79                     | 1.16              |
| 1:WJ:197:LEU:HD12 | 1:WK:175:SER:OG   | 1.42                     | 1.16              |
| 5:L:11:ILE:HG21   | 1:AH:372:ILE:CG2  | 1.74                     | 1.15              |
| 6:U:78:VAL:HG11   | 1:1:299:ASN:ND2   | 1.61                     | 1.15              |
| 1:WA:158:ALA:HB2  | 1:WW:200:SER:O    | 1.44                     | 1.15              |
| 1:WR:197:LEU:HD12 | 1:WS:175:SER:CB   | 1.75                     | 1.14              |
| 1:WD:168:GLU:CD   | 1:WD:170:LYS:CE   | 2.21                     | 1.14              |
| 1:WK:197:LEU:HD12 | 1:WL:175:SER:CB   | 1.77                     | 1.14              |
| 1:UJ:103:GLN:HB3  | 1:WD:182:PRO:HB3  | 1.20                     | 1.14              |
| 5:O:21:ALA:CB     | 1:x:278:THR:HG21  | 1.78                     | 1.14              |
| 1:WI:197:LEU:HD12 | 1:WJ:175:SER:OG   | 1.47                     | 1.13              |
| 1:WE:166:VAL:CG2  | 4:I:160:GLN:HA    | 1.78                     | 1.13              |
| 1:WK:193:ALA:HB1  | 1:WL:213:VAL:HG21 | 1.28                     | 1.13              |
| 6:T:68:THR:HG21   | 1:7:367:GLU:OE1   | 1.49                     | 1.13              |
| 6:U:68:THR:HG21   | 1:1:367:GLU:OE1   | 1.49                     | 1.13              |
| 1:WS:200:SER:O    | 1:WT:158:ALA:HB2  | 1.46                     | 1.12              |
| 1:WA:128:GLU:HG2  | 1:WB:126:PHE:HD2  | 0.96                     | 1.12              |
| 1:WO:181:GLU:HB2  | 1:WO:184:ARG:HG3  | 1.14                     | 1.12              |
| 1:WR:112:GLY:HA2  | 1:WR:135:ALA:HA   | 1.27                     | 1.12              |
| 5:M:11:ILE:HD12   | 5:M:12:SER:N      | 1.64                     | 1.12              |
| 5:P:7:ILE:HG21    | 1:t:278:THR:HG21  | 1.21                     | 1.12              |
| 1:WJ:164:LEU:HD22 | 3:E:145:TRP:CD1   | 1.83                     | 1.12              |
| 1:WP:166:VAL:HG22 | 4:F:160:GLN:CB    | 1.79                     | 1.12              |
| 5:K:14:LEU:HD23   | 1:AL:278:THR:CG2  | 1.78                     | 1.12              |
| 1:WL:197:LEU:HD12 | 1:WM:175:SER:OG   | 1.49                     | 1.11              |
| 1:WG:181:GLU:HB2  | 1:WG:184:ARG:HG3  | 1.14                     | 1.11              |
| 1:WJ:164:LEU:HB2  | 3:E:145:TRP:NE1   | 1.65                     | 1.11              |
| 1:WK:181:GLU:HB2  | 1:WK:184:ARG:HG3  | 1.14                     | 1.11              |
| 1:WP:181:GLU:HB2  | 1:WP:184:ARG:HG3  | 1.14                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:U:78:VAL:CG1    | 1:1:299:ASN:ND2   | 2.13                     | 1.11              |
| 1:WF:181:GLU:HB2  | 1:WF:184:ARG:HG3  | 1.14                     | 1.10              |
| 1:WO:200:SER:OG   | 1:WP:175:SER:HB2  | 1.50                     | 1.10              |
| 5:K:7:ILE:HG21    | 1:AM:278:THR:HG21 | 1.20                     | 1.10              |
| 5:P:19:MET:HA     | 1:AP:276:GLU:OE2  | 1.51                     | 1.10              |
| 1:WE:181:GLU:HB2  | 1:WE:184:ARG:HG3  | 1.14                     | 1.10              |
| 1:WU:197:LEU:HD12 | 1:WV:175:SER:OG   | 1.51                     | 1.10              |
| 5:P:21:ALA:CB     | 1:AP:278:THR:HG21 | 1.80                     | 1.10              |
| 1:UN:167:ARG:NH2  | 1:WQ:188:GLU:HB3  | 1.68                     | 1.09              |
| 5:L:14:LEU:HD21   | 1:AH:370:ARG:HH21 | 1.07                     | 1.09              |
| 1:WA:197:LEU:HD12 | 1:WB:175:SER:OG   | 1.50                     | 1.09              |
| 1:WU:181:GLU:HB2  | 1:WU:184:ARG:HG3  | 1.14                     | 1.09              |
| 5:M:7:ILE:HB      | 1:AB:278:THR:HG21 | 1.16                     | 1.09              |
| 1:WC:121:PHE:CZ   | 2:C:15:LYS:NZ     | 2.02                     | 1.09              |
| 1:WA:181:GLU:HB2  | 1:WA:184:ARG:HG3  | 1.14                     | 1.09              |
| 1:WR:181:GLU:HB2  | 1:WR:184:ARG:HG3  | 1.14                     | 1.09              |
| 5:L:4:ILE:HG12    | 1:AI:372:ILE:CG2  | 1.81                     | 1.09              |
| 1:WA:158:ALA:CB   | 1:WW:200:SER:O    | 2.00                     | 1.08              |
| 1:WW:181:GLU:HB2  | 1:WW:184:ARG:HG3  | 1.14                     | 1.08              |
| 1:WQ:181:GLU:HB2  | 1:WQ:184:ARG:HG3  | 1.13                     | 1.08              |
| 1:WV:181:GLU:HB2  | 1:WV:184:ARG:HG3  | 1.14                     | 1.08              |
| 5:P:21:ALA:HB1    | 1:AP:278:THR:HG21 | 1.29                     | 1.08              |
| 1:WJ:197:LEU:HD12 | 1:WK:175:SER:CB   | 1.82                     | 1.08              |
| 1:WN:181:GLU:HB2  | 1:WN:184:ARG:HG3  | 1.14                     | 1.08              |
| 1:WT:181:GLU:HB2  | 1:WT:184:ARG:HG3  | 1.14                     | 1.08              |
| 1:WE:112:GLY:HA2  | 1:WE:135:ALA:HA   | 1.31                     | 1.08              |
| 1:WD:181:GLU:HB2  | 1:WD:184:ARG:HG3  | 1.14                     | 1.08              |
| 1:WL:181:GLU:HB2  | 1:WL:184:ARG:HG3  | 1.14                     | 1.08              |
| 1:WS:181:GLU:HB2  | 1:WS:184:ARG:HG3  | 1.13                     | 1.07              |
| 1:WM:181:GLU:HB2  | 1:WM:184:ARG:HG3  | 1.14                     | 1.07              |
| 5:L:11:ILE:HG22   | 1:AH:372:ILE:HD13 | 1.36                     | 1.07              |
| 1:WE:166:VAL:HG22 | 4:I:160:GLN:HA    | 1.11                     | 1.07              |
| 5:K:7:ILE:CG2     | 1:AM:278:THR:HG21 | 1.85                     | 1.07              |
| 6:S:72:HIS:ND1    | 1:AD:365:ASN:HB3  | 1.67                     | 1.07              |
| 1:WB:181:GLU:HB2  | 1:WB:184:ARG:HG3  | 1.14                     | 1.07              |
| 1:WI:181:GLU:HB2  | 1:WI:184:ARG:HG3  | 1.14                     | 1.07              |
| 5:K:21:ALA:CB     | 1:AK:278:THR:HG21 | 1.83                     | 1.07              |
| 5:N:21:ALA:CB     | 1:4:278:THR:HG21  | 1.84                     | 1.07              |
| 1:WN:196:HIS:HB3  | 1:WO:211:THR:HG21 | 1.34                     | 1.07              |
| 1:UK:207:PRO:HB2  | 1:WE:187:ASP:OD1  | 1.56                     | 1.06              |
| 1:WG:200:SER:OG   | 1:WH:175:SER:HB2  | 1.54                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WH:181:GLU:HB2  | 1:WH:184:ARG:HG3  | 1.13                     | 1.06              |
| 1:WJ:181:GLU:HB2  | 1:WJ:184:ARG:HG3  | 1.14                     | 1.06              |
| 5:L:7:ILE:CD1     | 1:AI:370:ARG:HH21 | 1.67                     | 1.06              |
| 1:UK:207:PRO:HD2  | 1:WE:187:ASP:CG   | 1.80                     | 1.06              |
| 1:WK:196:HIS:HB3  | 1:WL:211:THR:HG21 | 1.33                     | 1.06              |
| 1:WS:164:LEU:HB2  | 2:A:89:GLY:O      | 1.54                     | 1.06              |
| 6:S:65:LEU:HB2    | 1:AD:295:SER:HB2  | 1.35                     | 1.06              |
| 1:j:318:ASN:HD21  | 1:4:357:SER:HB2   | 1.20                     | 1.06              |
| 1:WC:186:LEU:HD22 | 1:WC:190:GLN:HG2  | 1.38                     | 1.05              |
| 5:O:7:ILE:CG2     | 1:z:278:THR:CG2   | 2.25                     | 1.05              |
| 6:T:68:THR:OG1    | 6:T:72:HIS:CE1    | 2.07                     | 1.05              |
| 1:UK:207:PRO:CB   | 1:WE:187:ASP:OD1  | 2.04                     | 1.05              |
| 5:K:14:LEU:HD23   | 1:AL:278:THR:HG21 | 1.37                     | 1.05              |
| 1:WG:112:GLY:HA2  | 1:WG:135:ALA:HA   | 1.36                     | 1.05              |
| 1:WS:112:GLY:HA2  | 1:WS:135:ALA:HA   | 1.12                     | 1.05              |
| 1:UJ:103:GLN:HB3  | 1:WD:182:PRO:CB   | 1.85                     | 1.05              |
| 1:WN:201:ALA:HA   | 1:WO:158:ALA:HB2  | 1.33                     | 1.05              |
| 1:WM:143:THR:OG1  | 1:WN:154:ARG:HG2  | 1.57                     | 1.04              |
| 6:S:72:HIS:CB     | 1:AE:295:SER:HB3  | 1.87                     | 1.04              |
| 1:WJ:164:LEU:HB2  | 3:E:145:TRP:HE1   | 1.14                     | 1.04              |
| 1:WF:122:GLY:HA2  | 2:D:68:TRP:HE1    | 1.20                     | 1.04              |
| 5:M:11:ILE:HG22   | 1:AB:372:ILE:CG2  | 1.87                     | 1.04              |
| 1:WD:200:SER:O    | 1:WE:158:ALA:HB2  | 1.58                     | 1.04              |
| 5:L:11:ILE:HG22   | 1:AH:372:ILE:HD12 | 1.38                     | 1.04              |
| 5:O:7:ILE:HG21    | 1:z:278:THR:HG22  | 1.36                     | 1.04              |
| 1:WJ:164:LEU:CD1  | 3:E:145:TRP:CD1   | 2.41                     | 1.03              |
| 1:WS:124:SER:HB2  | 2:A:8:MET:HE2     | 1.38                     | 1.03              |
| 1:WM:200:SER:OG   | 1:WN:175:SER:HB2  | 1.58                     | 1.03              |
| 5:L:7:ILE:HD11    | 1:AI:370:ARG:HH21 | 1.00                     | 1.03              |
| 1:WE:166:VAL:HG22 | 4:I:160:GLN:CA    | 1.86                     | 1.03              |
| 1:WK:197:LEU:HD12 | 1:WL:175:SER:HB3  | 1.07                     | 1.03              |
| 5:P:7:ILE:HG21    | 1:t:278:THR:CG2   | 1.87                     | 1.03              |
| 6:T:55:ARG:NH2    | 1:5:299:ASN:ND2   | 2.06                     | 1.03              |
| 1:WJ:128:GLU:HG2  | 1:WK:126:PHE:HD2  | 1.22                     | 1.03              |
| 1:WL:197:LEU:HD12 | 1:WM:175:SER:CB   | 1.88                     | 1.03              |
| 1:WV:112:GLY:HA2  | 1:WV:135:ALA:HA   | 1.40                     | 1.03              |
| 6:R:73:ILE:HG13   | 1:AK:295:SER:HB2  | 1.38                     | 1.02              |
| 1:WL:197:LEU:CD1  | 1:WM:175:SER:OG   | 2.06                     | 1.02              |
| 1:WO:197:LEU:HD12 | 1:WP:175:SER:OG   | 1.58                     | 1.02              |
| 1:WD:168:GLU:CG   | 1:WD:170:LYS:CE   | 2.37                     | 1.02              |
| 1:WR:197:LEU:CD1  | 1:WS:175:SER:OG   | 2.07                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WT:197:LEU:HD12 | 1:WU:175:SER:OG   | 1.57                     | 1.02              |
| 1:WN:200:SER:O    | 1:WO:158:ALA:CB   | 2.07                     | 1.02              |
| 1:WF:197:LEU:HD12 | 1:WG:175:SER:CB   | 1.89                     | 1.02              |
| 1:WH:203:ALA:HB1  | 1:WI:160:PRO:HB3  | 1.39                     | 1.02              |
| 1:WA:128:GLU:HG3  | 1:WB:126:PHE:CE2  | 1.95                     | 1.01              |
| 1:WW:165:PHE:HE1  | 2:B:89:GLY:HA2    | 1.20                     | 1.01              |
| 5:M:11:ILE:HD12   | 5:M:11:ILE:C      | 1.84                     | 1.01              |
| 6:U:65:LEU:CD2    | 1:1:297:GLN:HB2   | 1.90                     | 1.01              |
| 1:UJ:103:GLN:OE1  | 1:WD:182:PRO:HB3  | 1.58                     | 1.01              |
| 1:WW:164:LEU:HD12 | 2:B:89:GLY:O      | 1.60                     | 1.01              |
| 1:WE:167:ARG:HD3  | 4:I:161:GLY:HA2   | 1.40                     | 1.01              |
| 1:WG:164:LEU:O    | 4:J:241:GLN:HG2   | 1.58                     | 1.01              |
| 1:WJ:164:LEU:HD22 | 3:E:145:TRP:HD1   | 1.26                     | 1.01              |
| 1:WN:200:SER:O    | 1:WO:158:ALA:HB3  | 1.59                     | 1.01              |
| 1:WT:196:HIS:HB3  | 1:WU:211:THR:HG21 | 1.41                     | 1.01              |
| 1:WA:112:GLY:HA2  | 1:WA:135:ALA:HA   | 1.41                     | 1.00              |
| 5:N:21:ALA:HB3    | 1:4:278:THR:HG21  | 1.43                     | 1.00              |
| 1:WA:160:PRO:HB3  | 1:WW:203:ALA:HB1  | 1.38                     | 1.00              |
| 5:O:21:ALA:HB1    | 1:x:278:THR:HG21  | 1.43                     | 1.00              |
| 1:WJ:164:LEU:CD2  | 3:E:145:TRP:HD1   | 1.74                     | 1.00              |
| 6:U:78:VAL:HG11   | 1:1:299:ASN:HD22  | 0.86                     | 1.00              |
| 1:UP:62:ASP:OD2   | 1:WV:184:ARG:NH2  | 1.95                     | 1.00              |
| 1:WS:200:SER:O    | 1:WT:158:ALA:CB   | 2.09                     | 1.00              |
| 1:WD:168:GLU:HG2  | 1:WD:170:LYS:HE3  | 1.42                     | 0.99              |
| 5:M:11:ILE:CG2    | 1:AB:372:ILE:HG21 | 1.92                     | 0.99              |
| 1:WC:164:LEU:O    | 4:I:241:GLN:HG2   | 1.61                     | 0.99              |
| 1:WH:200:SER:O    | 1:WI:158:ALA:HB2  | 1.62                     | 0.99              |
| 1:WJ:197:LEU:CD1  | 1:WK:175:SER:OG   | 2.11                     | 0.99              |
| 1:UO:103:GLN:CD   | 1:WU:182:PRO:HB3  | 1.87                     | 0.99              |
| 1:WD:200:SER:OG   | 1:WE:175:SER:HB2  | 1.59                     | 0.99              |
| 1:WM:193:ALA:HB1  | 1:WN:213:VAL:HG11 | 1.44                     | 0.99              |
| 1:UK:207:PRO:HD2  | 1:WE:187:ASP:OD2  | 1.61                     | 0.99              |
| 1:WA:128:GLU:HG3  | 1:WB:126:PHE:CD2  | 1.96                     | 0.98              |
| 1:UM:125:GLN:O    | 1:UM:129:GLN:N    | 1.97                     | 0.98              |
| 1:UK:73:MET:CE    | 1:UK:99:ARG:HD3   | 1.93                     | 0.98              |
| 1:UN:125:GLN:O    | 1:UN:129:GLN:N    | 1.97                     | 0.98              |
| 1:UO:125:GLN:O    | 1:UO:129:GLN:N    | 1.97                     | 0.98              |
| 5:M:11:ILE:CG2    | 1:AB:372:ILE:CG2  | 2.42                     | 0.98              |
| 1:UN:73:MET:CE    | 1:UN:99:ARG:HD3   | 1.93                     | 0.98              |
| 1:UP:125:GLN:O    | 1:UP:129:GLN:N    | 1.97                     | 0.98              |
| 1:WF:197:LEU:CD1  | 1:WG:175:SER:OG   | 2.11                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UJ:73:MET:CE    | 1:UJ:99:ARG:HD3   | 1.93                     | 0.98              |
| 1:UP:73:MET:CE    | 1:UP:99:ARG:HD3   | 1.93                     | 0.98              |
| 1:WK:164:LEU:HD12 | 3:E:248:PHE:HB3   | 1.46                     | 0.98              |
| 3:E:185:MET:O     | 3:E:189:PRO:HD2   | 1.64                     | 0.97              |
| 1:WC:164:LEU:O    | 4:I:241:GLN:CG    | 2.12                     | 0.97              |
| 5:O:14:LEU:HD11   | 1:z:370:ARG:HH21  | 1.29                     | 0.97              |
| 1:UL:73:MET:CE    | 1:UL:99:ARG:HD3   | 1.93                     | 0.97              |
| 1:UO:73:MET:CE    | 1:UO:99:ARG:HD3   | 1.93                     | 0.97              |
| 6:T:78:VAL:C      | 1:7:299:ASN:HD21  | 1.70                     | 0.97              |
| 1:UL:219:LEU:HD22 | 1:u:247:ARG:NH1   | 1.79                     | 0.97              |
| 5:M:14:LEU:HB3    | 1:AA:278:THR:HG21 | 1.45                     | 0.97              |
| 1:UI:73:MET:CE    | 1:UI:99:ARG:HD3   | 1.93                     | 0.97              |
| 1:WI:197:LEU:CD1  | 1:WJ:175:SER:OG   | 2.12                     | 0.97              |
| 5:L:11:ILE:HG21   | 1:AH:372:ILE:HG21 | 1.34                     | 0.97              |
| 1:WT:197:LEU:HD12 | 1:WU:175:SER:CB   | 1.94                     | 0.96              |
| 1:UI:125:GLN:O    | 1:UI:129:GLN:N    | 1.97                     | 0.96              |
| 1:UM:73:MET:CE    | 1:UM:99:ARG:HD3   | 1.93                     | 0.96              |
| 1:WC:121:PHE:HZ   | 2:C:15:LYS:CE     | 1.76                     | 0.96              |
| 1:UK:125:GLN:O    | 1:UK:129:GLN:N    | 1.97                     | 0.96              |
| 1:WI:196:HIS:HB3  | 1:WJ:211:THR:HG21 | 1.45                     | 0.96              |
| 1:WP:166:VAL:HG22 | 4:F:160:GLN:HB3   | 0.99                     | 0.96              |
| 6:T:78:VAL:O      | 1:7:299:ASN:ND2   | 1.99                     | 0.96              |
| 1:UL:125:GLN:O    | 1:UL:129:GLN:N    | 1.97                     | 0.96              |
| 1:WK:164:LEU:HD12 | 3:E:248:PHE:CB    | 1.96                     | 0.96              |
| 1:WE:197:LEU:HD12 | 1:WF:175:SER:OG   | 1.63                     | 0.96              |
| 5:M:11:ILE:HG22   | 1:AB:372:ILE:HG21 | 1.44                     | 0.96              |
| 6:U:72:HIS:HD2    | 1:1:365:ASN:HB3   | 0.98                     | 0.96              |
| 1:UJ:125:GLN:O    | 1:UJ:129:GLN:N    | 1.97                     | 0.96              |
| 1:WT:112:GLY:HA2  | 1:WT:135:ALA:HA   | 1.48                     | 0.95              |
| 1:WA:200:SER:OG   | 1:WB:175:SER:HB2  | 1.64                     | 0.95              |
| 5:L:4:ILE:CG1     | 1:AI:372:ILE:CG2  | 2.44                     | 0.95              |
| 1:WH:200:SER:OG   | 1:WI:175:SER:HB2  | 1.67                     | 0.95              |
| 5:L:11:ILE:CG2    | 1:AH:372:ILE:CG2  | 2.38                     | 0.95              |
| 6:R:72:HIS:CE1    | 1:AJ:365:ASN:HB3  | 2.02                     | 0.95              |
| 1:UP:133:GLN:NE2  | 1:UP:157:LEU:O    | 2.00                     | 0.95              |
| 1:WC:200:SER:O    | 1:WD:158:ALA:HB2  | 1.64                     | 0.95              |
| 1:WD:165:PHE:HB3  | 4:I:143:ARG:HA    | 1.48                     | 0.95              |
| 1:WK:197:LEU:CD1  | 1:WL:175:SER:HB3  | 1.96                     | 0.95              |
| 1:UI:133:GLN:NE2  | 1:UI:157:LEU:O    | 2.00                     | 0.94              |
| 1:UJ:133:GLN:NE2  | 1:UJ:157:LEU:O    | 2.00                     | 0.94              |
| 1:WE:200:SER:OG   | 1:WF:175:SER:HB2  | 1.67                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WH:193:ALA:HB1  | 1:WI:213:VAL:HG11 | 1.46                     | 0.94              |
| 1:UK:133:GLN:NE2  | 1:UK:157:LEU:O    | 2.00                     | 0.94              |
| 1:UM:103:GLN:CD   | 1:WQ:182:PRO:HB3  | 1.93                     | 0.94              |
| 1:UM:133:GLN:NE2  | 1:UM:157:LEU:O    | 2.00                     | 0.94              |
| 1:UN:133:GLN:NE2  | 1:UN:157:LEU:O    | 2.00                     | 0.94              |
| 1:UL:133:GLN:NE2  | 1:UL:157:LEU:O    | 2.00                     | 0.94              |
| 5:O:7:ILE:HG21    | 1:z:278:THR:HG21  | 1.31                     | 0.94              |
| 1:WI:197:LEU:HD12 | 1:WJ:175:SER:HB3  | 1.47                     | 0.94              |
| 1:UM:62:ASP:OD2   | 1:WP:184:ARG:NH2  | 1.99                     | 0.94              |
| 1:WS:112:GLY:CA   | 1:WS:135:ALA:HA   | 1.97                     | 0.94              |
| 1:WT:200:SER:O    | 1:WU:158:ALA:CB   | 2.15                     | 0.93              |
| 6:Q:65:LEU:HD22   | 1:AQ:295:SER:HB2  | 1.49                     | 0.93              |
| 1:UO:133:GLN:NE2  | 1:UO:157:LEU:O    | 2.00                     | 0.93              |
| 1:WV:120:LYS:HZ3  | 1:WV:123:ILE:HD11 | 1.34                     | 0.93              |
| 6:S:72:HIS:HB2    | 1:AE:295:SER:HB3  | 1.48                     | 0.93              |
| 1:UK:207:PRO:CG   | 1:WE:187:ASP:OD1  | 2.16                     | 0.93              |
| 5:L:4:ILE:HD11    | 1:AI:372:ILE:HG22 | 1.49                     | 0.93              |
| 1:j:318:ASN:ND2   | 1:4:357:SER:HB2   | 1.84                     | 0.93              |
| 5:L:4:ILE:HG12    | 1:AI:372:ILE:CB   | 1.98                     | 0.92              |
| 1:WP:200:SER:OG   | 1:WQ:175:SER:HB2  | 1.69                     | 0.92              |
| 1:WS:112:GLY:HA2  | 1:WS:135:ALA:CA   | 1.99                     | 0.92              |
| 6:T:72:HIS:HD2    | 1:7:365:ASN:HB3   | 1.15                     | 0.92              |
| 1:WA:197:LEU:HD12 | 1:WB:175:SER:CB   | 1.99                     | 0.92              |
| 1:WR:112:GLY:CA   | 1:WR:135:ALA:HA   | 2.00                     | 0.92              |
| 1:UN:62:ASP:OD2   | 1:WR:184:ARG:NH2  | 2.02                     | 0.92              |
| 1:WF:181:GLU:CB   | 1:WF:184:ARG:HG3  | 2.00                     | 0.91              |
| 1:WP:181:GLU:CB   | 1:WP:184:ARG:HG3  | 2.01                     | 0.91              |
| 1:WT:181:GLU:CB   | 1:WT:184:ARG:HG3  | 2.00                     | 0.91              |
| 1:WA:181:GLU:CB   | 1:WA:184:ARG:HG3  | 2.01                     | 0.91              |
| 1:WM:181:GLU:CB   | 1:WM:184:ARG:HG3  | 2.01                     | 0.91              |
| 1:WE:181:GLU:CB   | 1:WE:184:ARG:HG3  | 2.01                     | 0.91              |
| 1:WB:181:GLU:CB   | 1:WB:184:ARG:HG3  | 2.01                     | 0.91              |
| 1:WI:164:LEU:HD22 | 4:J:148:ALA:HB2   | 1.50                     | 0.91              |
| 1:WS:121:PHE:HE1  | 1:WT:120:LYS:HZ3  | 0.94                     | 0.91              |
| 1:WS:124:SER:HB2  | 2:A:8:MET:CE      | 2.00                     | 0.90              |
| 5:L:14:LEU:CD2    | 1:AH:370:ARG:HH21 | 1.83                     | 0.90              |
| 1:WQ:181:GLU:CB   | 1:WQ:184:ARG:HG3  | 2.00                     | 0.90              |
| 5:K:14:LEU:CD2    | 1:AL:278:THR:HG21 | 2.01                     | 0.90              |
| 1:WU:181:GLU:CB   | 1:WU:184:ARG:HG3  | 2.00                     | 0.90              |
| 1:WI:181:GLU:CB   | 1:WI:184:ARG:HG3  | 2.01                     | 0.90              |
| 1:WG:181:GLU:CB   | 1:WG:184:ARG:HG3  | 2.01                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:O:14:LEU:HB3    | 1:y:278:THR:HG21  | 1.52                     | 0.90              |
| 1:WD:181:GLU:CB   | 1:WD:184:ARG:HG3  | 2.01                     | 0.90              |
| 6:S:73:ILE:HD13   | 1:AE:297:GLN:HB2  | 1.54                     | 0.90              |
| 1:WJ:164:LEU:CD2  | 3:E:145:TRP:CD1   | 2.53                     | 0.90              |
| 1:WG:165:PHE:CZ   | 4:I:153:LEU:HD21  | 2.07                     | 0.90              |
| 1:WG:165:PHE:HE1  | 4:J:240:ALA:HB3   | 1.36                     | 0.90              |
| 1:d:319:GLN:CD    | 1:AM:357:SER:OG   | 2.15                     | 0.90              |
| 1:WH:181:GLU:CB   | 1:WH:184:ARG:HG3  | 2.00                     | 0.89              |
| 1:WM:197:LEU:HD12 | 1:WN:175:SER:OG   | 1.72                     | 0.89              |
| 5:O:7:ILE:CB      | 1:z:278:THR:HG21  | 2.01                     | 0.89              |
| 1:WJ:128:GLU:CG   | 1:WK:126:PHE:HD2  | 1.84                     | 0.89              |
| 1:WK:181:GLU:CB   | 1:WK:184:ARG:HG3  | 2.01                     | 0.89              |
| 1:WD:168:GLU:HG2  | 1:WD:170:LYS:CE   | 2.00                     | 0.89              |
| 1:WV:181:GLU:CB   | 1:WV:184:ARG:HG3  | 2.01                     | 0.89              |
| 3:E:158:PRO:HG2   | 3:E:162:ASN:HD21  | 1.35                     | 0.89              |
| 5:K:14:LEU:HD23   | 1:AL:278:THR:HG22 | 1.55                     | 0.89              |
| 1:WB:197:LEU:HD12 | 1:WC:175:SER:OG   | 1.72                     | 0.89              |
| 5:O:21:ALA:HB3    | 1:x:278:THR:HG21  | 1.54                     | 0.89              |
| 1:WD:115:LEU:HD22 | 1:WD:134:ARG:HD2  | 1.54                     | 0.89              |
| 1:WR:197:LEU:HD12 | 1:WS:175:SER:HB3  | 1.54                     | 0.89              |
| 1:WW:165:PHE:CE1  | 2:B:89:GLY:HA2    | 2.07                     | 0.89              |
| 6:T:55:ARG:CZ     | 1:5:299:ASN:ND2   | 2.35                     | 0.89              |
| 1:WD:200:SER:O    | 1:WE:158:ALA:CB   | 2.20                     | 0.89              |
| 1:WI:164:LEU:HD22 | 4:J:148:ALA:CB    | 2.02                     | 0.89              |
| 1:WO:181:GLU:CB   | 1:WO:184:ARG:HG3  | 2.00                     | 0.89              |
| 1:WJ:181:GLU:CB   | 1:WJ:184:ARG:HG3  | 2.00                     | 0.88              |
| 1:WR:181:GLU:CB   | 1:WR:184:ARG:HG3  | 2.01                     | 0.88              |
| 1:WW:181:GLU:CB   | 1:WW:184:ARG:HG3  | 2.01                     | 0.88              |
| 6:S:65:LEU:HB2    | 1:AD:295:SER:CB   | 2.03                     | 0.88              |
| 1:UM:126:PHE:CE1  | 1:UM:130:VAL:HG21 | 2.09                     | 0.88              |
| 1:WN:181:GLU:CB   | 1:WN:184:ARG:HG3  | 2.01                     | 0.88              |
| 1:UN:126:PHE:O    | 1:UN:130:VAL:N    | 2.07                     | 0.88              |
| 1:UP:126:PHE:CE1  | 1:UP:130:VAL:HG21 | 2.09                     | 0.88              |
| 1:UK:126:PHE:CE1  | 1:UK:130:VAL:HG21 | 2.09                     | 0.88              |
| 1:UM:126:PHE:O    | 1:UM:130:VAL:N    | 2.07                     | 0.87              |
| 1:UO:126:PHE:CE1  | 1:UO:130:VAL:HG21 | 2.09                     | 0.87              |
| 1:WS:181:GLU:CB   | 1:WS:184:ARG:HG3  | 2.00                     | 0.87              |
| 6:T:72:HIS:HD2    | 1:7:365:ASN:CB    | 1.87                     | 0.87              |
| 1:UO:126:PHE:O    | 1:UO:130:VAL:N    | 2.07                     | 0.87              |
| 1:WT:121:PHE:CZ   | 1:WU:122:GLY:O    | 2.27                     | 0.87              |
| 1:UI:126:PHE:CE1  | 1:UI:130:VAL:HG21 | 2.09                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WL:181:GLU:CB   | 1:WL:184:ARG:HG3  | 2.01                     | 0.87              |
| 5:L:4:ILE:HG12    | 1:AI:372:ILE:HB   | 1.54                     | 0.87              |
| 1:UK:126:PHE:O    | 1:UK:130:VAL:N    | 2.07                     | 0.87              |
| 1:WV:200:SER:O    | 1:WW:158:ALA:HB2  | 1.73                     | 0.87              |
| 1:UJ:126:PHE:CE1  | 1:UJ:130:VAL:HG21 | 2.09                     | 0.87              |
| 1:UL:126:PHE:CE1  | 1:UL:130:VAL:HG21 | 2.09                     | 0.87              |
| 1:WD:165:PHE:HE2  | 4:I:141:GLN:HA    | 1.39                     | 0.87              |
| 1:UN:126:PHE:CE1  | 1:UN:130:VAL:HG21 | 2.09                     | 0.87              |
| 1:UP:126:PHE:O    | 1:UP:130:VAL:N    | 2.07                     | 0.87              |
| 1:UJ:126:PHE:O    | 1:UJ:130:VAL:N    | 2.07                     | 0.86              |
| 1:WK:200:SER:O    | 1:WL:158:ALA:HB3  | 1.75                     | 0.86              |
| 1:WC:121:PHE:CZ   | 2:C:15:LYS:CE     | 2.56                     | 0.86              |
| 1:WD:203:ALA:HB1  | 1:WE:160:PRO:HB3  | 1.57                     | 0.86              |
| 6:S:73:ILE:HD12   | 1:AE:297:GLN:HB2  | 1.57                     | 0.86              |
| 1:WC:200:SER:O    | 1:WD:158:ALA:CB   | 2.23                     | 0.86              |
| 1:WM:139:GLU:HB3  | 1:WN:154:ARG:HH21 | 1.39                     | 0.86              |
| 5:L:4:ILE:HG12    | 1:AI:372:ILE:HG21 | 1.57                     | 0.86              |
| 1:WK:132:TYR:HB2  | 1:WL:126:PHE:HZ   | 1.40                     | 0.86              |
| 1:WA:196:HIS:HB3  | 1:WB:211:THR:HG21 | 1.57                     | 0.86              |
| 1:WB:200:SER:OG   | 1:WC:175:SER:HB2  | 1.76                     | 0.86              |
| 1:WK:193:ALA:HB1  | 1:WL:213:VAL:CG2  | 2.06                     | 0.86              |
| 1:WO:166:VAL:HG23 | 4:F:139:LEU:O     | 1.75                     | 0.86              |
| 1:WS:121:PHE:HE1  | 1:WT:120:LYS:NZ   | 1.74                     | 0.86              |
| 5:L:4:ILE:CG1     | 1:AI:372:ILE:HG21 | 2.04                     | 0.86              |
| 1:UL:126:PHE:O    | 1:UL:130:VAL:N    | 2.07                     | 0.85              |
| 1:UJ:103:GLN:CB   | 1:WD:182:PRO:HB3  | 2.04                     | 0.85              |
| 1:WR:196:HIS:HB3  | 1:WS:211:THR:HG21 | 1.56                     | 0.85              |
| 1:WR:200:SER:O    | 1:WS:158:ALA:CB   | 2.24                     | 0.85              |
| 5:K:21:ALA:HB1    | 1:AK:278:THR:HG21 | 1.56                     | 0.85              |
| 1:UI:126:PHE:O    | 1:UI:130:VAL:N    | 2.07                     | 0.85              |
| 1:UJ:126:PHE:O    | 1:UJ:130:VAL:HG23 | 1.77                     | 0.85              |
| 1:d:319:GLN:CD    | 1:AM:357:SER:HG   | 1.84                     | 0.85              |
| 1:UM:103:GLN:CG   | 1:WQ:182:PRO:HB3  | 2.06                     | 0.85              |
| 1:WH:200:SER:O    | 1:WI:158:ALA:CB   | 2.23                     | 0.85              |
| 1:WK:167:ARG:CG   | 3:E:156:THR:HG22  | 2.04                     | 0.85              |
| 6:U:65:LEU:HD22   | 1:I:297:GLN:HB2   | 1.57                     | 0.85              |
| 1:UI:126:PHE:O    | 1:UI:130:VAL:HG23 | 1.77                     | 0.85              |
| 1:WV:200:SER:O    | 1:WW:158:ALA:CB   | 2.25                     | 0.85              |
| 1:WM:197:LEU:HD12 | 1:WN:175:SER:CB   | 2.05                     | 0.84              |
| 1:WS:125:GLN:HB2  | 2:A:4:GLU:HB2     | 1.57                     | 0.84              |
| 1:WJ:164:LEU:CD1  | 3:E:145:TRP:HD1   | 1.82                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:T:68:THR:HG1    | 6:T:72:HIS:CE1    | 1.94                     | 0.84              |
| 1:UN:126:PHE:O    | 1:UN:130:VAL:HG23 | 1.77                     | 0.84              |
| 1:WU:197:LEU:HD12 | 1:WV:175:SER:CB   | 2.07                     | 0.84              |
| 6:T:78:VAL:HG12   | 1:6:361:ASN:HD22  | 1.40                     | 0.84              |
| 1:WC:165:PHE:HD2  | 4:H:152:ARG:HH21  | 1.21                     | 0.84              |
| 1:WA:175:SER:HB2  | 1:WW:200:SER:OG   | 1.76                     | 0.84              |
| 1:WA:175:SER:CB   | 1:WW:197:LEU:HD12 | 2.08                     | 0.84              |
| 1:WF:122:GLY:HA2  | 2:D:68:TRP:NE1    | 1.93                     | 0.84              |
| 1:UK:126:PHE:O    | 1:UK:130:VAL:HG23 | 1.77                     | 0.84              |
| 1:UO:103:GLN:NE2  | 1:WU:182:PRO:HB3  | 1.92                     | 0.84              |
| 1:UP:126:PHE:O    | 1:UP:130:VAL:HG23 | 1.77                     | 0.84              |
| 1:UL:126:PHE:O    | 1:UL:130:VAL:HG23 | 1.77                     | 0.84              |
| 5:L:4:ILE:CD1     | 1:AI:372:ILE:HG22 | 2.08                     | 0.84              |
| 6:Q:88:ARG:NH1    | 6:Q:105:GLU:OE1   | 2.10                     | 0.84              |
| 1:WT:200:SER:O    | 1:WU:158:ALA:HB2  | 1.77                     | 0.84              |
| 6:S:76:GLN:O      | 1:AD:297:GLN:OE1  | 1.96                     | 0.84              |
| 1:UJ:167:ARG:NH2  | 1:WB:188:GLU:HB3  | 1.92                     | 0.83              |
| 3:E:182:ASN:HB3   | 3:E:239:PHE:HZ    | 1.43                     | 0.83              |
| 5:M:7:ILE:HB      | 1:AB:278:THR:CG2  | 2.07                     | 0.83              |
| 1:UO:126:PHE:O    | 1:UO:130:VAL:HG23 | 1.77                     | 0.83              |
| 1:UJ:103:GLN:OE1  | 1:WD:182:PRO:CB   | 2.26                     | 0.83              |
| 1:UM:126:PHE:O    | 1:UM:130:VAL:HG23 | 1.77                     | 0.83              |
| 1:UN:94:HIS:HB3   | 1:UN:146:THR:HG21 | 1.60                     | 0.83              |
| 1:WJ:164:LEU:CG   | 3:E:145:TRP:HD1   | 1.91                     | 0.83              |
| 1:WQ:200:SER:OG   | 1:WR:175:SER:HB2  | 1.78                     | 0.83              |
| 5:P:7:ILE:CG2     | 1:t:278:THR:CG2   | 2.52                     | 0.83              |
| 1:UK:207:PRO:CD   | 1:WE:187:ASP:CG   | 2.51                     | 0.83              |
| 1:UP:94:HIS:HB3   | 1:UP:146:THR:HG21 | 1.61                     | 0.83              |
| 1:UL:94:HIS:HB3   | 1:UL:146:THR:HG21 | 1.60                     | 0.83              |
| 5:L:14:LEU:HD21   | 1:AH:370:ARG:NH2  | 1.91                     | 0.83              |
| 1:UO:94:HIS:HB3   | 1:UO:146:THR:HG21 | 1.60                     | 0.83              |
| 1:WP:166:VAL:CG2  | 4:F:160:GLN:CB    | 2.46                     | 0.83              |
| 6:T:55:ARG:NH2    | 1:5:299:ASN:HD22  | 1.75                     | 0.83              |
| 1:WG:200:SER:O    | 1:WH:158:ALA:HB2  | 1.79                     | 0.83              |
| 1:WT:197:LEU:CD1  | 1:WU:175:SER:OG   | 2.27                     | 0.82              |
| 1:WJ:164:LEU:CG   | 3:E:145:TRP:CD1   | 2.62                     | 0.82              |
| 5:L:7:ILE:HD11    | 1:AI:370:ARG:CZ   | 2.08                     | 0.82              |
| 1:UI:94:HIS:HB3   | 1:UI:146:THR:HG21 | 1.60                     | 0.82              |
| 1:UJ:167:ARG:HH22 | 1:WB:188:GLU:HB3  | 1.44                     | 0.82              |
| 1:UK:207:PRO:CD   | 1:WE:187:ASP:OD1  | 2.27                     | 0.82              |
| 1:WW:125:GLN:OE1  | 2:B:2:THR:CG2     | 2.28                     | 0.82              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:21:ALA:HB1   | 1:O:278:THR:HG21  | 1.62                     | 0.82              |
| 5:N:11:ILE:HG22  | 1:6:372:ILE:HD12  | 1.62                     | 0.82              |
| 7:Z:6:ILE:HG21   | 7:Z:122:VAL:HG11  | 1.59                     | 0.82              |
| 5:O:14:LEU:HD23  | 1:y:278:THR:CG2   | 2.09                     | 0.82              |
| 6:U:78:VAL:HG12  | 1:1:299:ASN:ND2   | 1.93                     | 0.82              |
| 1:UL:128:GLU:O   | 1:UL:132:TYR:N    | 2.13                     | 0.81              |
| 1:UP:127:SER:O   | 1:UP:131:ASN:N    | 2.13                     | 0.81              |
| 1:UK:128:GLU:O   | 1:UK:132:TYR:N    | 2.13                     | 0.81              |
| 1:UO:127:SER:O   | 1:UO:131:ASN:N    | 2.13                     | 0.81              |
| 1:WK:196:HIS:CB  | 1:WL:211:THR:HG21 | 2.10                     | 0.81              |
| 1:UJ:73:MET:HE1  | 1:UJ:99:ARG:HD3   | 1.62                     | 0.81              |
| 1:UM:103:GLN:HG2 | 1:WQ:182:PRO:HB3  | 1.61                     | 0.81              |
| 1:WJ:164:LEU:CD2 | 3:E:144:LEU:HB2   | 2.10                     | 0.81              |
| 2:C:28:ALA:HB1   | 2:C:54:LYS:HE3    | 1.60                     | 0.81              |
| 5:P:21:ALA:HB1   | 1:AP:278:THR:CG2  | 2.10                     | 0.81              |
| 1:UI:127:SER:O   | 1:UI:131:ASN:N    | 2.13                     | 0.81              |
| 1:UJ:94:HIS:HB3  | 1:UJ:146:THR:HG21 | 1.60                     | 0.81              |
| 1:UL:127:SER:O   | 1:UL:131:ASN:N    | 2.13                     | 0.81              |
| 1:UM:94:HIS:HB3  | 1:UM:146:THR:HG21 | 1.60                     | 0.81              |
| 1:WI:200:SER:O   | 1:WJ:158:ALA:CB   | 2.29                     | 0.81              |
| 6:U:33:ALA:O     | 6:U:98:ASN:ND2    | 2.13                     | 0.81              |
| 1:UJ:128:GLU:O   | 1:UJ:132:TYR:N    | 2.13                     | 0.81              |
| 1:UK:94:HIS:HB3  | 1:UK:146:THR:HG21 | 1.60                     | 0.81              |
| 1:WS:124:SER:CB  | 2:A:8:MET:HE2     | 2.11                     | 0.81              |
| 1:UN:127:SER:O   | 1:UN:131:ASN:N    | 2.13                     | 0.81              |
| 1:UI:73:MET:HE1  | 1:UI:99:ARG:HD3   | 1.62                     | 0.81              |
| 1:UJ:127:SER:O   | 1:UJ:131:ASN:N    | 2.13                     | 0.80              |
| 1:UK:127:SER:O   | 1:UK:131:ASN:N    | 2.13                     | 0.80              |
| 1:UM:73:MET:HE1  | 1:UM:99:ARG:HD3   | 1.62                     | 0.80              |
| 1:UM:127:SER:O   | 1:UM:131:ASN:N    | 2.13                     | 0.80              |
| 1:WA:197:LEU:CD1 | 1:WB:175:SER:OG   | 2.28                     | 0.80              |
| 1:WK:143:THR:CB  | 1:WL:156:HIS:HE2  | 1.94                     | 0.80              |
| 6:U:72:HIS:HD2   | 1:1:365:ASN:CB    | 1.88                     | 0.80              |
| 1:WK:165:PHE:HA  | 3:E:149:LEU:HD13  | 1.62                     | 0.80              |
| 1:WP:200:SER:O   | 1:WQ:158:ALA:HB2  | 1.80                     | 0.80              |
| 1:UI:128:GLU:O   | 1:UI:132:TYR:N    | 2.13                     | 0.80              |
| 1:UP:73:MET:HE1  | 1:UP:99:ARG:HD3   | 1.62                     | 0.80              |
| 1:WT:121:PHE:CE1 | 1:WU:122:GLY:O    | 2.34                     | 0.80              |
| 1:WG:165:PHE:CE1 | 4:J:240:ALA:HB3   | 2.17                     | 0.80              |
| 1:WH:143:THR:OG1 | 1:WI:154:ARG:HG2  | 1.82                     | 0.80              |
| 5:M:11:ILE:HG22  | 1:AB:372:ILE:CB   | 2.11                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:14:LEU:HB3    | 1:AQ:278:THR:HG21 | 1.64                     | 0.80              |
| 1:WJ:164:LEU:CD2  | 3:E:144:LEU:CB    | 2.60                     | 0.80              |
| 5:M:7:ILE:HD11    | 1:AC:370:ARG:HE   | 1.46                     | 0.80              |
| 1:WU:200:SER:OG   | 1:WV:175:SER:HB2  | 1.82                     | 0.79              |
| 1:WV:197:LEU:HD12 | 1:WW:175:SER:CB   | 2.12                     | 0.79              |
| 7:Y:6:ILE:HG21    | 7:Y:122:VAL:HG21  | 1.62                     | 0.79              |
| 1:WG:197:LEU:HD12 | 1:WH:175:SER:OG   | 1.82                     | 0.79              |
| 1:WH:181:GLU:HB2  | 1:WH:184:ARG:CG   | 2.07                     | 0.79              |
| 1:UK:73:MET:HE1   | 1:UK:99:ARG:HD3   | 1.62                     | 0.79              |
| 1:UN:73:MET:HE1   | 1:UN:99:ARG:HD3   | 1.62                     | 0.79              |
| 1:WM:181:GLU:HB2  | 1:WM:184:ARG:CG   | 2.07                     | 0.79              |
| 4:J:83:ALA:HB3    | 4:J:84:PRO:HD3    | 1.62                     | 0.79              |
| 1:WB:164:LEU:O    | 4:H:152:ARG:HD3   | 1.81                     | 0.79              |
| 1:UO:73:MET:HE1   | 1:UO:99:ARG:HD3   | 1.62                     | 0.79              |
| 1:WJ:181:GLU:HB2  | 1:WJ:184:ARG:CG   | 2.07                     | 0.79              |
| 1:WF:200:SER:OG   | 1:WG:175:SER:HB2  | 1.81                     | 0.79              |
| 1:WG:143:THR:OG1  | 1:WH:154:ARG:HG2  | 1.83                     | 0.79              |
| 1:WO:181:GLU:HB2  | 1:WO:184:ARG:CG   | 2.07                     | 0.79              |
| 1:UM:128:GLU:O    | 1:UM:132:TYR:N    | 2.13                     | 0.79              |
| 1:WA:175:SER:OG   | 1:WW:197:LEU:HD12 | 1.83                     | 0.79              |
| 1:WJ:197:LEU:HD12 | 1:WK:175:SER:HB3  | 1.63                     | 0.79              |
| 1:WP:165:PHE:HB3  | 4:F:160:GLN:O     | 1.83                     | 0.79              |
| 1:WN:201:ALA:CA   | 1:WO:158:ALA:HB2  | 2.13                     | 0.79              |
| 1:WA:175:SER:HB3  | 1:WW:197:LEU:HD12 | 1.64                     | 0.79              |
| 1:UL:73:MET:HE1   | 1:UL:99:ARG:HD3   | 1.62                     | 0.78              |
| 1:UO:128:GLU:O    | 1:UO:132:TYR:N    | 2.14                     | 0.78              |
| 1:WI:181:GLU:HB2  | 1:WI:184:ARG:CG   | 2.07                     | 0.78              |
| 1:UI:98:LEU:HD22  | 1:UI:147:LEU:HD21 | 1.66                     | 0.78              |
| 1:UJ:98:LEU:HD22  | 1:UJ:147:LEU:HD21 | 1.66                     | 0.78              |
| 1:WE:167:ARG:CD   | 4:I:161:GLY:HA2   | 2.12                     | 0.78              |
| 1:WQ:113:PHE:HB3  | 1:WR:134:ARG:HE   | 1.48                     | 0.78              |
| 2:B:39:GLN:NE2    | 2:B:46:GLU:O      | 2.13                     | 0.78              |
| 6:S:35:THR:HG22   | 7:X:49:PHE:HB3    | 1.65                     | 0.78              |
| 1:WL:181:GLU:HB2  | 1:WL:184:ARG:CG   | 2.07                     | 0.78              |
| 1:UJ:103:GLN:HB3  | 1:WD:182:PRO:CA   | 2.13                     | 0.78              |
| 1:WK:162:PRO:HB2  | 3:E:249:ASN:HB2   | 1.64                     | 0.78              |
| 1:WP:197:LEU:HD12 | 1:WQ:175:SER:OG   | 1.84                     | 0.78              |
| 5:N:11:ILE:HG22   | 1:6:372:ILE:CD1   | 2.14                     | 0.78              |
| 1:UP:128:GLU:O    | 1:UP:132:TYR:N    | 2.13                     | 0.78              |
| 4:F:141:GLN:HE22  | 4:F:243:PHE:HB3   | 1.48                     | 0.78              |
| 6:R:67:LEU:HD11   | 6:R:74:PRO:HA     | 1.64                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UK:207:PRO:CD   | 1:WE:187:ASP:OD2  | 2.31                     | 0.78              |
| 1:WP:200:SER:O    | 1:WQ:158:ALA:CB   | 2.31                     | 0.78              |
| 1:WV:120:LYS:NZ   | 1:WV:123:ILE:HD11 | 1.99                     | 0.78              |
| 1:WS:200:SER:OG   | 1:WT:175:SER:HB2  | 1.83                     | 0.78              |
| 1:WU:197:LEU:CD1  | 1:WV:175:SER:OG   | 2.29                     | 0.78              |
| 1:WA:167:ARG:NH2  | 1:WA:168:GLU:OE2  | 2.17                     | 0.78              |
| 1:UO:98:LEU:HD22  | 1:UO:147:LEU:HD21 | 1.66                     | 0.77              |
| 6:S:72:HIS:HA     | 1:AE:295:SER:OG   | 1.83                     | 0.77              |
| 1:WJ:143:THR:OG1  | 1:WK:154:ARG:HG2  | 1.83                     | 0.77              |
| 1:UM:98:LEU:HD22  | 1:UM:147:LEU:HD21 | 1.66                     | 0.77              |
| 1:WF:187:ASP:HB3  | 1:WF:190:GLN:HG3  | 1.66                     | 0.77              |
| 1:WJ:128:GLU:CG   | 1:WK:126:PHE:CD2  | 2.67                     | 0.77              |
| 1:UK:98:LEU:HD22  | 1:UK:147:LEU:HD21 | 1.66                     | 0.77              |
| 1:UP:98:LEU:HD22  | 1:UP:147:LEU:HD21 | 1.66                     | 0.77              |
| 1:WF:128:GLU:HG2  | 1:WG:126:PHE:HD2  | 1.48                     | 0.77              |
| 1:WT:197:LEU:HD12 | 1:WU:175:SER:HB3  | 1.65                     | 0.77              |
| 1:WD:197:LEU:HD12 | 1:WE:175:SER:OG   | 1.85                     | 0.77              |
| 6:S:72:HIS:ND1    | 1:AD:365:ASN:CB   | 2.47                     | 0.77              |
| 1:f:319:GLN:HB3   | 1:AG:303:GLN:HE22 | 1.50                     | 0.77              |
| 1:UJ:167:ARG:HH11 | 1:2:236:LYS:NZ    | 1.83                     | 0.77              |
| 5:O:14:LEU:HD23   | 1:y:278:THR:HG22  | 1.66                     | 0.77              |
| 5:P:19:MET:CA     | 1:AP:276:GLU:OE2  | 2.32                     | 0.77              |
| 1:UJ:261:LEU:HB3  | 1:UJ:270:THR:HG23 | 1.67                     | 0.77              |
| 1:UL:98:LEU:HD22  | 1:UL:147:LEU:HD21 | 1.66                     | 0.77              |
| 1:UN:128:GLU:O    | 1:UN:132:TYR:N    | 2.13                     | 0.77              |
| 1:UN:167:ARG:HH22 | 1:WQ:188:GLU:HB3  | 1.47                     | 0.77              |
| 1:WK:165:PHE:HA   | 3:E:149:LEU:CD1   | 2.15                     | 0.77              |
| 1:WK:197:LEU:CD1  | 1:WL:175:SER:CB   | 2.59                     | 0.77              |
| 1:WO:203:ALA:HB1  | 1:WP:160:PRO:HB3  | 1.66                     | 0.77              |
| 4:J:62:THR:HG23   | 4:J:101:MET:HE2   | 1.66                     | 0.77              |
| 6:S:73:ILE:HD11   | 1:AE:297:GLN:HB2  | 1.63                     | 0.77              |
| 1:WJ:125:GLN:HG3  | 3:E:242:HIS:ND1   | 1.99                     | 0.76              |
| 1:WM:197:LEU:HD12 | 1:WN:175:SER:HB3  | 1.67                     | 0.76              |
| 5:N:21:ALA:HB1    | 1:4:278:THR:HG21  | 1.65                     | 0.76              |
| 1:UP:212:LEU:HB3  | 1:UP:221:THR:HG23 | 1.67                     | 0.76              |
| 1:WK:181:GLU:HB2  | 1:WK:184:ARG:CG   | 2.07                     | 0.76              |
| 1:WQ:181:GLU:HB2  | 1:WQ:184:ARG:CG   | 2.07                     | 0.76              |
| 5:M:11:ILE:C      | 5:M:11:ILE:CD1    | 2.57                     | 0.76              |
| 1:WD:193:ALA:HB1  | 1:WE:213:VAL:HG11 | 1.67                     | 0.76              |
| 1:WN:200:SER:HA   | 1:WO:173:SER:OG   | 1.85                     | 0.76              |
| 1:WT:200:SER:O    | 1:WU:158:ALA:HB3  | 1.84                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UL:167:ARG:NH1  | 1:WF:188:GLU:OE2  | 2.19                     | 0.76              |
| 1:WQ:197:LEU:CD1  | 1:WR:175:SER:OG   | 2.26                     | 0.76              |
| 1:WW:125:GLN:HB2  | 2:B:2:THR:HG21    | 1.66                     | 0.76              |
| 5:M:21:ALA:CB     | 1:O:278:THR:HG21  | 2.15                     | 0.76              |
| 1:WP:196:HIS:HB3  | 1:WQ:211:THR:HG21 | 1.66                     | 0.76              |
| 6:U:73:ILE:HG13   | 1:2:295:SER:HB2   | 1.67                     | 0.76              |
| 6:R:73:ILE:HG13   | 1:AK:295:SER:CB   | 2.14                     | 0.76              |
| 1:UM:212:LEU:HB3  | 1:UM:221:THR:HG23 | 1.67                     | 0.76              |
| 1:UN:98:LEU:HD22  | 1:UN:147:LEU:HD21 | 1.66                     | 0.76              |
| 1:WA:211:THR:HG21 | 1:WW:196:HIS:HB3  | 1.67                     | 0.76              |
| 1:WN:197:LEU:HD12 | 1:WO:175:SER:HB3  | 1.68                     | 0.76              |
| 1:WW:181:GLU:HB2  | 1:WW:184:ARG:CG   | 2.07                     | 0.76              |
| 1:UI:212:LEU:HB3  | 1:UI:221:THR:HG23 | 1.67                     | 0.76              |
| 1:WA:181:GLU:HB2  | 1:WA:184:ARG:CG   | 2.07                     | 0.76              |
| 1:WP:181:GLU:HB2  | 1:WP:184:ARG:CG   | 2.07                     | 0.76              |
| 1:UN:212:LEU:HB3  | 1:UN:221:THR:HG23 | 1.67                     | 0.76              |
| 1:WB:163:SER:HB2  | 1:WB:166:VAL:HG22 | 1.67                     | 0.76              |
| 1:WT:160:PRO:HD3  | 1:WT:172:PRO:HA   | 1.66                     | 0.76              |
| 2:D:55:ILE:HD11   | 4:I:205:MET:HE1   | 1.67                     | 0.76              |
| 1:UL:212:LEU:HB3  | 1:UL:221:THR:HG23 | 1.67                     | 0.75              |
| 1:UO:212:LEU:HB3  | 1:UO:221:THR:HG23 | 1.67                     | 0.75              |
| 1:WJ:164:LEU:C    | 4:J:152:ARG:HH22  | 1.95                     | 0.75              |
| 1:WA:199:SER:HA   | 1:WA:205:LEU:HD23 | 1.69                     | 0.75              |
| 1:WC:199:SER:HA   | 1:WC:205:LEU:HD23 | 1.69                     | 0.75              |
| 1:WD:112:GLY:HA2  | 1:WD:135:ALA:HA   | 1.67                     | 0.75              |
| 1:WD:199:SER:HA   | 1:WD:205:LEU:HD23 | 1.69                     | 0.75              |
| 5:N:7:ILE:CG2     | 1:6:278:THR:HG21  | 2.17                     | 0.75              |
| 5:P:4:ILE:CD1     | 1:u:374:HIS:HB2   | 2.16                     | 0.75              |
| 1:UK:73:MET:HE1   | 1:UK:99:ARG:CD    | 2.17                     | 0.75              |
| 1:WF:196:HIS:HB3  | 1:WG:211:THR:HG21 | 1.67                     | 0.75              |
| 1:WN:199:SER:HA   | 1:WN:205:LEU:HD23 | 1.69                     | 0.75              |
| 1:WE:199:SER:HA   | 1:WE:205:LEU:HD23 | 1.68                     | 0.75              |
| 1:WP:199:SER:HA   | 1:WP:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:U:68:THR:CG2    | 1:1:294:ARG:CD    | 2.65                     | 0.75              |
| 1:WF:199:SER:HA   | 1:WF:205:LEU:HD23 | 1.69                     | 0.75              |
| 1:UL:73:MET:HE1   | 1:UL:99:ARG:CD    | 2.17                     | 0.75              |
| 1:WC:200:SER:OG   | 1:WD:175:SER:HB2  | 1.86                     | 0.75              |
| 1:WI:199:SER:HA   | 1:WI:205:LEU:HD23 | 1.69                     | 0.75              |
| 1:WO:166:VAL:HG11 | 4:F:147:LEU:HD12  | 1.66                     | 0.75              |
| 1:WW:199:SER:HA   | 1:WW:205:LEU:HD23 | 1.69                     | 0.75              |
| 1:WO:199:SER:HA   | 1:WO:205:LEU:HD23 | 1.69                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WR:181:GLU:HB2  | 1:WR:184:ARG:CG   | 2.07                     | 0.75              |
| 1:UM:139:GLU:OE1  | 1:UM:142:ARG:NH2  | 2.20                     | 0.75              |
| 1:WB:199:SER:HA   | 1:WB:205:LEU:HD23 | 1.68                     | 0.75              |
| 1:WJ:128:GLU:HG2  | 1:WK:126:PHE:CD2  | 2.15                     | 0.75              |
| 1:WW:125:GLN:OE1  | 2:B:2:THR:HG22    | 1.86                     | 0.75              |
| 5:M:4:ILE:HD12    | 1:AC:374:HIS:HB2  | 1.68                     | 0.75              |
| 5:N:7:ILE:HG21    | 1:6:278:THR:CG2   | 2.15                     | 0.75              |
| 1:UK:212:LEU:HB3  | 1:UK:221:THR:HG23 | 1.67                     | 0.74              |
| 1:WG:199:SER:HA   | 1:WG:205:LEU:HD23 | 1.69                     | 0.74              |
| 6:T:55:ARG:CZ     | 1:5:299:ASN:HD21  | 1.97                     | 0.74              |
| 1:e:312:VAL:O     | 1:e:317:SER:OG    | 2.05                     | 0.74              |
| 1:WI:200:SER:O    | 1:WJ:158:ALA:HB3  | 1.87                     | 0.74              |
| 1:WR:200:SER:O    | 1:WS:158:ALA:HB2  | 1.87                     | 0.74              |
| 1:UK:94:HIS:CB    | 1:UK:146:THR:HG21 | 2.17                     | 0.74              |
| 1:WC:193:ALA:HB1  | 1:WD:213:VAL:HG11 | 1.68                     | 0.74              |
| 1:UI:73:MET:HE1   | 1:UI:99:ARG:CD    | 2.17                     | 0.74              |
| 1:UJ:73:MET:HE1   | 1:UJ:99:ARG:CD    | 2.17                     | 0.74              |
| 1:WD:149:PRO:HG2  | 1:WD:190:GLN:HE22 | 1.52                     | 0.74              |
| 1:WJ:164:LEU:HB2  | 3:E:145:TRP:CD1   | 2.22                     | 0.74              |
| 4:G:135:ARG:NH2   | 4:G:165:VAL:O     | 2.21                     | 0.74              |
| 7:X:6:ILE:HG21    | 7:X:122:VAL:HG21  | 1.69                     | 0.74              |
| 1:UO:94:HIS:CB    | 1:UO:146:THR:HG21 | 2.17                     | 0.74              |
| 1:WT:199:SER:HA   | 1:WT:205:LEU:HD23 | 1.69                     | 0.74              |
| 1:WV:197:LEU:HD12 | 1:WW:175:SER:OG   | 1.88                     | 0.74              |
| 1:WN:197:LEU:HD12 | 1:WO:175:SER:CB   | 2.17                     | 0.74              |
| 1:WO:164:LEU:O    | 4:F:144:GLU:N     | 2.21                     | 0.74              |
| 5:K:21:ALA:HB1    | 1:AK:278:THR:CG2  | 2.17                     | 0.74              |
| 1:UL:94:HIS:CB    | 1:UL:146:THR:HG21 | 2.17                     | 0.74              |
| 1:WQ:199:SER:HA   | 1:WQ:205:LEU:HD23 | 1.69                     | 0.74              |
| 1:WR:199:SER:HA   | 1:WR:205:LEU:HD23 | 1.69                     | 0.74              |
| 1:WS:199:SER:HA   | 1:WS:205:LEU:HD23 | 1.69                     | 0.74              |
| 1:WV:199:SER:HA   | 1:WV:205:LEU:HD23 | 1.69                     | 0.74              |
| 3:E:23:VAL:HA     | 3:E:150:LEU:HD21  | 1.69                     | 0.74              |
| 5:M:4:ILE:HG12    | 1:AC:372:ILE:HB   | 1.68                     | 0.74              |
| 1:WJ:199:SER:HA   | 1:WJ:205:LEU:HD23 | 1.69                     | 0.74              |
| 1:WN:181:GLU:HB2  | 1:WN:184:ARG:CG   | 2.07                     | 0.74              |
| 1:UP:73:MET:HE1   | 1:UP:99:ARG:CD    | 2.17                     | 0.74              |
| 1:WB:163:SER:HB3  | 1:WB:169:GLN:HG2  | 1.70                     | 0.74              |
| 1:WK:199:SER:HA   | 1:WK:205:LEU:HD23 | 1.69                     | 0.74              |
| 5:K:75:MET:HE1    | 5:P:88:VAL:HG22   | 1.69                     | 0.74              |
| 5:O:14:LEU:HD11   | 1:z:370:ARG:NH2   | 2.02                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UN:94:HIS:CB    | 1:UN:146:THR:HG21 | 2.17                     | 0.74              |
| 1:UO:139:GLU:OE1  | 1:UO:142:ARG:NH2  | 2.20                     | 0.74              |
| 1:WH:199:SER:HA   | 1:WH:205:LEU:HD23 | 1.69                     | 0.74              |
| 1:WP:164:LEU:HD13 | 4:F:148:ALA:HA    | 1.69                     | 0.74              |
| 5:O:7:ILE:HB      | 1:z:278:THR:HG21  | 1.69                     | 0.74              |
| 1:UJ:94:HIS:CB    | 1:UJ:146:THR:HG21 | 2.17                     | 0.73              |
| 1:UL:139:GLU:OE1  | 1:UL:142:ARG:NH2  | 2.20                     | 0.73              |
| 1:WC:197:LEU:HD12 | 1:WD:175:SER:OG   | 1.88                     | 0.73              |
| 1:WK:143:THR:HG1  | 1:WL:156:HIS:CE1  | 2.04                     | 0.73              |
| 6:U:65:LEU:HB2    | 1:1:295:SER:HB2   | 1.69                     | 0.73              |
| 1:UK:103:GLN:NE2  | 1:WF:182:PRO:HB3  | 2.01                     | 0.73              |
| 1:UM:94:HIS:CB    | 1:UM:146:THR:HG21 | 2.17                     | 0.73              |
| 1:WE:166:VAL:HG21 | 4:I:160:GLN:HG2   | 1.69                     | 0.73              |
| 5:K:89:ARG:NH1    | 5:P:102:MET:SD    | 2.61                     | 0.73              |
| 5:N:94:ALA:O      | 5:N:98:GLU:HG3    | 1.88                     | 0.73              |
| 1:UL:73:MET:CE    | 1:UL:99:ARG:CD    | 2.66                     | 0.73              |
| 1:UN:73:MET:CE    | 1:UN:99:ARG:CD    | 2.66                     | 0.73              |
| 1:UO:73:MET:HE1   | 1:UO:99:ARG:CD    | 2.17                     | 0.73              |
| 1:WB:197:LEU:HD12 | 1:WC:175:SER:CB   | 2.18                     | 0.73              |
| 1:UI:94:HIS:CB    | 1:UI:146:THR:HG21 | 2.17                     | 0.73              |
| 1:WB:181:GLU:HB2  | 1:WB:184:ARG:CG   | 2.07                     | 0.73              |
| 1:WW:167:ARG:HD2  | 4:H:140:ARG:O     | 1.87                     | 0.73              |
| 7:X:79:GLU:HG2    | 7:X:82:ASN:HB2    | 1.69                     | 0.73              |
| 7:Z:6:ILE:HD13    | 7:Z:122:VAL:HG21  | 1.71                     | 0.73              |
| 1:UK:73:MET:CE    | 1:UK:99:ARG:CD    | 2.66                     | 0.73              |
| 1:UM:73:MET:HE1   | 1:UM:99:ARG:CD    | 2.17                     | 0.73              |
| 1:WA:158:ALA:HB3  | 1:WW:200:SER:O    | 1.87                     | 0.73              |
| 1:WJ:164:LEU:HD21 | 3:E:144:LEU:CB    | 2.17                     | 0.73              |
| 1:WR:200:SER:OG   | 1:WS:175:SER:HB2  | 1.88                     | 0.73              |
| 1:WU:199:SER:HA   | 1:WU:205:LEU:HD23 | 1.69                     | 0.73              |
| 7:V:55:PRO:HG3    | 1:AP:359:GLN:NE2  | 2.04                     | 0.73              |
| 1:UN:139:GLU:OE1  | 1:UN:142:ARG:NH2  | 2.20                     | 0.73              |
| 1:WD:164:LEU:O    | 4:I:144:GLU:HG2   | 1.88                     | 0.73              |
| 1:WP:123:ILE:HG23 | 2:A:67:PRO:HB3    | 1.70                     | 0.73              |
| 2:C:29:LEU:HB2    | 2:D:52:ILE:HG13   | 1.71                     | 0.73              |
| 6:S:73:ILE:CD1    | 1:AE:297:GLN:CB   | 2.56                     | 0.73              |
| 1:UN:73:MET:HE1   | 1:UN:99:ARG:CD    | 2.17                     | 0.73              |
| 1:UP:94:HIS:CB    | 1:UP:146:THR:HG21 | 2.17                     | 0.73              |
| 1:WT:200:SER:OG   | 1:WU:175:SER:HB2  | 1.88                     | 0.73              |
| 1:UK:139:GLU:OE1  | 1:UK:142:ARG:NH2  | 2.20                     | 0.73              |
| 1:UP:73:MET:CE    | 1:UP:99:ARG:CD    | 2.66                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WK:193:ALA:CB   | 1:WL:213:VAL:HG21 | 2.13                     | 0.73              |
| 5:K:21:ALA:CB     | 1:AK:278:THR:CG2  | 2.64                     | 0.73              |
| 6:S:42:ASP:OD2    | 6:S:43:ILE:N      | 2.22                     | 0.73              |
| 7:X:3:LEU:HB2     | 7:X:126:MET:HE3   | 1.70                     | 0.73              |
| 1:UP:139:GLU:OE1  | 1:UP:142:ARG:NH2  | 2.20                     | 0.73              |
| 1:WM:200:SER:O    | 1:WN:158:ALA:CB   | 2.37                     | 0.73              |
| 1:UI:139:GLU:OE1  | 1:UI:142:ARG:NH2  | 2.20                     | 0.72              |
| 1:WK:132:TYR:HB2  | 1:WL:126:PHE:CZ   | 2.23                     | 0.72              |
| 1:UM:73:MET:CE    | 1:UM:99:ARG:CD    | 2.66                     | 0.72              |
| 1:UI:73:MET:CE    | 1:UI:99:ARG:CD    | 2.66                     | 0.72              |
| 1:WL:199:SER:HA   | 1:WL:205:LEU:HD23 | 1.69                     | 0.72              |
| 1:WM:199:SER:HA   | 1:WM:205:LEU:HD23 | 1.69                     | 0.72              |
| 1:WS:181:GLU:HB2  | 1:WS:184:ARG:CG   | 2.07                     | 0.72              |
| 1:WC:197:LEU:HD12 | 1:WD:175:SER:CB   | 2.18                     | 0.72              |
| 1:WU:181:GLU:HB2  | 1:WU:184:ARG:CG   | 2.07                     | 0.72              |
| 5:L:11:ILE:CG2    | 1:AH:372:ILE:HD13 | 2.16                     | 0.72              |
| 1:WM:197:LEU:HA   | 1:WN:175:SER:OG   | 1.89                     | 0.72              |
| 5:M:4:ILE:HG13    | 1:AC:372:ILE:CG2  | 2.20                     | 0.72              |
| 1:WG:181:GLU:HB2  | 1:WG:184:ARG:CG   | 2.07                     | 0.72              |
| 5:L:11:ILE:CG2    | 1:AH:372:ILE:CB   | 2.67                     | 0.72              |
| 1:UO:73:MET:CE    | 1:UO:99:ARG:CD    | 2.66                     | 0.72              |
| 5:L:11:ILE:HG21   | 1:AH:372:ILE:CB   | 2.18                     | 0.72              |
| 6:R:46:ALA:O      | 6:R:50:LYS:HG3    | 1.90                     | 0.72              |
| 1:UJ:73:MET:CE    | 1:UJ:99:ARG:CD    | 2.66                     | 0.72              |
| 1:WD:197:LEU:HA   | 1:WE:175:SER:OG   | 1.89                     | 0.72              |
| 1:WV:181:GLU:HB2  | 1:WV:184:ARG:CG   | 2.07                     | 0.72              |
| 5:K:7:ILE:CG2     | 1:AM:278:THR:CG2  | 2.53                     | 0.72              |
| 7:W:6:ILE:HG21    | 7:W:122:VAL:HG21  | 1.72                     | 0.72              |
| 1:UJ:98:LEU:CD1   | 1:UJ:146:THR:OG1  | 2.38                     | 0.71              |
| 1:WE:181:GLU:HB2  | 1:WE:184:ARG:CG   | 2.07                     | 0.71              |
| 1:UL:98:LEU:CD1   | 1:UL:146:THR:OG1  | 2.39                     | 0.71              |
| 1:UJ:139:GLU:OE1  | 1:UJ:142:ARG:NH2  | 2.20                     | 0.71              |
| 1:WJ:164:LEU:HD21 | 3:E:144:LEU:HB3   | 1.72                     | 0.71              |
| 5:P:76:GLN:HE21   | 7:V:123:LYS:HB2   | 1.54                     | 0.71              |
| 1:UM:98:LEU:CD1   | 1:UM:146:THR:OG1  | 2.39                     | 0.71              |
| 1:WC:165:PHE:CD2  | 4:H:152:ARG:NH2   | 2.52                     | 0.71              |
| 6:U:72:HIS:CE1    | 1:2:294:ARG:HG3   | 2.25                     | 0.71              |
| 1:UI:62:ASP:OD2   | 1:WA:184:ARG:NH2  | 2.24                     | 0.71              |
| 1:UI:98:LEU:CD1   | 1:UI:146:THR:OG1  | 2.38                     | 0.71              |
| 1:UN:126:PHE:CD1  | 1:UN:130:VAL:HG21 | 2.26                     | 0.71              |
| 1:WC:165:PHE:HD2  | 4:H:152:ARG:NH2   | 1.88                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UP:126:PHE:CD1  | 1:UP:130:VAL:HG21 | 2.26                     | 0.71              |
| 1:WT:181:GLU:HB2  | 1:WT:184:ARG:CG   | 2.07                     | 0.71              |
| 1:WV:197:LEU:HD12 | 1:WW:175:SER:HB3  | 1.71                     | 0.71              |
| 4:J:139:LEU:O     | 4:J:142:THR:HG22  | 1.89                     | 0.71              |
| 5:K:21:ALA:HB3    | 1:AK:278:THR:HG21 | 1.71                     | 0.71              |
| 5:M:4:ILE:CD1     | 1:AC:374:HIS:HB2  | 2.20                     | 0.71              |
| 1:WH:193:ALA:HB1  | 1:WI:213:VAL:CG1  | 2.18                     | 0.71              |
| 2:D:48:THR:OG1    | 4:I:206:ALA:O     | 2.08                     | 0.71              |
| 1:UK:126:PHE:CD1  | 1:UK:130:VAL:HG21 | 2.26                     | 0.71              |
| 1:WD:181:GLU:HB2  | 1:WD:184:ARG:CG   | 2.07                     | 0.71              |
| 5:P:11:ILE:CG2    | 1:t:372:ILE:HG21  | 2.21                     | 0.71              |
| 6:R:72:HIS:ND1    | 1:AJ:365:ASN:CB   | 2.40                     | 0.71              |
| 1:UN:98:LEU:CD1   | 1:UN:146:THR:OG1  | 2.39                     | 0.71              |
| 1:WF:181:GLU:HB2  | 1:WF:184:ARG:CG   | 2.07                     | 0.71              |
| 1:WK:200:SER:HA   | 1:WL:173:SER:OG   | 1.91                     | 0.71              |
| 2:B:39:GLN:HE21   | 2:B:49:LEU:HD12   | 1.56                     | 0.71              |
| 6:T:78:VAL:HG12   | 1:6:361:ASN:ND2   | 2.06                     | 0.71              |
| 1:WR:200:SER:O    | 1:WS:158:ALA:HB3  | 1.90                     | 0.71              |
| 6:U:68:THR:HG22   | 1:1:294:ARG:HD3   | 1.73                     | 0.71              |
| 1:UK:98:LEU:CD1   | 1:UK:146:THR:OG1  | 2.38                     | 0.70              |
| 1:UL:103:GLN:HG2  | 1:WH:182:PRO:HB3  | 1.72                     | 0.70              |
| 1:UM:126:PHE:CD1  | 1:UM:130:VAL:HG21 | 2.26                     | 0.70              |
| 1:UP:98:LEU:CD1   | 1:UP:146:THR:OG1  | 2.38                     | 0.70              |
| 3:E:187:ALA:O     | 3:E:188:LEU:C     | 2.34                     | 0.70              |
| 1:UK:126:PHE:O    | 1:UK:130:VAL:CG2  | 2.40                     | 0.70              |
| 1:WD:190:GLN:HG3  | 1:WE:217:GLY:HA3  | 1.72                     | 0.70              |
| 1:WE:128:GLU:HB3  | 1:WF:126:PHE:CE2  | 2.25                     | 0.70              |
| 2:D:84:LEU:HD21   | 4:J:185:ILE:HG23  | 1.72                     | 0.70              |
| 6:U:68:THR:HG21   | 1:1:294:ARG:HD2   | 1.71                     | 0.70              |
| 1:UO:126:PHE:CD1  | 1:UO:130:VAL:HG21 | 2.26                     | 0.70              |
| 1:WE:197:LEU:HD12 | 1:WF:175:SER:CB   | 2.21                     | 0.70              |
| 1:WM:139:GLU:HB3  | 1:WN:154:ARG:NH2  | 2.06                     | 0.70              |
| 1:UI:126:PHE:O    | 1:UI:130:VAL:CG2  | 2.40                     | 0.70              |
| 1:UJ:126:PHE:O    | 1:UJ:130:VAL:CG2  | 2.40                     | 0.70              |
| 1:WA:200:SER:O    | 1:WB:158:ALA:CB   | 2.40                     | 0.70              |
| 1:WB:200:SER:O    | 1:WC:158:ALA:HB2  | 1.91                     | 0.70              |
| 1:WD:165:PHE:CE2  | 4:I:141:GLN:HA    | 2.26                     | 0.70              |
| 1:WF:167:ARG:C    | 4:I:152:ARG:NH1   | 2.49                     | 0.70              |
| 1:WP:193:ALA:HB1  | 1:WQ:213:VAL:HG11 | 1.74                     | 0.70              |
| 6:R:71:HIS:HB2    | 1:AK:294:ARG:HG2  | 1.74                     | 0.70              |
| 1:UN:126:PHE:O    | 1:UN:130:VAL:CG2  | 2.40                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UO:98:LEU:CD1   | 1:UO:146:THR:OG1  | 2.38                     | 0.70              |
| 2:D:13:ALA:HB1    | 4:J:195:ILE:HD11  | 1.73                     | 0.70              |
| 1:UI:167:ARG:HH22 | 1:WW:188:GLU:HB3  | 1.57                     | 0.70              |
| 1:UM:139:GLU:CD   | 1:UM:142:ARG:HH21 | 2.00                     | 0.70              |
| 1:WD:165:PHE:CB   | 4:I:143:ARG:HA    | 2.22                     | 0.70              |
| 1:WW:167:ARG:CD   | 4:H:140:ARG:O     | 2.40                     | 0.70              |
| 1:WR:112:GLY:HA2  | 1:WR:135:ALA:CA   | 2.16                     | 0.70              |
| 3:E:182:ASN:HB3   | 3:E:239:PHE:CZ    | 2.26                     | 0.70              |
| 5:K:14:LEU:HB3    | 1:AL:278:THR:HG21 | 1.72                     | 0.70              |
| 1:WS:121:PHE:CE1  | 1:WT:120:LYS:NZ   | 2.55                     | 0.69              |
| 1:UL:62:ASP:OD2   | 1:WG:184:ARG:NH2  | 2.25                     | 0.69              |
| 1:UL:126:PHE:CD1  | 1:UL:130:VAL:HG21 | 2.26                     | 0.69              |
| 1:WM:193:ALA:HB1  | 1:WN:213:VAL:CG1  | 2.22                     | 0.69              |
| 6:T:91:ASP:OD2    | 6:T:104:ARG:NH1   | 2.25                     | 0.69              |
| 1:UJ:126:PHE:CD1  | 1:UJ:130:VAL:HG21 | 2.26                     | 0.69              |
| 1:WJ:164:LEU:CB   | 3:E:145:TRP:HE1   | 1.99                     | 0.69              |
| 1:j:318:ASN:HD21  | 1:4:357:SER:CB    | 2.02                     | 0.69              |
| 1:UI:126:PHE:CD1  | 1:UI:130:VAL:HG21 | 2.26                     | 0.69              |
| 1:UL:126:PHE:O    | 1:UL:130:VAL:CG2  | 2.40                     | 0.69              |
| 6:S:72:HIS:HB3    | 1:AE:295:SER:HB3  | 1.72                     | 0.69              |
| 1:UL:126:PHE:O    | 1:UL:130:VAL:CB   | 2.41                     | 0.69              |
| 1:WA:175:SER:OG   | 1:WW:197:LEU:HA   | 1.93                     | 0.69              |
| 1:WE:166:VAL:HG21 | 4:I:160:GLN:CG    | 2.23                     | 0.69              |
| 1:UI:126:PHE:O    | 1:UI:130:VAL:CB   | 2.41                     | 0.69              |
| 1:UN:126:PHE:O    | 1:UN:130:VAL:CB   | 2.41                     | 0.69              |
| 1:UO:126:PHE:O    | 1:UO:130:VAL:CG2  | 2.40                     | 0.69              |
| 3:E:188:LEU:HB3   | 3:E:189:PRO:CD    | 2.22                     | 0.69              |
| 4:J:143:ARG:HB3   | 4:J:146:ASP:OD2   | 1.92                     | 0.69              |
| 1:UJ:126:PHE:O    | 1:UJ:130:VAL:CB   | 2.41                     | 0.69              |
| 1:UO:139:GLU:CD   | 1:UO:142:ARG:HH21 | 2.00                     | 0.69              |
| 1:UP:139:GLU:CD   | 1:UP:142:ARG:HH21 | 2.00                     | 0.69              |
| 1:WF:167:ARG:C    | 4:I:152:ARG:HH12  | 2.00                     | 0.69              |
| 1:WL:197:LEU:HD13 | 1:WM:175:SER:OG   | 1.91                     | 0.69              |
| 5:M:77:LYS:NZ     | 6:S:13:GLN:OE1    | 2.26                     | 0.69              |
| 1:UJ:139:GLU:CD   | 1:UJ:142:ARG:HH21 | 2.00                     | 0.69              |
| 1:UM:126:PHE:O    | 1:UM:130:VAL:CB   | 2.41                     | 0.69              |
| 1:UN:139:GLU:CD   | 1:UN:142:ARG:HH21 | 2.00                     | 0.69              |
| 1:WK:164:LEU:HD12 | 3:E:248:PHE:HB2   | 1.74                     | 0.69              |
| 1:WN:200:SER:CA   | 1:WO:173:SER:OG   | 2.41                     | 0.69              |
| 2:C:13:ALA:HB1    | 4:I:195:ILE:HD11  | 1.75                     | 0.69              |
| 5:M:11:ILE:HG22   | 1:AB:372:ILE:HB   | 1.74                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:R:36:PRO:HG2    | 1:e:311:GLY:H     | 1.56                     | 0.69              |
| 1:UI:139:GLU:CD   | 1:UI:142:ARG:HH21 | 2.00                     | 0.69              |
| 1:WA:167:ARG:HH21 | 4:H:162:PRO:CD    | 2.06                     | 0.69              |
| 4:H:153:LEU:HD22  | 4:I:99:PHE:HB3    | 1.75                     | 0.69              |
| 6:U:76:GLN:N      | 1:1:297:GLN:HE22  | 1.91                     | 0.69              |
| 1:WA:128:GLU:HG3  | 1:WB:126:PHE:HE2  | 1.54                     | 0.69              |
| 1:WA:213:VAL:HG11 | 1:WW:193:ALA:HB1  | 1.73                     | 0.69              |
| 1:WG:165:PHE:CZ   | 4:I:153:LEU:CD2   | 2.75                     | 0.69              |
| 1:WK:197:LEU:HA   | 1:WL:175:SER:HB2  | 1.74                     | 0.69              |
| 1:WP:190:GLN:HG2  | 1:WQ:217:GLY:HA3  | 1.75                     | 0.69              |
| 5:M:4:ILE:CG1     | 1:AC:372:ILE:CG2  | 2.70                     | 0.69              |
| 1:UM:126:PHE:O    | 1:UM:130:VAL:CG2  | 2.40                     | 0.68              |
| 1:UO:126:PHE:O    | 1:UO:130:VAL:CB   | 2.41                     | 0.68              |
| 1:UP:126:PHE:O    | 1:UP:130:VAL:CG2  | 2.40                     | 0.68              |
| 1:WD:196:HIS:HB3  | 1:WE:211:THR:HG21 | 1.75                     | 0.68              |
| 5:P:7:ILE:HG22    | 1:t:278:THR:HG21  | 1.73                     | 0.68              |
| 6:R:68:THR:CG2    | 1:AJ:294:ARG:HD3  | 2.23                     | 0.68              |
| 1:UJ:167:ARG:HH11 | 1:2:236:LYS:HZ3   | 1.40                     | 0.68              |
| 1:UL:139:GLU:CD   | 1:UL:142:ARG:HH21 | 2.00                     | 0.68              |
| 1:UP:126:PHE:O    | 1:UP:130:VAL:CB   | 2.41                     | 0.68              |
| 1:WC:197:LEU:HD12 | 1:WD:175:SER:HB3  | 1.76                     | 0.68              |
| 1:WA:167:ARG:HH21 | 4:H:162:PRO:HD3   | 1.58                     | 0.68              |
| 4:F:109:TYR:HA    | 4:F:113:TYR:HB2   | 1.74                     | 0.68              |
| 1:UK:139:GLU:CD   | 1:UK:142:ARG:HH21 | 2.00                     | 0.68              |
| 1:WB:193:ALA:HB1  | 1:WC:213:VAL:HG11 | 1.76                     | 0.68              |
| 1:WD:197:LEU:HD12 | 1:WE:175:SER:CB   | 2.23                     | 0.68              |
| 1:UK:126:PHE:O    | 1:UK:130:VAL:CB   | 2.41                     | 0.68              |
| 1:WS:197:LEU:HD12 | 1:WT:175:SER:OG   | 1.94                     | 0.68              |
| 1:WS:197:LEU:HD12 | 1:WT:175:SER:CB   | 2.24                     | 0.68              |
| 1:UJ:125:GLN:HA   | 1:UJ:128:GLU:HB2  | 1.76                     | 0.68              |
| 1:UL:98:LEU:HD12  | 1:UL:146:THR:OG1  | 1.94                     | 0.68              |
| 1:WD:193:ALA:HB1  | 1:WE:213:VAL:CG1  | 2.23                     | 0.68              |
| 1:WJ:125:GLN:CB   | 3:E:242:HIS:HB2   | 2.23                     | 0.68              |
| 1:j:318:ASN:ND2   | 1:4:357:SER:CB    | 2.57                     | 0.68              |
| 1:WA:128:GLU:CG   | 1:WB:126:PHE:CE2  | 2.64                     | 0.67              |
| 1:WD:165:PHE:CB   | 4:I:142:THR:O     | 2.29                     | 0.67              |
| 1:WN:200:SER:O    | 1:WO:173:SER:OG   | 2.12                     | 0.67              |
| 1:WW:164:LEU:CD1  | 2:B:89:GLY:O      | 2.40                     | 0.67              |
| 2:B:58:VAL:HG21   | 4:H:207:LEU:HD11  | 1.75                     | 0.67              |
| 1:UM:125:GLN:HA   | 1:UM:128:GLU:HB2  | 1.76                     | 0.67              |
| 1:WE:134:ARG:HB3  | 1:WE:134:ARG:HH21 | 1.57                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UM:98:LEU:HD12  | 1:UM:146:THR:OG1  | 1.94                     | 0.67              |
| 1:UP:98:LEU:HD12  | 1:UP:146:THR:OG1  | 1.94                     | 0.67              |
| 4:F:59:LEU:HD21   | 5:K:102:MET:HE1   | 1.75                     | 0.67              |
| 5:L:4:ILE:CG1     | 1:AI:372:ILE:HG22 | 2.25                     | 0.67              |
| 1:WP:197:LEU:HD12 | 1:WQ:175:SER:CB   | 2.25                     | 0.67              |
| 1:UL:125:GLN:HA   | 1:UL:128:GLU:HB2  | 1.76                     | 0.67              |
| 1:UO:125:GLN:HA   | 1:UO:128:GLU:HB2  | 1.76                     | 0.67              |
| 1:WE:166:VAL:CG2  | 4:I:160:GLN:HG2   | 2.25                     | 0.67              |
| 1:WQ:197:LEU:HD12 | 1:WR:175:SER:CB   | 2.23                     | 0.67              |
| 1:UN:98:LEU:HD12  | 1:UN:146:THR:OG1  | 1.94                     | 0.67              |
| 1:UN:103:GLN:HG2  | 1:WS:182:PRO:HB3  | 1.75                     | 0.67              |
| 1:WG:200:SER:O    | 1:WH:158:ALA:CB   | 2.42                     | 0.67              |
| 2:B:14:MET:HG3    | 2:C:59:PHE:HE1    | 1.58                     | 0.67              |
| 1:UJ:98:LEU:HD12  | 1:UJ:146:THR:OG1  | 1.94                     | 0.67              |
| 1:WE:112:GLY:HA3  | 1:WE:139:GLU:OE1  | 1.95                     | 0.67              |
| 1:WF:197:LEU:HD12 | 1:WG:175:SER:HB3  | 1.74                     | 0.67              |
| 5:O:7:ILE:HD11    | 1:1:370:ARG:HE    | 1.58                     | 0.67              |
| 1:WA:197:LEU:HD12 | 1:WB:175:SER:HB3  | 1.75                     | 0.67              |
| 1:WD:115:LEU:CD2  | 1:WD:134:ARG:HD2  | 2.24                     | 0.67              |
| 1:WH:164:LEU:O    | 4:J:143:ARG:HG3   | 1.95                     | 0.67              |
| 1:UI:125:GLN:HA   | 1:UI:128:GLU:HB2  | 1.76                     | 0.67              |
| 1:UK:98:LEU:HD12  | 1:UK:146:THR:OG1  | 1.94                     | 0.67              |
| 1:WA:200:SER:O    | 1:WB:158:ALA:HB3  | 1.95                     | 0.67              |
| 1:WO:167:ARG:O    | 1:WO:168:GLU:HB2  | 1.93                     | 0.67              |
| 1:WR:113:PHE:HA   | 1:WS:134:ARG:HH12 | 1.58                     | 0.67              |
| 3:E:166:SER:O     | 3:E:168:ALA:N     | 2.26                     | 0.67              |
| 5:P:21:ALA:HB3    | 1:AP:278:THR:HG21 | 1.73                     | 0.67              |
| 6:U:36:PRO:HB3    | 6:U:96:ASP:HB2    | 1.77                     | 0.67              |
| 1:WW:186:LEU:HA   | 1:WW:190:GLN:OE1  | 1.96                     | 0.66              |
| 4:H:68:ILE:HD11   | 5:M:104:VAL:HG22  | 1.76                     | 0.66              |
| 6:U:65:LEU:HD21   | 1:1:297:GLN:HB2   | 1.73                     | 0.66              |
| 1:UO:98:LEU:HD12  | 1:UO:146:THR:OG1  | 1.94                     | 0.66              |
| 1:WB:190:GLN:HG2  | 1:WC:216:SER:O    | 1.94                     | 0.66              |
| 1:WE:112:GLY:HA2  | 1:WE:135:ALA:CA   | 2.18                     | 0.66              |
| 1:w:391:VAL:HG21  | 1:w:409:MET:HE1   | 1.78                     | 0.66              |
| 1:x:391:VAL:HG21  | 1:x:409:MET:HE1   | 1.78                     | 0.66              |
| 4:F:43:GLN:OE1    | 6:Q:4:ARG:NH1     | 2.28                     | 0.66              |
| 1:z:391:VAL:HG21  | 1:z:409:MET:HE1   | 1.78                     | 0.66              |
| 1:AD:391:VAL:HG21 | 1:AD:409:MET:HE1  | 1.78                     | 0.66              |
| 1:AF:391:VAL:HG21 | 1:AF:409:MET:HE1  | 1.78                     | 0.66              |
| 1:UO:62:ASP:OD2   | 1:WT:184:ARG:NH2  | 2.28                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UP:125:GLN:HA   | 1:UP:128:GLU:HB2  | 1.76                     | 0.66              |
| 3:E:193:LEU:HD22  | 3:E:228:LEU:HD11  | 1.77                     | 0.66              |
| 5:N:14:LEU:HB3    | 1:5:278:THR:HG21  | 1.77                     | 0.66              |
| 1:y:391:VAL:HG21  | 1:y:409:MET:HE1   | 1.78                     | 0.66              |
| 1:AE:391:VAL:HG21 | 1:AE:409:MET:HE1  | 1.78                     | 0.66              |
| 1:AG:391:VAL:HG21 | 1:AG:409:MET:HE1  | 1.78                     | 0.66              |
| 1:UK:207:PRO:CG   | 1:WE:187:ASP:CG   | 2.68                     | 0.66              |
| 5:P:15:GLN:HB2    | 1:AQ:374:HIS:CD2  | 2.30                     | 0.66              |
| 1:v:391:VAL:HG21  | 1:v:409:MET:HE1   | 1.78                     | 0.66              |
| 1:AH:391:VAL:HG21 | 1:AH:409:MET:HE1  | 1.78                     | 0.66              |
| 1:AI:391:VAL:HG21 | 1:AI:409:MET:HE1  | 1.78                     | 0.66              |
| 1:WD:200:SER:HG   | 1:WE:175:SER:HB2  | 1.61                     | 0.66              |
| 5:K:7:ILE:CB      | 1:AM:278:THR:HG21 | 2.24                     | 0.66              |
| 4:I:194:LEU:HD11  | 4:J:220:PRO:HG2   | 1.77                     | 0.66              |
| 7:V:6:ILE:HG21    | 7:V:122:VAL:HG21  | 1.76                     | 0.66              |
| 1:k:312:VAL:O     | 1:k:317:SER:OG    | 2.11                     | 0.66              |
| 1:l:391:VAL:HG21  | 1:l:409:MET:HE1   | 1.78                     | 0.66              |
| 1:AC:391:VAL:HG21 | 1:AC:409:MET:HE1  | 1.78                     | 0.66              |
| 1:AJ:391:VAL:HG21 | 1:AJ:409:MET:HE1  | 1.78                     | 0.66              |
| 7:Z:37:PRO:HB2    | 1:j:330:THR:HG23  | 1.78                     | 0.66              |
| 1:u:391:VAL:HG21  | 1:u:409:MET:HE1   | 1.78                     | 0.66              |
| 1:3:391:VAL:HG21  | 1:3:409:MET:HE1   | 1.78                     | 0.66              |
| 1:WA:112:GLY:HA3  | 1:WA:139:GLU:OE1  | 1.95                     | 0.66              |
| 6:U:123:LEU:HD23  | 7:Z:132:LEU:HD11  | 1.77                     | 0.66              |
| 1:2:391:VAL:HG21  | 1:2:409:MET:HE1   | 1.78                     | 0.66              |
| 1:AB:391:VAL:HG21 | 1:AB:409:MET:HE1  | 1.78                     | 0.66              |
| 5:N:7:ILE:HG21    | 1:6:278:THR:HG21  | 1.76                     | 0.65              |
| 5:O:21:ALA:HB1    | 1:x:278:THR:CG2   | 2.22                     | 0.65              |
| 1:t:391:VAL:HG21  | 1:t:409:MET:HE1   | 1.78                     | 0.65              |
| 1:AA:391:VAL:HG21 | 1:AA:409:MET:HE1  | 1.78                     | 0.65              |
| 1:AK:391:VAL:HG21 | 1:AK:409:MET:HE1  | 1.78                     | 0.65              |
| 1:WF:128:GLU:HG2  | 1:WG:126:PHE:CD2  | 2.29                     | 0.65              |
| 1:WU:167:ARG:HH12 | 4:G:158:PRO:HD3   | 1.61                     | 0.65              |
| 6:T:78:VAL:C      | 1:7:299:ASN:ND2   | 2.48                     | 0.65              |
| 1:AQ:391:VAL:HG21 | 1:AQ:409:MET:HE1  | 1.78                     | 0.65              |
| 1:UI:98:LEU:HD12  | 1:UI:146:THR:OG1  | 1.94                     | 0.65              |
| 1:WH:203:ALA:CB   | 1:WI:160:PRO:HB3  | 2.19                     | 0.65              |
| 1:WO:197:LEU:HD12 | 1:WP:175:SER:CB   | 2.26                     | 0.65              |
| 5:O:11:ILE:HG22   | 1:z:372:ILE:HB    | 1.77                     | 0.65              |
| 1:4:391:VAL:HG21  | 1:4:409:MET:HE1   | 1.78                     | 0.65              |
| 1:0:391:VAL:HG21  | 1:0:409:MET:HE1   | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UK:125:GLN:HA   | 1:UK:128:GLU:HB2  | 1.76                     | 0.65              |
| 1:9:391:VAL:HG21  | 1:9:409:MET:HE1   | 1.78                     | 0.65              |
| 1:AL:391:VAL:HG21 | 1:AL:409:MET:HE1  | 1.78                     | 0.65              |
| 1:AM:391:VAL:HG21 | 1:AM:409:MET:HE1  | 1.78                     | 0.65              |
| 4:H:66:ARG:NH2    | 4:H:242:SER:OG    | 2.30                     | 0.65              |
| 5:N:7:ILE:HD11    | 1:7:370:ARG:HH21  | 1.61                     | 0.65              |
| 1:1:389:VAL:HG21  | 1:1:416:THR:HG21  | 1.79                     | 0.65              |
| 1:3:389:VAL:HG21  | 1:3:416:THR:HG21  | 1.79                     | 0.65              |
| 1:4:389:VAL:HG21  | 1:4:416:THR:HG21  | 1.79                     | 0.65              |
| 1:AM:389:VAL:HG21 | 1:AM:416:THR:HG21 | 1.79                     | 0.65              |
| 1:5:391:VAL:HG21  | 1:5:409:MET:HE1   | 1.78                     | 0.65              |
| 1:AI:389:VAL:HG21 | 1:AI:416:THR:HG21 | 1.79                     | 0.65              |
| 1:AK:389:VAL:HG21 | 1:AK:416:THR:HG21 | 1.79                     | 0.65              |
| 1:AP:391:VAL:HG21 | 1:AP:409:MET:HE1  | 1.78                     | 0.65              |
| 6:S:72:HIS:HA     | 1:AE:295:SER:CB   | 2.27                     | 0.65              |
| 6:U:72:HIS:CD2    | 1:1:365:ASN:CB    | 2.60                     | 0.65              |
| 1:2:389:VAL:HG21  | 1:2:416:THR:HG21  | 1.79                     | 0.65              |
| 1:8:391:VAL:HG21  | 1:8:409:MET:HE1   | 1.78                     | 0.65              |
| 1:AN:389:VAL:HG21 | 1:AN:416:THR:HG21 | 1.79                     | 0.65              |
| 1:AO:391:VAL:HG21 | 1:AO:409:MET:HE1  | 1.78                     | 0.65              |
| 1:UK:103:GLN:CD   | 1:WF:182:PRO:HB3  | 2.21                     | 0.65              |
| 1:UN:125:GLN:HA   | 1:UN:128:GLU:HB2  | 1.76                     | 0.65              |
| 1:WP:128:GLU:HG3  | 1:WQ:126:PHE:HE2  | 1.62                     | 0.65              |
| 1:WW:134:ARG:HB3  | 1:WW:134:ARG:HH21 | 1.61                     | 0.65              |
| 4:J:138:MET:HE1   | 4:J:171:LEU:HD23  | 1.78                     | 0.65              |
| 6:U:76:GLN:H      | 1:1:297:GLN:NE2   | 1.95                     | 0.65              |
| 1:AJ:389:VAL:HG21 | 1:AJ:416:THR:HG21 | 1.79                     | 0.65              |
| 1:AL:389:VAL:HG21 | 1:AL:416:THR:HG21 | 1.79                     | 0.65              |
| 1:AN:391:VAL:HG21 | 1:AN:409:MET:HE1  | 1.78                     | 0.65              |
| 1:WM:200:SER:O    | 1:WN:158:ALA:HB2  | 1.97                     | 0.65              |
| 1:WT:128:GLU:HG2  | 1:WU:126:PHE:HD2  | 1.60                     | 0.65              |
| 1:y:389:VAL:HG21  | 1:y:416:THR:HG21  | 1.79                     | 0.65              |
| 1:z:389:VAL:HG21  | 1:z:416:THR:HG21  | 1.79                     | 0.65              |
| 1:6:389:VAL:HG21  | 1:6:416:THR:HG21  | 1.79                     | 0.65              |
| 1:7:391:VAL:HG21  | 1:7:409:MET:HE1   | 1.78                     | 0.65              |
| 1:AG:389:VAL:HG21 | 1:AG:416:THR:HG21 | 1.79                     | 0.65              |
| 4:F:58:LEU:O      | 4:F:62:THR:OG1    | 2.14                     | 0.64              |
| 4:H:135:ARG:NH1   | 4:H:165:VAL:O     | 2.30                     | 0.64              |
| 1:5:389:VAL:HG21  | 1:5:416:THR:HG21  | 1.79                     | 0.64              |
| 1:6:391:VAL:HG21  | 1:6:409:MET:HE1   | 1.78                     | 0.64              |
| 1:7:389:VAL:HG21  | 1:7:416:THR:HG21  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WA:154:ARG:HG2  | 1:WW:143:THR:OG1  | 1.97                     | 0.64              |
| 1:w:389:VAL:HG21  | 1:w:416:THR:HG21  | 1.79                     | 0.64              |
| 1:AP:389:VAL:HG21 | 1:AP:416:THR:HG21 | 1.79                     | 0.64              |
| 1:WE:123:ILE:HB   | 1:WE:128:GLU:OE1  | 1.95                     | 0.64              |
| 1:WE:166:VAL:CG2  | 4:I:160:GLN:CA    | 2.60                     | 0.64              |
| 1:WI:167:ARG:HG3  | 4:J:160:GLN:O     | 1.98                     | 0.64              |
| 1:WP:164:LEU:HD21 | 4:F:151:ALA:HB2   | 1.79                     | 0.64              |
| 5:M:4:ILE:HG13    | 1:AC:372:ILE:HG21 | 1.79                     | 0.64              |
| 6:R:36:PRO:HB3    | 6:R:96:ASP:HB2    | 1.79                     | 0.64              |
| 6:U:68:THR:CG2    | 1:1:294:ARG:HD2   | 2.25                     | 0.64              |
| 1:AO:389:VAL:HG21 | 1:AO:416:THR:HG21 | 1.79                     | 0.64              |
| 1:WR:143:THR:OG1  | 1:WS:154:ARG:HG2  | 1.97                     | 0.64              |
| 1:t:389:VAL:HG21  | 1:t:416:THR:HG21  | 1.79                     | 0.64              |
| 1:8:389:VAL:HG21  | 1:8:416:THR:HG21  | 1.79                     | 0.64              |
| 1:WD:168:GLU:OE2  | 1:WD:170:LYS:HE3  | 1.94                     | 0.64              |
| 1:u:389:VAL:HG21  | 1:u:416:THR:HG21  | 1.79                     | 0.64              |
| 1:v:389:VAL:HG21  | 1:v:416:THR:HG21  | 1.79                     | 0.64              |
| 1:AE:389:VAL:HG21 | 1:AE:416:THR:HG21 | 1.79                     | 0.64              |
| 1:AH:389:VAL:HG21 | 1:AH:416:THR:HG21 | 1.79                     | 0.64              |
| 6:R:74:PRO:O      | 6:R:75:ALA:C      | 2.40                     | 0.64              |
| 1:x:389:VAL:HG21  | 1:x:416:THR:HG21  | 1.79                     | 0.64              |
| 1:y:235:LEU:HD22  | 1:z:244:ARG:HH12  | 1.63                     | 0.64              |
| 1:AJ:235:LEU:HD22 | 1:AK:244:ARG:HH12 | 1.63                     | 0.64              |
| 1:AL:235:LEU:HD22 | 1:AM:244:ARG:HH12 | 1.63                     | 0.64              |
| 1:AM:287:ASP:HB3  | 1:AM:290:LYS:HE2  | 1.80                     | 0.64              |
| 1:WH:197:LEU:HD11 | 1:WI:156:HIS:HD2  | 1.63                     | 0.64              |
| 1:WH:197:LEU:HD12 | 1:WI:175:SER:OG   | 1.97                     | 0.64              |
| 1:WR:122:GLY:O    | 1:WR:123:ILE:C    | 2.39                     | 0.64              |
| 5:P:55:GLN:NE2    | 5:P:74:ASP:OD2    | 2.31                     | 0.64              |
| 1:5:394:LYS:HA    | 1:5:394:LYS:HE3   | 1.80                     | 0.64              |
| 1:8:394:LYS:HA    | 1:8:394:LYS:HE3   | 1.80                     | 0.64              |
| 1:9:389:VAL:HG21  | 1:9:416:THR:HG21  | 1.79                     | 0.64              |
| 1:0:394:LYS:HA    | 1:0:394:LYS:HE3   | 1.80                     | 0.64              |
| 1:AE:394:LYS:HA   | 1:AE:394:LYS:HE3  | 1.80                     | 0.64              |
| 1:AN:235:LEU:HD22 | 1:AO:244:ARG:HH12 | 1.63                     | 0.64              |
| 1:AQ:389:VAL:HG21 | 1:AQ:416:THR:HG21 | 1.79                     | 0.64              |
| 1:WN:196:HIS:CB   | 1:WO:211:THR:HG21 | 2.19                     | 0.64              |
| 5:N:7:ILE:HD11    | 1:7:370:ARG:HE    | 1.62                     | 0.64              |
| 1:u:235:LEU:HD22  | 1:v:244:ARG:HH12  | 1.63                     | 0.64              |
| 1:6:394:LYS:HA    | 1:6:394:LYS:HE3   | 1.80                     | 0.64              |
| 1:0:235:LEU:HD22  | 1:AA:244:ARG:HH12 | 1.63                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:235:LEU:HD22 | 1:AC:244:ARG:HH12 | 1.63                     | 0.64              |
| 1:AC:394:LYS:HA   | 1:AC:394:LYS:HE3  | 1.80                     | 0.64              |
| 1:WH:166:VAL:HG11 | 4:J:147:LEU:HD12  | 1.80                     | 0.64              |
| 3:E:24:LEU:HB3    | 5:K:89:ARG:NH2    | 2.12                     | 0.64              |
| 5:P:21:ALA:CB     | 1:AP:278:THR:CG2  | 2.67                     | 0.64              |
| 6:T:72:HIS:CD2    | 1:7:365:ASN:CB    | 2.66                     | 0.64              |
| 1:w:235:LEU:HD22  | 1:x:244:ARG:HH12  | 1.63                     | 0.64              |
| 1:1:235:LEU:HD22  | 1:2:244:ARG:HH12  | 1.63                     | 0.64              |
| 1:3:394:LYS:HE3   | 1:3:394:LYS:HA    | 1.80                     | 0.64              |
| 1:7:394:LYS:HA    | 1:7:394:LYS:HE3   | 1.80                     | 0.64              |
| 1:8:235:LEU:HD22  | 1:9:244:ARG:HH12  | 1.63                     | 0.64              |
| 1:AA:394:LYS:HE3  | 1:AA:394:LYS:HA   | 1.80                     | 0.64              |
| 1:AF:389:VAL:HG21 | 1:AF:416:THR:HG21 | 1.79                     | 0.64              |
| 1:AG:394:LYS:HA   | 1:AG:394:LYS:HE3  | 1.80                     | 0.64              |
| 1:WF:167:ARG:O    | 4:I:152:ARG:NH1   | 2.31                     | 0.64              |
| 5:M:3:ALA:C       | 1:AC:372:ILE:CD1  | 2.70                     | 0.64              |
| 1:4:287:ASP:HB3   | 1:4:290:LYS:HE2   | 1.80                     | 0.64              |
| 1:5:287:ASP:HB3   | 1:5:290:LYS:HE2   | 1.80                     | 0.64              |
| 1:AA:389:VAL:HG21 | 1:AA:416:THR:HG21 | 1.79                     | 0.64              |
| 1:AB:394:LYS:HA   | 1:AB:394:LYS:HE3  | 1.80                     | 0.64              |
| 1:AC:389:VAL:HG21 | 1:AC:416:THR:HG21 | 1.79                     | 0.64              |
| 1:AL:287:ASP:HB3  | 1:AL:290:LYS:HE2  | 1.80                     | 0.64              |
| 1:WG:139:GLU:HB3  | 1:WH:154:ARG:HH21 | 1.63                     | 0.63              |
| 4:I:204:LEU:HD22  | 4:I:212:VAL:HG11  | 1.78                     | 0.63              |
| 5:N:11:ILE:CG2    | 1:6:372:ILE:HG21  | 2.28                     | 0.63              |
| 5:O:11:ILE:CG2    | 1:z:372:ILE:HG21  | 2.28                     | 0.63              |
| 5:P:7:ILE:HD12    | 1:u:372:ILE:HD12  | 1.80                     | 0.63              |
| 1:t:244:ARG:HH12  | 1:AQ:235:LEU:HD22 | 1.63                     | 0.63              |
| 1:3:235:LEU:HD22  | 1:4:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:0:389:VAL:HG21  | 1:0:416:THR:HG21  | 1.79                     | 0.63              |
| 1:AB:389:VAL:HG21 | 1:AB:416:THR:HG21 | 1.79                     | 0.63              |
| 1:AD:389:VAL:HG21 | 1:AD:416:THR:HG21 | 1.79                     | 0.63              |
| 1:AN:287:ASP:HB3  | 1:AN:290:LYS:HE2  | 1.80                     | 0.63              |
| 1:AP:235:LEU:HD22 | 1:AQ:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:WL:197:LEU:HD12 | 1:WM:175:SER:HB3  | 1.80                     | 0.63              |
| 2:C:75:ASP:O      | 2:C:79:THR:HG23   | 1.98                     | 0.63              |
| 3:E:158:PRO:CG    | 3:E:162:ASN:HD21  | 2.09                     | 0.63              |
| 1:3:287:ASP:HB3   | 1:3:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:9:394:LYS:HA    | 1:9:394:LYS:HE3   | 1.80                     | 0.63              |
| 1:AD:394:LYS:HE3  | 1:AD:394:LYS:HA   | 1.80                     | 0.63              |
| 1:AE:235:LEU:HD22 | 1:AF:244:ARG:HH12 | 1.63                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WB:200:SER:O    | 1:WC:158:ALA:CB   | 2.45                     | 0.63              |
| 1:WH:197:LEU:HD12 | 1:WI:175:SER:CB   | 2.28                     | 0.63              |
| 1:WH:197:LEU:HA   | 1:WI:175:SER:OG   | 1.97                     | 0.63              |
| 2:D:58:VAL:HG11   | 4:J:207:LEU:HD11  | 1.79                     | 0.63              |
| 6:T:66:THR:OG1    | 1:7:294:ARG:HG2   | 1.98                     | 0.63              |
| 1:1:394:LYS:HA    | 1:1:394:LYS:HE3   | 1.80                     | 0.63              |
| 1:5:235:LEU:HD22  | 1:6:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:AD:235:LEU:HD22 | 1:AE:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:AF:394:LYS:HA   | 1:AF:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:AH:235:LEU:HD22 | 1:AI:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:AH:394:LYS:HA   | 1:AH:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:WB:166:VAL:O    | 4:H:152:ARG:HD2   | 1.97                     | 0.63              |
| 1:WJ:164:LEU:CD2  | 3:E:144:LEU:HB3   | 2.27                     | 0.63              |
| 5:K:14:LEU:CD2    | 1:AL:278:THR:CG2  | 2.62                     | 0.63              |
| 6:S:22:ARG:NH2    | 6:S:108:GLN:OE1   | 2.31                     | 0.63              |
| 7:V:55:PRO:HG3    | 1:AP:359:GLN:CD   | 2.23                     | 0.63              |
| 1:2:394:LYS:HA    | 1:2:394:LYS:HE3   | 1.80                     | 0.63              |
| 1:4:394:LYS:HA    | 1:4:394:LYS:HE3   | 1.80                     | 0.63              |
| 1:6:235:LEU:HD22  | 1:7:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:9:287:ASP:HB3   | 1:9:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:AC:235:LEU:HD22 | 1:AD:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:AG:235:LEU:HD22 | 1:AH:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:WO:196:HIS:HB3  | 1:WP:211:THR:HG21 | 1.80                     | 0.63              |
| 6:U:72:HIS:HE1    | 1:2:294:ARG:HE    | 1.43                     | 0.63              |
| 1:0:287:ASP:HB3   | 1:0:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:AO:235:LEU:HD22 | 1:AP:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:WH:166:VAL:CG1  | 4:J:147:LEU:HD12  | 2.28                     | 0.63              |
| 1:WP:214:ASP:OD1  | 1:WP:218:HIS:HB2  | 1.99                     | 0.63              |
| 1:WU:128:GLU:HG2  | 1:WV:126:PHE:HD2  | 1.64                     | 0.63              |
| 1:6:287:ASP:HB3   | 1:6:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:7:235:LEU:HD22  | 1:8:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:9:235:LEU:HD22  | 1:0:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:AF:235:LEU:HD22 | 1:AG:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:AH:287:ASP:HB3  | 1:AH:290:LYS:HE2  | 1.80                     | 0.63              |
| 1:AI:394:LYS:HA   | 1:AI:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:WG:139:GLU:HB3  | 1:WH:154:ARG:NH2  | 2.14                     | 0.63              |
| 1:WH:166:VAL:HG11 | 4:J:147:LEU:CD1   | 2.28                     | 0.63              |
| 6:U:84:ASP:OD2    | 1:y:303:GLN:NE2   | 2.31                     | 0.63              |
| 1:v:287:ASP:HB3   | 1:v:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:w:287:ASP:HB3   | 1:w:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:AA:287:ASP:HB3  | 1:AA:290:LYS:HE2  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:287:ASP:HB3  | 1:AK:290:LYS:HE2  | 1.80                     | 0.63              |
| 1:AO:287:ASP:HB3  | 1:AO:290:LYS:HE2  | 1.80                     | 0.63              |
| 1:WG:193:ALA:HB1  | 1:WH:213:VAL:HG11 | 1.81                     | 0.63              |
| 1:t:235:LEU:HD22  | 1:u:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:4:235:LEU:HD22  | 1:5:244:ARG:HH12  | 1.63                     | 0.63              |
| 1:8:287:ASP:HB3   | 1:8:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:AJ:394:LYS:HA   | 1:AJ:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:WS:168:GLU:HB3  | 1:WS:170:LYS:HE3  | 1.81                     | 0.63              |
| 4:H:116:PHE:O     | 6:S:4:ARG:NH2     | 2.30                     | 0.63              |
| 6:R:65:LEU:HD21   | 1:AI:363:THR:HG23 | 1.80                     | 0.63              |
| 7:X:20:ARG:NH1    | 1:g:313:PRO:O     | 2.32                     | 0.63              |
| 1:u:287:ASP:HB3   | 1:u:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:2:287:ASP:HB3   | 1:2:290:LYS:HE2   | 1.80                     | 0.63              |
| 1:AA:235:LEU:HD22 | 1:AB:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:AI:235:LEU:HD22 | 1:AJ:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:AI:287:ASP:HB3  | 1:AI:290:LYS:HE2  | 1.80                     | 0.63              |
| 1:AM:235:LEU:HD22 | 1:AN:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:WL:186:LEU:HA   | 1:WL:190:GLN:OE1  | 1.99                     | 0.62              |
| 6:R:73:ILE:CG1    | 1:AK:295:SER:HB2  | 2.22                     | 0.62              |
| 6:S:76:GLN:H      | 1:AD:297:GLN:HE22 | 1.46                     | 0.62              |
| 1:z:394:LYS:HA    | 1:z:394:LYS:HE3   | 1.80                     | 0.62              |
| 1:UM:103:GLN:CD   | 1:WQ:182:PRO:CB   | 2.71                     | 0.62              |
| 1:WA:187:ASP:CG   | 1:WA:190:GLN:HG3  | 2.24                     | 0.62              |
| 1:WI:200:SER:OG   | 1:WJ:175:SER:HB2  | 1.99                     | 0.62              |
| 1:WU:165:PHE:HA   | 4:G:148:ALA:HB1   | 1.80                     | 0.62              |
| 4:F:60:MET:HE1    | 4:G:91:GLY:HA3    | 1.80                     | 0.62              |
| 1:t:287:ASP:HB3   | 1:t:290:LYS:HE2   | 1.80                     | 0.62              |
| 1:t:394:LYS:HA    | 1:t:394:LYS:HE3   | 1.80                     | 0.62              |
| 1:v:235:LEU:HD22  | 1:w:244:ARG:HH12  | 1.63                     | 0.62              |
| 1:x:287:ASP:HB3   | 1:x:290:LYS:HE2   | 1.80                     | 0.62              |
| 1:AG:287:ASP:HB3  | 1:AG:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:AO:394:LYS:HE3  | 1:AO:394:LYS:HA   | 1.80                     | 0.62              |
| 2:C:23:PRO:O      | 2:C:27:VAL:HG12   | 1.99                     | 0.62              |
| 4:J:229:VAL:O     | 4:J:230:ASP:C     | 2.41                     | 0.62              |
| 5:L:11:ILE:HG23   | 1:AH:372:ILE:HG21 | 1.76                     | 0.62              |
| 5:M:4:ILE:CG1     | 1:AC:372:ILE:HG22 | 2.29                     | 0.62              |
| 1:u:394:LYS:HA    | 1:u:394:LYS:HE3   | 1.80                     | 0.62              |
| 1:AD:287:ASP:HB3  | 1:AD:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:AK:235:LEU:HD22 | 1:AL:244:ARG:HH12 | 1.63                     | 0.62              |
| 1:AK:394:LYS:HA   | 1:AK:394:LYS:HE3  | 1.80                     | 0.62              |
| 1:UI:167:ARG:NH2  | 1:WW:188:GLU:HB3  | 2.13                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WQ:128:GLU:HG2  | 1:WR:126:PHE:CD2  | 2.34                     | 0.62              |
| 6:S:72:HIS:CB     | 1:AE:295:SER:CB   | 2.73                     | 0.62              |
| 1:w:394:LYS:HA    | 1:w:394:LYS:HE3   | 1.80                     | 0.62              |
| 1:y:394:LYS:HE3   | 1:y:394:LYS:HA    | 1.80                     | 0.62              |
| 4:F:162:PRO:HD2   | 4:F:163:GLU:N     | 2.14                     | 0.62              |
| 1:x:235:LEU:HD22  | 1:y:244:ARG:HH12  | 1.63                     | 0.62              |
| 1:2:235:LEU:HD22  | 1:3:244:ARG:HH12  | 1.63                     | 0.62              |
| 1:WS:197:LEU:HD12 | 1:WT:175:SER:HB3  | 1.81                     | 0.62              |
| 3:E:105:GLN:NE2   | 4:F:216:THR:O     | 2.33                     | 0.62              |
| 4:G:67:ILE:HD12   | 4:G:239:LEU:HD13  | 1.81                     | 0.62              |
| 4:J:45:LEU:HG     | 5:P:89:ARG:HD3    | 1.81                     | 0.62              |
| 1:AE:287:ASP:HB3  | 1:AE:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:AP:394:LYS:HA   | 1:AP:394:LYS:HE3  | 1.80                     | 0.62              |
| 1:WQ:128:GLU:HG2  | 1:WR:126:PHE:HD2  | 1.65                     | 0.62              |
| 2:B:24:LEU:HD22   | 2:B:58:VAL:HG13   | 1.81                     | 0.62              |
| 6:U:78:VAL:HG12   | 1:1:299:ASN:HD21  | 1.62                     | 0.62              |
| 1:7:287:ASP:HB3   | 1:7:290:LYS:HE2   | 1.80                     | 0.62              |
| 1:AC:287:ASP:HB3  | 1:AC:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:WE:166:VAL:CG2  | 4:I:160:GLN:CG    | 2.78                     | 0.62              |
| 1:AJ:287:ASP:HB3  | 1:AJ:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:WK:197:LEU:HD11 | 1:WL:156:HIS:HD2  | 1.63                     | 0.62              |
| 4:H:52:THR:OG1    | 5:M:91:LYS:NZ     | 2.28                     | 0.62              |
| 5:L:4:ILE:HG13    | 1:AI:372:ILE:HG21 | 1.82                     | 0.62              |
| 6:S:65:LEU:C      | 6:S:65:LEU:HD12   | 2.25                     | 0.62              |
| 6:S:72:HIS:CE1    | 1:AD:365:ASN:HB3  | 2.33                     | 0.62              |
| 1:x:394:LYS:HA    | 1:x:394:LYS:HE3   | 1.80                     | 0.62              |
| 1:AL:394:LYS:HA   | 1:AL:394:LYS:HE3  | 1.80                     | 0.62              |
| 1:UO:103:GLN:NE2  | 1:WU:182:PRO:CB   | 2.63                     | 0.62              |
| 1:UP:167:ARG:HH11 | 1:8:236:LYS:HE2   | 1.63                     | 0.62              |
| 3:E:185:MET:O     | 3:E:186:LEU:C     | 2.42                     | 0.62              |
| 1:y:287:ASP:HB3   | 1:y:290:LYS:HE2   | 1.80                     | 0.62              |
| 1:z:235:LEU:HD22  | 1:1:244:ARG:HH12  | 1.63                     | 0.62              |
| 1:AP:287:ASP:HB3  | 1:AP:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:AQ:394:LYS:HA   | 1:AQ:394:LYS:HE3  | 1.80                     | 0.62              |
| 1:UK:161:LYS:O    | 1:UK:162:PRO:C    | 2.43                     | 0.61              |
| 5:M:75:MET:HE1    | 6:R:122:VAL:HG13  | 1.82                     | 0.61              |
| 1:1:287:ASP:HB3   | 1:1:290:LYS:HE2   | 1.80                     | 0.61              |
| 1:AB:287:ASP:HB3  | 1:AB:290:LYS:HE2  | 1.80                     | 0.61              |
| 1:AN:394:LYS:HA   | 1:AN:394:LYS:HE3  | 1.80                     | 0.61              |
| 1:WT:128:GLU:HG2  | 1:WU:126:PHE:CD2  | 2.35                     | 0.61              |
| 2:D:46:GLU:HB2    | 2:D:49:LEU:HD23   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:70:LEU:O     | 2:D:74:LEU:HG     | 2.01                     | 0.61              |
| 1:UM:161:LYS:O   | 1:UM:162:PRO:C    | 2.43                     | 0.61              |
| 1:UN:73:MET:HE3  | 1:UN:99:ARG:HD3   | 1.81                     | 0.61              |
| 1:WO:197:LEU:CD1 | 1:WP:175:SER:OG   | 2.42                     | 0.61              |
| 1:l:319:GLN:NE2  | 1:y:305:GLY:O     | 2.33                     | 0.61              |
| 1:AF:277:GLN:HB3 | 1:AF:377:MET:HE1  | 1.83                     | 0.61              |
| 1:AF:287:ASP:HB3 | 1:AF:290:LYS:HE2  | 1.80                     | 0.61              |
| 1:AM:394:LYS:HA  | 1:AM:394:LYS:HE3  | 1.80                     | 0.61              |
| 1:AQ:287:ASP:HB3 | 1:AQ:290:LYS:HE2  | 1.80                     | 0.61              |
| 1:WI:190:GLN:HG2 | 1:WJ:217:GLY:HA3  | 1.82                     | 0.61              |
| 3:E:114:VAL:HG12 | 4:G:213:PRO:HB3   | 1.81                     | 0.61              |
| 4:J:83:ALA:O     | 4:J:84:PRO:C      | 2.39                     | 0.61              |
| 1:AA:277:GLN:HB3 | 1:AA:377:MET:HE1  | 1.83                     | 0.61              |
| 1:AE:277:GLN:HB3 | 1:AE:377:MET:HE1  | 1.83                     | 0.61              |
| 1:UK:73:MET:HE3  | 1:UK:99:ARG:HD3   | 1.81                     | 0.61              |
| 1:UL:208:GLY:N   | 1:WG:187:ASP:OD2  | 2.33                     | 0.61              |
| 1:WB:212:LEU:HB3 | 1:WB:221:THR:HG23 | 1.81                     | 0.61              |
| 1:WI:190:GLN:NE2 | 1:WJ:216:SER:O    | 2.33                     | 0.61              |
| 1:WO:128:GLU:HG2 | 1:WP:126:PHE:HD2  | 1.64                     | 0.61              |
| 2:D:9:MET:HE2    | 4:J:191:ILE:HG13  | 1.81                     | 0.61              |
| 1:AC:277:GLN:HB3 | 1:AC:377:MET:HE1  | 1.83                     | 0.61              |
| 1:AH:277:GLN:HB3 | 1:AH:377:MET:HE1  | 1.83                     | 0.61              |
| 4:G:82:SER:HA    | 5:K:103:GLN:NE2   | 2.15                     | 0.61              |
| 5:M:11:ILE:CD1   | 5:M:12:SER:N      | 2.55                     | 0.61              |
| 1:AD:277:GLN:HB3 | 1:AD:377:MET:HE1  | 1.83                     | 0.61              |
| 1:AJ:277:GLN:HB3 | 1:AJ:377:MET:HE1  | 1.83                     | 0.61              |
| 1:UO:161:LYS:O   | 1:UO:162:PRO:C    | 2.43                     | 0.61              |
| 1:WW:125:GLN:OE1 | 2:B:2:THR:HG21    | 1.98                     | 0.61              |
| 2:A:66:GLY:HA2   | 2:A:69:MET:HE2    | 1.82                     | 0.61              |
| 5:O:14:LEU:CD1   | 1:z:370:ARG:HH21  | 2.10                     | 0.61              |
| 5:P:11:ILE:CG2   | 1:t:372:ILE:CG2   | 2.78                     | 0.61              |
| 6:Q:23:GLN:NE2   | 7:V:125:MET:HE1   | 2.15                     | 0.61              |
| 1:v:394:LYS:HA   | 1:v:394:LYS:HE3   | 1.80                     | 0.61              |
| 1:AB:277:GLN:HB3 | 1:AB:377:MET:HE1  | 1.83                     | 0.61              |
| 1:AI:277:GLN:HB3 | 1:AI:377:MET:HE1  | 1.83                     | 0.61              |
| 1:UL:161:LYS:O   | 1:UL:162:PRO:C    | 2.43                     | 0.61              |
| 5:M:11:ILE:HD12  | 5:M:12:SER:CA     | 2.31                     | 0.61              |
| 1:z:287:ASP:HB3  | 1:z:290:LYS:HE2   | 1.80                     | 0.61              |
| 1:AG:277:GLN:HB3 | 1:AG:377:MET:HE1  | 1.83                     | 0.61              |
| 1:UM:73:MET:HE3  | 1:UM:99:ARG:HD3   | 1.81                     | 0.61              |
| 1:UP:73:MET:HE3  | 1:UP:99:ARG:HD3   | 1.81                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WP:128:GLU:HG3  | 1:WQ:126:PHE:CE2  | 2.35                     | 0.61              |
| 1:WP:190:GLN:NE2  | 1:WQ:216:SER:O    | 2.33                     | 0.61              |
| 4:F:52:THR:OG1    | 5:K:91:LYS:NZ     | 2.34                     | 0.61              |
| 5:M:3:ALA:C       | 1:AC:372:ILE:HD13 | 2.26                     | 0.61              |
| 6:R:51:LYS:NZ     | 6:R:84:ASP:OD1    | 2.34                     | 0.61              |
| 7:W:27:ASN:OD1    | 7:W:42:TYR:OH     | 2.19                     | 0.61              |
| 1:O:277:GLN:HB3   | 1:O:377:MET:HE1   | 1.83                     | 0.61              |
| 1:AL:277:GLN:HB3  | 1:AL:377:MET:HE1  | 1.83                     | 0.61              |
| 1:WJ:164:LEU:CB   | 3:E:145:TRP:CD1   | 2.83                     | 0.61              |
| 1:WJ:186:LEU:HA   | 1:WJ:190:GLN:OE1  | 2.00                     | 0.61              |
| 1:WR:212:LEU:HB3  | 1:WR:221:THR:HG23 | 1.82                     | 0.61              |
| 2:A:56:VAL:O      | 2:A:60:ILE:HG12   | 2.01                     | 0.61              |
| 4:G:66:ARG:NE     | 4:G:178:GLU:OE1   | 2.33                     | 0.61              |
| 1:AK:277:GLN:HB3  | 1:AK:377:MET:HE1  | 1.83                     | 0.61              |
| 1:UP:161:LYS:O    | 1:UP:162:PRO:C    | 2.43                     | 0.60              |
| 1:WC:193:ALA:HB1  | 1:WD:213:VAL:CG1  | 2.30                     | 0.60              |
| 1:WH:197:LEU:HD12 | 1:WI:175:SER:HB3  | 1.83                     | 0.60              |
| 1:WM:200:SER:O    | 1:WN:158:ALA:HB3  | 2.01                     | 0.60              |
| 1:w:277:GLN:HB3   | 1:w:377:MET:HE1   | 1.83                     | 0.60              |
| 1:9:277:GLN:HB3   | 1:9:377:MET:HE1   | 1.83                     | 0.60              |
| 1:WD:117:ASP:O    | 1:WD:118:GLN:C    | 2.44                     | 0.60              |
| 1:WI:164:LEU:HD23 | 1:WI:165:PHE:HB3  | 1.83                     | 0.60              |
| 3:E:106:MET:SD    | 3:E:225:GLY:HA3   | 2.40                     | 0.60              |
| 4:F:123:MET:HE3   | 4:F:124:GLN:HG2   | 1.81                     | 0.60              |
| 5:O:14:LEU:HD23   | 1:y:278:THR:HG21  | 1.83                     | 0.60              |
| 7:Z:12:SER:OG     | 7:Z:62:VAL:O      | 2.19                     | 0.60              |
| 1:1:277:GLN:HB3   | 1:1:377:MET:HE1   | 1.83                     | 0.60              |
| 1:2:277:GLN:HB3   | 1:2:377:MET:HE1   | 1.83                     | 0.60              |
| 1:AN:277:GLN:HB3  | 1:AN:377:MET:HE1  | 1.83                     | 0.60              |
| 1:UI:161:LYS:O    | 1:UI:162:PRO:C    | 2.43                     | 0.60              |
| 1:UJ:161:LYS:O    | 1:UJ:162:PRO:C    | 2.43                     | 0.60              |
| 1:UM:126:PHE:CE1  | 1:UM:130:VAL:CG2  | 2.84                     | 0.60              |
| 1:WA:197:LEU:HA   | 1:WB:175:SER:OG   | 2.00                     | 0.60              |
| 1:WS:117:ASP:O    | 1:WS:118:GLN:C    | 2.44                     | 0.60              |
| 4:I:83:ALA:HB3    | 4:I:84:PRO:HD3    | 1.83                     | 0.60              |
| 1:v:277:GLN:HB3   | 1:v:377:MET:HE1   | 1.83                     | 0.60              |
| 1:WA:175:SER:CB   | 1:WW:197:LEU:HA   | 2.31                     | 0.60              |
| 1:UK:127:SER:O    | 1:UK:131:ASN:CB   | 2.50                     | 0.60              |
| 1:UP:103:GLN:HG2  | 1:WW:182:PRO:HB3  | 0.71                     | 0.60              |
| 1:WE:197:LEU:CD1  | 1:WF:175:SER:OG   | 2.44                     | 0.60              |
| 1:WS:165:PHE:CE1  | 2:A:89:GLY:C      | 2.79                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WV:164:LEU:HB3  | 4:G:152:ARG:NH1   | 2.17                     | 0.60              |
| 1:x:277:GLN:HB3   | 1:x:377:MET:HE1   | 1.83                     | 0.60              |
| 1:8:277:GLN:HB3   | 1:8:377:MET:HE1   | 1.83                     | 0.60              |
| 1:AM:277:GLN:HB3  | 1:AM:377:MET:HE1  | 1.83                     | 0.60              |
| 1:UM:103:GLN:NE2  | 1:WQ:182:PRO:HB3  | 2.17                     | 0.60              |
| 1:UO:73:MET:HE3   | 1:UO:99:ARG:HD3   | 1.81                     | 0.60              |
| 1:WF:190:GLN:HA   | 1:WG:217:GLY:O    | 2.01                     | 0.60              |
| 1:WK:197:LEU:HA   | 1:WL:175:SER:CB   | 2.32                     | 0.60              |
| 1:WR:186:LEU:HA   | 1:WR:190:GLN:OE1  | 2.00                     | 0.60              |
| 1:4:402:LEU:HD12  | 1:4:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:AM:402:LEU:HD12 | 1:AM:403:PRO:HD2  | 1.84                     | 0.60              |
| 1:UP:167:ARG:NH1  | 1:8:236:LYS:HE2   | 2.15                     | 0.60              |
| 1:WH:193:ALA:CB   | 1:WI:213:VAL:HG11 | 2.26                     | 0.60              |
| 2:B:14:MET:HG3    | 2:C:59:PHE:CE1    | 2.36                     | 0.60              |
| 2:D:74:LEU:HD11   | 4:J:228:LEU:HD13  | 1.83                     | 0.60              |
| 1:5:402:LEU:HD12  | 1:5:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:UN:161:LYS:O    | 1:UN:162:PRO:C    | 2.43                     | 0.60              |
| 1:WK:197:LEU:HD11 | 1:WL:156:HIS:CD2  | 2.35                     | 0.60              |
| 1:z:277:GLN:HB3   | 1:z:377:MET:HE1   | 1.83                     | 0.60              |
| 1:1:402:LEU:HD12  | 1:1:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:UI:127:SER:O    | 1:UI:131:ASN:CB   | 2.50                     | 0.60              |
| 1:WH:167:ARG:HH22 | 4:J:162:PRO:CG    | 2.14                     | 0.60              |
| 1:WJ:212:LEU:HB3  | 1:WJ:221:THR:HG23 | 1.84                     | 0.60              |
| 4:J:83:ALA:CB     | 4:J:84:PRO:HD3    | 2.30                     | 0.60              |
| 6:T:55:ARG:NH2    | 1:5:299:ASN:HD21  | 1.91                     | 0.60              |
| 1:7:277:GLN:HB3   | 1:7:377:MET:HE1   | 1.83                     | 0.60              |
| 1:7:402:LEU:HD12  | 1:7:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:UK:126:PHE:CE1  | 1:UK:130:VAL:CG2  | 2.84                     | 0.60              |
| 1:WI:200:SER:O    | 1:WJ:158:ALA:HB2  | 2.02                     | 0.60              |
| 1:WM:143:THR:OG1  | 1:WN:154:ARG:CG   | 2.41                     | 0.60              |
| 4:J:184:GLN:O     | 4:J:188:THR:HG23  | 2.02                     | 0.60              |
| 1:2:402:LEU:HD12  | 1:2:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:8:402:LEU:HD12  | 1:8:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:AL:402:LEU:HD12 | 1:AL:403:PRO:HD2  | 1.84                     | 0.60              |
| 1:UI:73:MET:HE3   | 1:UI:99:ARG:HD3   | 1.81                     | 0.59              |
| 1:UI:126:PHE:CE1  | 1:UI:130:VAL:CG2  | 2.84                     | 0.59              |
| 1:UN:127:SER:O    | 1:UN:131:ASN:CB   | 2.50                     | 0.59              |
| 1:UN:208:GLY:N    | 1:WR:187:ASP:OD1  | 2.35                     | 0.59              |
| 1:UO:126:PHE:CE1  | 1:UO:130:VAL:CG2  | 2.84                     | 0.59              |
| 1:UP:127:SER:O    | 1:UP:131:ASN:CB   | 2.50                     | 0.59              |
| 1:WD:168:GLU:CG   | 1:WD:170:LYS:HE2  | 2.31                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:U:32:ASN:ND2    | 7:Z:60:GLY:O      | 2.35                     | 0.59              |
| 7:Y:109:SER:O     | 7:Y:113:GLN:HG3   | 2.02                     | 0.59              |
| 1:u:277:GLN:HB3   | 1:u:377:MET:HE1   | 1.83                     | 0.59              |
| 1:3:402:LEU:HD12  | 1:3:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:AG:402:LEU:HD12 | 1:AG:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:AN:402:LEU:HD12 | 1:AN:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:AO:277:GLN:HB3  | 1:AO:377:MET:HE1  | 1.83                     | 0.59              |
| 1:AP:277:GLN:HB3  | 1:AP:377:MET:HE1  | 1.83                     | 0.59              |
| 1:UL:127:SER:O    | 1:UL:131:ASN:CB   | 2.50                     | 0.59              |
| 1:UM:127:SER:O    | 1:UM:131:ASN:CB   | 2.50                     | 0.59              |
| 1:WG:212:LEU:HB3  | 1:WG:221:THR:HG23 | 1.83                     | 0.59              |
| 2:C:52:ILE:O      | 2:C:56:VAL:HG22   | 2.02                     | 0.59              |
| 5:M:11:ILE:CG2    | 1:AB:372:ILE:HG22 | 2.31                     | 0.59              |
| 5:O:14:LEU:CB     | 1:y:278:THR:HG21  | 2.31                     | 0.59              |
| 6:Q:94:SER:O      | 1:d:324:ASN:ND2   | 2.35                     | 0.59              |
| 6:U:68:THR:CG2    | 1:1:294:ARG:HD3   | 2.30                     | 0.59              |
| 7:V:20:ARG:HD3    | 7:V:108:ALA:HB2   | 1.84                     | 0.59              |
| 1:6:277:GLN:HB3   | 1:6:377:MET:HE1   | 1.83                     | 0.59              |
| 1:6:402:LEU:HD12  | 1:6:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:AH:402:LEU:HD12 | 1:AH:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:WB:197:LEU:CD1  | 1:WC:175:SER:OG   | 2.48                     | 0.59              |
| 1:WS:193:ALA:HB1  | 1:WT:213:VAL:HG11 | 1.84                     | 0.59              |
| 1:WV:190:GLN:NE2  | 1:WW:216:SER:O    | 2.34                     | 0.59              |
| 1:WW:117:ASP:O    | 1:WW:118:GLN:C    | 2.44                     | 0.59              |
| 4:I:232:TRP:O     | 4:I:236:MET:HG2   | 2.02                     | 0.59              |
| 6:T:65:LEU:HB2    | 1:7:295:SER:CB    | 2.32                     | 0.59              |
| 1:z:402:LEU:HD12  | 1:z:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:3:277:GLN:HB3   | 1:3:377:MET:HE1   | 1.83                     | 0.59              |
| 1:UJ:127:SER:O    | 1:UJ:131:ASN:CB   | 2.50                     | 0.59              |
| 1:UO:127:SER:O    | 1:UO:131:ASN:CB   | 2.50                     | 0.59              |
| 1:WI:186:LEU:HA   | 1:WI:190:GLN:OE1  | 2.02                     | 0.59              |
| 1:WJ:128:GLU:OE2  | 1:WK:127:SER:OG   | 2.20                     | 0.59              |
| 1:WJ:164:LEU:HD13 | 3:E:145:TRP:CG    | 2.33                     | 0.59              |
| 1:WP:128:GLU:HG2  | 1:WQ:126:PHE:CD2  | 2.37                     | 0.59              |
| 1:WP:212:LEU:HB3  | 1:WP:221:THR:HG23 | 1.85                     | 0.59              |
| 6:S:115:LYS:HE3   | 7:Y:4:LEU:HD11    | 1.84                     | 0.59              |
| 1:9:402:LEU:HD12  | 1:9:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:AF:402:LEU:HD12 | 1:AF:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:UJ:73:MET:HE3   | 1:UJ:99:ARG:HD3   | 1.81                     | 0.59              |
| 1:WC:212:LEU:HB3  | 1:WC:221:THR:HG23 | 1.84                     | 0.59              |
| 1:WD:197:LEU:HD12 | 1:WE:175:SER:HB3  | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WP:193:ALA:HB1  | 1:WQ:213:VAL:CG1  | 2.32                     | 0.59              |
| 6:Q:46:ALA:O      | 6:Q:50:LYS:HG3    | 2.02                     | 0.59              |
| 6:R:68:THR:CG2    | 1:AJ:294:ARG:CD   | 2.80                     | 0.59              |
| 1:5:277:GLN:HB3   | 1:5:377:MET:HE1   | 1.83                     | 0.59              |
| 1:0:402:LEU:HD12  | 1:0:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:AQ:277:GLN:HB3  | 1:AQ:377:MET:HE1  | 1.83                     | 0.59              |
| 2:B:51:PHE:CZ     | 2:B:55:ILE:HD11   | 2.38                     | 0.59              |
| 4:F:66:ARG:NH2    | 4:F:243:PHE:O     | 2.36                     | 0.59              |
| 1:x:402:LEU:HD12  | 1:x:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:y:277:GLN:HB3   | 1:y:377:MET:HE1   | 1.83                     | 0.59              |
| 1:y:402:LEU:HD12  | 1:y:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:AI:402:LEU:HD12 | 1:AI:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:AO:402:LEU:HD12 | 1:AO:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:UL:126:PHE:CE1  | 1:UL:130:VAL:CG2  | 2.84                     | 0.59              |
| 1:WA:212:LEU:HB3  | 1:WA:221:THR:HG23 | 1.84                     | 0.59              |
| 1:WI:212:LEU:HB3  | 1:WI:221:THR:HG23 | 1.84                     | 0.59              |
| 1:WS:190:GLN:NE2  | 1:WT:216:SER:O    | 2.36                     | 0.59              |
| 2:A:84:LEU:HD13   | 4:G:188:THR:HG21  | 1.84                     | 0.59              |
| 1:AA:402:LEU:HD12 | 1:AA:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:AK:402:LEU:HD12 | 1:AK:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:WK:196:HIS:HB3  | 1:WL:211:THR:CG2  | 2.22                     | 0.59              |
| 5:L:7:ILE:CG2     | 1:AH:278:THR:HG21 | 2.33                     | 0.59              |
| 1:t:402:LEU:HD12  | 1:t:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:u:402:LEU:HD12  | 1:u:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:7:377:MET:SD    | 1:7:377:MET:N     | 2.76                     | 0.59              |
| 1:WK:186:LEU:HD22 | 1:WK:190:GLN:CD   | 2.28                     | 0.59              |
| 1:WK:197:LEU:CD1  | 1:WL:175:SER:OG   | 2.51                     | 0.59              |
| 1:u:377:MET:SD    | 1:u:377:MET:N     | 2.76                     | 0.59              |
| 1:9:377:MET:N     | 1:9:377:MET:SD    | 2.76                     | 0.59              |
| 1:AJ:252:ILE:HD11 | 1:AJ:419:ALA:HB2  | 1.85                     | 0.59              |
| 1:WK:203:ALA:HB1  | 1:WL:160:PRO:HA   | 1.84                     | 0.58              |
| 5:P:11:ILE:HG22   | 1:t:372:ILE:HG21  | 1.85                     | 0.58              |
| 1:w:377:MET:N     | 1:w:377:MET:SD    | 2.76                     | 0.58              |
| 1:w:402:LEU:HD12  | 1:w:403:PRO:HD2   | 1.84                     | 0.58              |
| 1:4:277:GLN:HB3   | 1:4:377:MET:HE1   | 1.83                     | 0.58              |
| 1:AC:252:ILE:HD11 | 1:AC:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AD:377:MET:N    | 1:AD:377:MET:SD   | 2.76                     | 0.58              |
| 1:AF:377:MET:N    | 1:AF:377:MET:SD   | 2.76                     | 0.58              |
| 1:AH:252:ILE:HD11 | 1:AH:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AI:252:ILE:HD11 | 1:AI:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:WJ:164:LEU:CB   | 3:E:145:TRP:NE1   | 2.54                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WS:196:HIS:HB3  | 1:WT:211:THR:HG21 | 1.84                     | 0.58              |
| 1:WT:116:LEU:HD13 | 1:WT:135:ALA:HB2  | 1.85                     | 0.58              |
| 1:5:377:MET:N     | 1:5:377:MET:SD    | 2.76                     | 0.58              |
| 1:AH:377:MET:SD   | 1:AH:377:MET:N    | 2.76                     | 0.58              |
| 1:AQ:377:MET:N    | 1:AQ:377:MET:SD   | 2.76                     | 0.58              |
| 1:WE:128:GLU:HB3  | 1:WF:126:PHE:CD2  | 2.38                     | 0.58              |
| 1:WT:212:LEU:HB3  | 1:WT:221:THR:HG23 | 1.84                     | 0.58              |
| 5:L:7:ILE:HD11    | 1:AI:370:ARG:NE   | 2.17                     | 0.58              |
| 5:L:11:ILE:CG2    | 1:AH:372:ILE:HB   | 2.33                     | 0.58              |
| 6:T:65:LEU:HB2    | 1:7:295:SER:HB2   | 1.84                     | 0.58              |
| 1:z:252:ILE:HD11  | 1:z:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:1:252:ILE:HD11  | 1:1:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:9:305:GLY:HA3   | 1:9:355:PRO:HG2   | 1.86                     | 0.58              |
| 1:AA:377:MET:N    | 1:AA:377:MET:SD   | 2.76                     | 0.58              |
| 1:AB:402:LEU:HD12 | 1:AB:403:PRO:HD2  | 1.84                     | 0.58              |
| 1:AC:377:MET:N    | 1:AC:377:MET:SD   | 2.76                     | 0.58              |
| 1:AD:252:ILE:HD11 | 1:AD:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AE:305:GLY:HA3  | 1:AE:355:PRO:HG2  | 1.86                     | 0.58              |
| 1:AE:402:LEU:HD12 | 1:AE:403:PRO:HD2  | 1.84                     | 0.58              |
| 1:AN:377:MET:N    | 1:AN:377:MET:SD   | 2.76                     | 0.58              |
| 1:AO:252:ILE:HD11 | 1:AO:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AP:377:MET:SD   | 1:AP:377:MET:N    | 2.76                     | 0.58              |
| 1:AQ:402:LEU:HD12 | 1:AQ:403:PRO:HD2  | 1.84                     | 0.58              |
| 1:WK:212:LEU:HB3  | 1:WK:221:THR:HG23 | 1.84                     | 0.58              |
| 6:S:67:LEU:HA     | 6:S:72:HIS:NE2    | 2.18                     | 0.58              |
| 1:t:277:GLN:HB3   | 1:t:377:MET:HE1   | 1.83                     | 0.58              |
| 1:x:252:ILE:HD11  | 1:x:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:3:252:ILE:HD11  | 1:3:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:4:305:GLY:HA3   | 1:4:355:PRO:HG2   | 1.86                     | 0.58              |
| 1:AB:377:MET:SD   | 1:AB:377:MET:N    | 2.76                     | 0.58              |
| 1:AD:305:GLY:HA3  | 1:AD:355:PRO:HG2  | 1.86                     | 0.58              |
| 1:AK:252:ILE:HD11 | 1:AK:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:WA:175:SER:OG   | 1:WW:197:LEU:CD1  | 2.51                     | 0.58              |
| 1:WO:166:VAL:HG22 | 4:F:142:THR:O     | 2.03                     | 0.58              |
| 6:R:66:THR:OG1    | 1:AJ:294:ARG:HG2  | 2.02                     | 0.58              |
| 7:Y:20:ARG:HD2    | 1:i:313:PRO:HG2   | 1.85                     | 0.58              |
| 1:3:377:MET:N     | 1:3:377:MET:SD    | 2.76                     | 0.58              |
| 1:4:252:ILE:HD11  | 1:4:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:5:305:GLY:HA3   | 1:5:355:PRO:HG2   | 1.86                     | 0.58              |
| 1:0:305:GLY:HA3   | 1:0:355:PRO:HG2   | 1.86                     | 0.58              |
| 1:AJ:402:LEU:HD12 | 1:AJ:403:PRO:HD2  | 1.84                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AP:402:LEU:HD12 | 1:AP:403:PRO:HD2  | 1.84                     | 0.58              |
| 1:WA:175:SER:HB2  | 1:WW:200:SER:HG   | 1.69                     | 0.58              |
| 6:Q:127:LEU:O     | 6:Q:131:MET:HG2   | 2.03                     | 0.58              |
| 6:S:42:ASP:OD1    | 6:S:88:ARG:NH2    | 2.36                     | 0.58              |
| 1:v:402:LEU:HD12  | 1:v:403:PRO:HD2   | 1.84                     | 0.58              |
| 1:AB:252:ILE:HD11 | 1:AB:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AE:252:ILE:HD11 | 1:AE:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AN:252:ILE:HD11 | 1:AN:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AO:377:MET:N    | 1:AO:377:MET:SD   | 2.76                     | 0.58              |
| 1:WE:212:LEU:HB3  | 1:WE:221:THR:HG23 | 1.85                     | 0.58              |
| 1:WW:125:GLN:CB   | 2:B:2:THR:HG21    | 2.34                     | 0.58              |
| 2:A:35:ILE:HD11   | 2:A:53:PRO:HB2    | 1.85                     | 0.58              |
| 1:w:252:ILE:HD11  | 1:w:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:y:252:ILE:HD11  | 1:y:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:4:377:MET:SD    | 1:4:377:MET:N     | 2.76                     | 0.58              |
| 1:6:252:ILE:HD11  | 1:6:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:AE:377:MET:SD   | 1:AE:377:MET:N    | 2.76                     | 0.58              |
| 1:AL:377:MET:N    | 1:AL:377:MET:SD   | 2.76                     | 0.58              |
| 1:AP:252:ILE:HD11 | 1:AP:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:WA:201:ALA:C    | 1:WB:158:ALA:HB2  | 2.28                     | 0.58              |
| 1:WU:164:LEU:HA   | 4:G:152:ARG:HG3   | 1.84                     | 0.58              |
| 1:WU:212:LEU:HB3  | 1:WU:221:THR:HG23 | 1.84                     | 0.58              |
| 1:WV:134:ARG:HB3  | 1:WV:134:ARG:HH21 | 1.69                     | 0.58              |
| 2:C:29:LEU:HD22   | 2:D:52:ILE:HG21   | 1.84                     | 0.58              |
| 4:J:82:SER:OG     | 5:N:104:VAL:O     | 2.20                     | 0.58              |
| 5:K:11:ILE:CD1    | 1:AL:276:GLU:OE2  | 2.52                     | 0.58              |
| 5:L:11:ILE:HG22   | 1:AH:372:ILE:CB   | 2.32                     | 0.58              |
| 5:M:7:ILE:CB      | 1:AB:278:THR:HG21 | 2.11                     | 0.58              |
| 1:UJ:167:ARG:CZ   | 1:WB:188:GLU:OE2  | 2.52                     | 0.58              |
| 1:WE:200:SER:O    | 1:WF:158:ALA:CB   | 2.52                     | 0.58              |
| 1:WH:167:ARG:NH2  | 4:J:162:PRO:HG2   | 2.18                     | 0.58              |
| 3:E:187:ALA:O     | 3:E:190:VAL:HG12  | 2.04                     | 0.58              |
| 4:H:83:ALA:HB3    | 4:H:84:PRO:HD3    | 1.85                     | 0.58              |
| 7:V:36:GLY:HA2    | 7:a:51:VAL:HG12   | 1.85                     | 0.58              |
| 7:V:50:GLN:HG3    | 7:V:65:ALA:HB2    | 1.85                     | 0.58              |
| 1:t:377:MET:N     | 1:t:377:MET:SD    | 2.76                     | 0.58              |
| 1:2:252:ILE:HD11  | 1:2:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:5:252:ILE:HD11  | 1:5:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:6:377:MET:N     | 1:6:377:MET:SD    | 2.76                     | 0.58              |
| 1:0:377:MET:N     | 1:0:377:MET:SD    | 2.76                     | 0.58              |
| 1:AA:305:GLY:HA3  | 1:AA:355:PRO:HG2  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AG:252:ILE:HD11 | 1:AG:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:AI:305:GLY:HA3  | 1:AI:355:PRO:HG2  | 1.86                     | 0.58              |
| 1:UP:126:PHE:CE1  | 1:UP:130:VAL:CG2  | 2.84                     | 0.58              |
| 1:WA:213:VAL:CG1  | 1:WW:193:ALA:HB1  | 2.32                     | 0.58              |
| 1:WB:186:LEU:HA   | 1:WB:190:GLN:OE1  | 2.04                     | 0.58              |
| 4:I:146:ASP:OD1   | 4:J:233:GLN:NE2   | 2.37                     | 0.58              |
| 1:7:252:ILE:HD11  | 1:7:419:ALA:HB2   | 1.85                     | 0.58              |
| 1:8:305:GLY:HA3   | 1:8:355:PRO:HG2   | 1.86                     | 0.58              |
| 1:AC:402:LEU:HD12 | 1:AC:403:PRO:HD2  | 1.84                     | 0.58              |
| 1:AJ:305:GLY:HA3  | 1:AJ:355:PRO:HG2  | 1.86                     | 0.58              |
| 1:AJ:377:MET:N    | 1:AJ:377:MET:SD   | 2.76                     | 0.58              |
| 1:AM:252:ILE:HD11 | 1:AM:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:WG:166:VAL:HG12 | 1:WG:168:GLU:HB3  | 1.86                     | 0.57              |
| 3:E:167:ASN:HD21  | 3:E:174:ARG:HH12  | 1.52                     | 0.57              |
| 1:z:377:MET:SD    | 1:z:377:MET:N     | 2.76                     | 0.57              |
| 1:3:305:GLY:HA3   | 1:3:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:6:305:GLY:HA3   | 1:6:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:AF:305:GLY:HA3  | 1:AF:355:PRO:HG2  | 1.86                     | 0.57              |
| 1:WD:168:GLU:OE1  | 1:WD:170:LYS:CE   | 2.51                     | 0.57              |
| 3:E:176:GLY:HA2   | 3:E:179:ILE:HD12  | 1.86                     | 0.57              |
| 5:M:19:MET:HA     | 1:O:276:GLU:OE2   | 2.04                     | 0.57              |
| 1:2:377:MET:N     | 1:2:377:MET:SD    | 2.76                     | 0.57              |
| 1:AD:402:LEU:HD12 | 1:AD:403:PRO:HD2  | 1.84                     | 0.57              |
| 1:AG:377:MET:N    | 1:AG:377:MET:SD   | 2.76                     | 0.57              |
| 1:AK:305:GLY:HA3  | 1:AK:355:PRO:HG2  | 1.85                     | 0.57              |
| 1:WV:212:LEU:HB3  | 1:WV:221:THR:HG23 | 1.84                     | 0.57              |
| 4:G:58:LEU:O      | 4:G:62:THR:OG1    | 2.22                     | 0.57              |
| 6:Q:67:LEU:HD11   | 6:Q:74:PRO:HA     | 1.85                     | 0.57              |
| 1:1:377:MET:N     | 1:1:377:MET:SD    | 2.76                     | 0.57              |
| 1:AC:305:GLY:HA3  | 1:AC:355:PRO:HG2  | 1.86                     | 0.57              |
| 1:UK:207:PRO:HG2  | 1:WE:187:ASP:CG   | 2.29                     | 0.57              |
| 1:UN:208:GLY:HA3  | 1:WR:187:ASP:OD1  | 2.05                     | 0.57              |
| 1:WJ:162:PRO:HA   | 1:WJ:169:GLN:CD   | 2.30                     | 0.57              |
| 1:WS:124:SER:CA   | 2:A:8:MET:HE2     | 2.34                     | 0.57              |
| 5:O:11:ILE:HG22   | 1:z:372:ILE:CB    | 2.34                     | 0.57              |
| 1:j:319:GLN:NE2   | 1:4:355:PRO:HB2   | 2.18                     | 0.57              |
| 1:t:305:GLY:HA3   | 1:t:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:v:252:ILE:HD11  | 1:v:419:ALA:HB2   | 1.85                     | 0.57              |
| 1:y:377:MET:N     | 1:y:377:MET:SD    | 2.76                     | 0.57              |
| 1:8:377:MET:N     | 1:8:377:MET:SD    | 2.76                     | 0.57              |
| 1:AH:305:GLY:HA3  | 1:AH:355:PRO:HG2  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AL:252:ILE:HD11 | 1:AL:419:ALA:HB2  | 1.85                     | 0.57              |
| 1:AQ:305:GLY:HA3  | 1:AQ:355:PRO:HG2  | 1.85                     | 0.57              |
| 1:UJ:126:PHE:CE1  | 1:UJ:130:VAL:CG2  | 2.84                     | 0.57              |
| 1:UL:69:GLN:HE22  | 1:WH:182:PRO:HG2  | 1.69                     | 0.57              |
| 1:WE:166:VAL:HG22 | 4:I:160:GLN:N     | 2.18                     | 0.57              |
| 1:WE:167:ARG:CD   | 4:I:161:GLY:CA    | 2.81                     | 0.57              |
| 1:WG:149:PRO:HG2  | 1:WG:190:GLN:NE2  | 2.19                     | 0.57              |
| 1:WG:197:LEU:HD12 | 1:WH:175:SER:CB   | 2.35                     | 0.57              |
| 1:WK:193:ALA:CB   | 1:WL:213:VAL:CG2  | 2.76                     | 0.57              |
| 1:WT:145:GLU:C    | 1:WT:147:LEU:H    | 2.12                     | 0.57              |
| 1:WV:197:LEU:CD1  | 1:WW:175:SER:OG   | 2.53                     | 0.57              |
| 3:E:170:MET:O     | 3:E:174:ARG:N     | 2.26                     | 0.57              |
| 5:M:4:ILE:HG12    | 1:AC:372:ILE:CB   | 2.34                     | 0.57              |
| 5:P:76:GLN:HG3    | 7:V:123:LYS:HD2   | 1.86                     | 0.57              |
| 6:T:103:ASP:OD1   | 7:Z:112:TYR:OH    | 2.14                     | 0.57              |
| 6:U:42:ASP:OD1    | 6:U:43:ILE:N      | 2.38                     | 0.57              |
| 6:U:72:HIS:HE1    | 1:2:294:ARG:NE    | 2.01                     | 0.57              |
| 1:AK:377:MET:N    | 1:AK:377:MET:SD   | 2.76                     | 0.57              |
| 1:AF:252:ILE:HD11 | 1:AF:419:ALA:HB2  | 1.85                     | 0.57              |
| 1:AP:305:GLY:HA3  | 1:AP:355:PRO:HG2  | 1.86                     | 0.57              |
| 1:WM:197:LEU:CD1  | 1:WN:175:SER:OG   | 2.48                     | 0.57              |
| 4:H:59:LEU:HD11   | 5:M:102:MET:HE1   | 1.87                     | 0.57              |
| 1:u:305:GLY:HA3   | 1:u:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:z:305:GLY:HA3   | 1:z:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:8:252:ILE:HD11  | 1:8:419:ALA:HB2   | 1.85                     | 0.57              |
| 1:AA:252:ILE:HD11 | 1:AA:419:ALA:HB2  | 1.85                     | 0.57              |
| 1:AI:377:MET:N    | 1:AI:377:MET:SD   | 2.76                     | 0.57              |
| 1:UP:126:PHE:O    | 1:UP:130:VAL:HB   | 2.05                     | 0.57              |
| 5:O:11:ILE:CG2    | 1:z:372:ILE:CG2   | 2.83                     | 0.57              |
| 6:S:65:LEU:CD1    | 1:AD:365:ASN:ND2  | 2.67                     | 0.57              |
| 1:t:252:ILE:HD11  | 1:t:419:ALA:HB2   | 1.85                     | 0.57              |
| 1:u:252:ILE:HD11  | 1:u:419:ALA:HB2   | 1.85                     | 0.57              |
| 1:v:305:GLY:HA3   | 1:v:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:v:377:MET:N     | 1:v:377:MET:SD    | 2.76                     | 0.57              |
| 1:AG:305:GLY:HA3  | 1:AG:355:PRO:HG2  | 1.86                     | 0.57              |
| 1:WC:196:HIS:HB3  | 1:WD:211:THR:HG21 | 1.87                     | 0.57              |
| 1:WQ:196:HIS:CD2  | 1:WR:219:LEU:HD22 | 2.40                     | 0.57              |
| 5:L:11:ILE:HG21   | 1:AH:372:ILE:HB   | 1.87                     | 0.57              |
| 1:w:305:GLY:HA3   | 1:w:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:y:305:GLY:HA3   | 1:y:355:PRO:HG2   | 1.86                     | 0.57              |
| 1:UK:207:PRO:HG2  | 1:WE:187:ASP:OD2  | 2.05                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:WG:197:LEU:HA   | 1:WH:175:SER:OG  | 2.05                     | 0.57              |
| 1:WO:200:SER:O    | 1:WP:158:ALA:HB2 | 2.04                     | 0.57              |
| 1:WQ:145:GLU:C    | 1:WQ:147:LEU:H   | 2.13                     | 0.57              |
| 1:WU:200:SER:O    | 1:WV:158:ALA:CB  | 2.52                     | 0.57              |
| 6:R:65:LEU:HD22   | 1:AJ:295:SER:HB2 | 1.86                     | 0.57              |
| 1:AB:305:GLY:HA3  | 1:AB:355:PRO:HG2 | 1.86                     | 0.57              |
| 1:AM:377:MET:N    | 1:AM:377:MET:SD  | 2.76                     | 0.57              |
| 1:AO:305:GLY:HA3  | 1:AO:355:PRO:HG2 | 1.86                     | 0.57              |
| 1:AQ:252:ILE:HD11 | 1:AQ:419:ALA:HB2 | 1.85                     | 0.57              |
| 1:UJ:126:PHE:O    | 1:UJ:130:VAL:HB  | 2.05                     | 0.56              |
| 1:UL:73:MET:HE3   | 1:UL:99:ARG:HD3  | 1.81                     | 0.56              |
| 1:UO:126:PHE:O    | 1:UO:130:VAL:HB  | 2.05                     | 0.56              |
| 1:WE:167:ARG:HD3  | 4:I:161:GLY:CA   | 2.27                     | 0.56              |
| 1:WK:170:LYS:O    | 1:WK:171:SER:C   | 2.47                     | 0.56              |
| 1:WK:187:ASP:OD1  | 1:WK:187:ASP:N   | 2.38                     | 0.56              |
| 1:WQ:124:SER:O    | 1:WQ:127:SER:N   | 2.37                     | 0.56              |
| 1:WS:145:GLU:C    | 1:WS:147:LEU:H   | 2.12                     | 0.56              |
| 1:WV:160:PRO:HB2  | 1:WV:170:LYS:HB2 | 1.87                     | 0.56              |
| 3:E:149:LEU:O     | 3:E:153:THR:HG23 | 2.05                     | 0.56              |
| 7:W:94:PRO:HB2    | 7:W:96:VAL:HG23  | 1.86                     | 0.56              |
| 1:7:305:GLY:HA3   | 1:7:355:PRO:HG2  | 1.86                     | 0.56              |
| 1:UI:126:PHE:O    | 1:UI:130:VAL:HB  | 2.05                     | 0.56              |
| 2:B:9:MET:HA      | 2:B:12:GLU:OE1   | 2.05                     | 0.56              |
| 5:L:8:GLU:O       | 5:L:11:ILE:HG13  | 2.05                     | 0.56              |
| 5:O:8:GLU:O       | 5:O:11:ILE:HG13  | 2.06                     | 0.56              |
| 1:9:252:ILE:HD11  | 1:9:419:ALA:HB2  | 1.85                     | 0.56              |
| 1:AN:305:GLY:HA3  | 1:AN:355:PRO:HG2 | 1.86                     | 0.56              |
| 1:UN:51:TYR:OH    | 1:UN:76:PRO:HB2  | 2.05                     | 0.56              |
| 1:UN:126:PHE:O    | 1:UN:130:VAL:HB  | 2.05                     | 0.56              |
| 1:WA:121:PHE:HB3  | 2:C:68:TRP:CD1   | 2.40                     | 0.56              |
| 1:WB:187:ASP:CG   | 1:WB:190:GLN:HG3 | 2.30                     | 0.56              |
| 1:WI:164:LEU:HD13 | 4:J:148:ALA:HB1  | 1.88                     | 0.56              |
| 5:P:8:GLU:O       | 5:P:11:ILE:HG13  | 2.06                     | 0.56              |
| 6:R:114:LEU:HD21  | 7:X:126:MET:SD   | 2.45                     | 0.56              |
| 1:x:305:GLY:HA3   | 1:x:355:PRO:HG2  | 1.86                     | 0.56              |
| 1:1:305:GLY:HA3   | 1:1:355:PRO:HG2  | 1.86                     | 0.56              |
| 1:UJ:103:GLN:CD   | 1:WD:182:PRO:HB3 | 2.28                     | 0.56              |
| 1:WA:213:VAL:HG21 | 1:WW:193:ALA:HB1 | 1.86                     | 0.56              |
| 1:WC:170:LYS:H    | 1:WC:170:LYS:HD2 | 1.69                     | 0.56              |
| 1:WM:201:ALA:C    | 1:WN:158:ALA:HB2 | 2.30                     | 0.56              |
| 1:WN:203:ALA:HB2  | 1:WO:160:PRO:HA  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WU:197:LEU:HD12 | 1:WV:175:SER:HB3  | 1.87                     | 0.56              |
| 5:K:8:GLU:O       | 5:K:11:ILE:HG13   | 2.05                     | 0.56              |
| 1:2:305:GLY:HA3   | 1:2:355:PRO:HG2   | 1.86                     | 0.56              |
| 1:0:252:ILE:HD11  | 1:0:419:ALA:HB2   | 1.85                     | 0.56              |
| 1:AL:305:GLY:HA3  | 1:AL:355:PRO:HG2  | 1.86                     | 0.56              |
| 1:UM:51:TYR:OH    | 1:UM:76:PRO:HB2   | 2.06                     | 0.56              |
| 1:WD:118:GLN:O    | 1:WD:119:GLU:C    | 2.49                     | 0.56              |
| 1:WI:170:LYS:O    | 1:WI:171:SER:OG   | 2.21                     | 0.56              |
| 2:C:4:GLU:C       | 2:C:6:VAL:H       | 2.13                     | 0.56              |
| 2:D:25:LEU:HD23   | 4:J:206:ALA:HB2   | 1.86                     | 0.56              |
| 5:L:11:ILE:HG22   | 1:AH:372:ILE:CG1  | 2.32                     | 0.56              |
| 6:Q:23:GLN:HE22   | 7:V:125:MET:HE1   | 1.69                     | 0.56              |
| 1:UI:51:TYR:OH    | 1:UI:76:PRO:HB2   | 2.05                     | 0.56              |
| 1:UJ:55:PHE:HB2   | 1:UJ:58:LEU:HD11  | 1.88                     | 0.56              |
| 1:WR:123:ILE:HB   | 1:WR:127:SER:OG   | 2.06                     | 0.56              |
| 3:E:205:ASN:HD21  | 4:F:211:MET:HB2   | 1.71                     | 0.56              |
| 1:UP:51:TYR:OH    | 1:UP:76:PRO:HB2   | 2.06                     | 0.56              |
| 1:UP:55:PHE:HB2   | 1:UP:58:LEU:HD11  | 1.88                     | 0.56              |
| 1:WA:216:SER:O    | 1:WW:190:GLN:NE2  | 2.39                     | 0.56              |
| 1:WB:143:THR:OG1  | 1:WC:154:ARG:HG2  | 2.06                     | 0.56              |
| 1:WU:200:SER:O    | 1:WV:158:ALA:HB2  | 2.06                     | 0.56              |
| 4:H:66:ARG:HG3    | 4:H:182:ALA:HB2   | 1.87                     | 0.56              |
| 7:W:72:ALA:O      | 7:W:95:ASN:ND2    | 2.38                     | 0.56              |
| 1:AM:305:GLY:HA3  | 1:AM:355:PRO:HG2  | 1.86                     | 0.56              |
| 1:UL:216:SER:C    | 1:UL:218:HIS:H    | 2.14                     | 0.56              |
| 1:UO:51:TYR:OH    | 1:UO:76:PRO:HB2   | 2.05                     | 0.56              |
| 1:WJ:200:SER:O    | 1:WK:158:ALA:CB   | 2.54                     | 0.56              |
| 1:WL:190:GLN:NE2  | 1:WM:216:SER:O    | 2.39                     | 0.56              |
| 1:WM:190:GLN:HG3  | 1:WN:217:GLY:HA3  | 1.88                     | 0.56              |
| 1:WT:187:ASP:OD1  | 1:WT:190:GLN:N    | 2.39                     | 0.56              |
| 3:E:93:ALA:HB2    | 4:F:88:VAL:HG21   | 1.87                     | 0.56              |
| 1:UI:55:PHE:HB2   | 1:UI:58:LEU:HD11  | 1.88                     | 0.56              |
| 1:UM:126:PHE:O    | 1:UM:130:VAL:HB   | 2.05                     | 0.56              |
| 1:UO:55:PHE:HB2   | 1:UO:58:LEU:HD11  | 1.88                     | 0.56              |
| 1:WI:145:GLU:C    | 1:WI:147:LEU:H    | 2.13                     | 0.56              |
| 5:K:14:LEU:CB     | 1:AL:278:THR:HG21 | 2.35                     | 0.56              |
| 5:N:14:LEU:HD11   | 1:6:370:ARG:HH21  | 1.71                     | 0.56              |
| 5:O:7:ILE:HG22    | 1:z:278:THR:HG21  | 1.78                     | 0.56              |
| 1:UL:126:PHE:O    | 1:UL:130:VAL:HB   | 2.05                     | 0.55              |
| 1:UO:102:GLN:HG2  | 1:UO:193:ALA:HB2  | 1.88                     | 0.55              |
| 1:UP:102:GLN:HG2  | 1:UP:193:ALA:HB2  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WB:197:LEU:HD12 | 1:WC:175:SER:HB3  | 1.87                     | 0.55              |
| 1:WJ:139:GLU:HB3  | 1:WK:154:ARG:HH21 | 1.70                     | 0.55              |
| 1:WP:145:GLU:C    | 1:WP:147:LEU:H    | 2.14                     | 0.55              |
| 1:UJ:126:PHE:CD1  | 1:UJ:130:VAL:CG2  | 2.90                     | 0.55              |
| 1:UL:126:PHE:CD1  | 1:UL:130:VAL:CG2  | 2.90                     | 0.55              |
| 1:WA:156:HIS:HD2  | 1:WW:197:LEU:HD11 | 1.71                     | 0.55              |
| 1:WD:143:THR:OG1  | 1:WE:154:ARG:HG2  | 2.06                     | 0.55              |
| 1:WG:190:GLN:NE2  | 1:WH:216:SER:O    | 2.39                     | 0.55              |
| 1:WJ:190:GLN:HG2  | 1:WK:216:SER:O    | 2.07                     | 0.55              |
| 4:H:58:LEU:O      | 4:H:62:THR:OG1    | 2.23                     | 0.55              |
| 4:J:75:ARG:NH1    | 4:J:86:ASN:OD1    | 2.36                     | 0.55              |
| 5:L:87:GLN:O      | 5:L:91:LYS:HG2    | 2.06                     | 0.55              |
| 6:Q:42:ASP:HB3    | 1:d:316:LEU:HD21  | 1.88                     | 0.55              |
| 6:Q:73:ILE:HG13   | 1:t:295:SER:HB2   | 1.88                     | 0.55              |
| 1:8:264:ALA:HB2   | 1:8:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:UN:55:PHE:HB2   | 1:UN:58:LEU:HD11  | 1.88                     | 0.55              |
| 1:WL:197:LEU:CD1  | 1:WM:175:SER:CB   | 2.72                     | 0.55              |
| 1:WO:128:GLU:HG2  | 1:WP:126:PHE:CD2  | 2.40                     | 0.55              |
| 1:WO:166:VAL:CG2  | 4:F:139:LEU:O     | 2.50                     | 0.55              |
| 3:E:166:SER:C     | 3:E:168:ALA:N     | 2.64                     | 0.55              |
| 5:M:12:SER:O      | 5:M:15:GLN:HG3    | 2.06                     | 0.55              |
| 1:v:264:ALA:HB2   | 1:v:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:UI:102:GLN:HG2  | 1:UI:193:ALA:HB2  | 1.89                     | 0.55              |
| 1:UN:126:PHE:CE1  | 1:UN:130:VAL:CG2  | 2.84                     | 0.55              |
| 1:WR:197:LEU:HA   | 1:WS:175:SER:OG   | 2.07                     | 0.55              |
| 1:WS:172:PRO:HD2  | 1:WS:204:GLY:O    | 2.07                     | 0.55              |
| 4:F:38:TRP:HB2    | 5:L:46:SER:OG     | 2.06                     | 0.55              |
| 5:P:89:ARG:NH2    | 5:P:90:ASN:OD1    | 2.39                     | 0.55              |
| 1:j:319:GLN:NE2   | 1:4:355:PRO:CB    | 2.69                     | 0.55              |
| 1:AQ:264:ALA:HB2  | 1:AQ:389:VAL:HG13 | 1.89                     | 0.55              |
| 1:WO:165:PHE:HE1  | 4:F:143:ARG:HH11  | 1.54                     | 0.55              |
| 1:WV:128:GLU:HG3  | 1:WW:126:PHE:CE2  | 2.42                     | 0.55              |
| 5:N:21:ALA:HB1    | 1:4:278:THR:CG2   | 2.35                     | 0.55              |
| 1:x:377:MET:N     | 1:x:377:MET:SD    | 2.76                     | 0.55              |
| 1:UI:211:THR:HG23 | 1:UI:219:LEU:HD11 | 1.89                     | 0.55              |
| 1:UK:51:TYR:OH    | 1:UK:76:PRO:HB2   | 2.05                     | 0.55              |
| 1:UM:102:GLN:HG2  | 1:UM:193:ALA:HB2  | 1.89                     | 0.55              |
| 1:WM:197:LEU:HD11 | 1:WN:156:HIS:HD2  | 1.71                     | 0.55              |
| 1:WP:123:ILE:CG2  | 2:A:67:PRO:HB3    | 2.35                     | 0.55              |
| 3:E:233:MET:O     | 3:E:236:ILE:HG12  | 2.06                     | 0.55              |
| 4:J:230:ASP:OD2   | 4:J:230:ASP:N     | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:11:ILE:HG21   | 1:AH:372:ILE:HG22 | 1.82                     | 0.55              |
| 1:u:264:ALA:HB2   | 1:u:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:y:264:ALA:HB2   | 1:y:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:5:264:ALA:HB2   | 1:5:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:AA:264:ALA:HB2  | 1:AA:389:VAL:HG13 | 1.89                     | 0.55              |
| 1:UJ:51:TYR:OH    | 1:UJ:76:PRO:HB2   | 2.06                     | 0.55              |
| 1:UK:126:PHE:O    | 1:UK:130:VAL:HB   | 2.05                     | 0.55              |
| 1:UM:211:THR:HG23 | 1:UM:219:LEU:HD11 | 1.89                     | 0.55              |
| 1:UN:102:GLN:HG2  | 1:UN:193:ALA:HB2  | 1.88                     | 0.55              |
| 1:UO:211:THR:HG23 | 1:UO:219:LEU:HD11 | 1.89                     | 0.55              |
| 1:WD:145:GLU:C    | 1:WD:147:LEU:H    | 2.15                     | 0.55              |
| 5:N:8:GLU:O       | 5:N:11:ILE:HG13   | 2.05                     | 0.55              |
| 1:u:409:MET:HE2   | 1:u:409:MET:HA    | 1.89                     | 0.55              |
| 1:v:409:MET:HE2   | 1:v:409:MET:HA    | 1.89                     | 0.55              |
| 1:x:409:MET:HE2   | 1:x:409:MET:HA    | 1.89                     | 0.55              |
| 1:y:409:MET:HE2   | 1:y:409:MET:HA    | 1.89                     | 0.55              |
| 1:6:264:ALA:HB2   | 1:6:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:AM:409:MET:HE2  | 1:AM:409:MET:HA   | 1.89                     | 0.55              |
| 1:UI:126:PHE:CD1  | 1:UI:130:VAL:CG2  | 2.90                     | 0.55              |
| 1:UJ:102:GLN:HG2  | 1:UJ:193:ALA:HB2  | 1.88                     | 0.55              |
| 1:UN:126:PHE:CD1  | 1:UN:130:VAL:CG2  | 2.90                     | 0.55              |
| 1:WP:197:LEU:HD12 | 1:WQ:175:SER:HB3  | 1.89                     | 0.55              |
| 1:WP:197:LEU:HA   | 1:WQ:175:SER:OG   | 2.07                     | 0.55              |
| 7:Z:17:GLN:NE2    | 7:Z:111:SER:OG    | 2.39                     | 0.55              |
| 1:w:409:MET:HA    | 1:w:409:MET:HE2   | 1.89                     | 0.55              |
| 1:x:264:ALA:HB2   | 1:x:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:2:264:ALA:HB2   | 1:2:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:AL:409:MET:HE2  | 1:AL:409:MET:HA   | 1.89                     | 0.55              |
| 1:UK:126:PHE:CD1  | 1:UK:130:VAL:CG2  | 2.90                     | 0.55              |
| 4:J:80:THR:HB     | 4:J:83:ALA:HB2    | 1.88                     | 0.55              |
| 5:O:59:PHE:CD2    | 6:T:118:MET:HE2   | 2.42                     | 0.55              |
| 7:Z:3:LEU:HB3     | 7:Z:126:MET:HE3   | 1.88                     | 0.55              |
| 1:t:409:MET:HA    | 1:t:409:MET:HE2   | 1.89                     | 0.55              |
| 1:AN:264:ALA:HB2  | 1:AN:389:VAL:HG13 | 1.89                     | 0.55              |
| 1:AN:409:MET:HE2  | 1:AN:409:MET:HA   | 1.89                     | 0.55              |
| 1:AO:409:MET:HE2  | 1:AO:409:MET:HA   | 1.89                     | 0.55              |
| 1:AP:264:ALA:HB2  | 1:AP:389:VAL:HG13 | 1.89                     | 0.55              |
| 1:AP:409:MET:HE2  | 1:AP:409:MET:HA   | 1.89                     | 0.55              |
| 1:UP:211:THR:HG23 | 1:UP:219:LEU:HD11 | 1.89                     | 0.55              |
| 1:WB:193:ALA:HB1  | 1:WC:213:VAL:CG1  | 2.36                     | 0.55              |
| 1:WC:121:PHE:CZ   | 2:C:15:LYS:HE3    | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WF:200:SER:O    | 1:WG:158:ALA:CB   | 2.55                     | 0.55              |
| 1:WP:165:PHE:CB   | 4:F:160:GLN:O     | 2.54                     | 0.55              |
| 1:WQ:172:PRO:HD2  | 1:WQ:204:GLY:O    | 2.07                     | 0.55              |
| 1:9:264:ALA:HB2   | 1:9:389:VAL:HG13  | 1.89                     | 0.55              |
| 1:AK:409:MET:HE2  | 1:AK:409:MET:HA   | 1.89                     | 0.55              |
| 1:UP:103:GLN:CB   | 1:WW:182:PRO:HB3  | 2.33                     | 0.54              |
| 1:WA:193:ALA:HB1  | 1:WB:213:VAL:HG11 | 1.89                     | 0.54              |
| 1:WT:190:GLN:NE2  | 1:WU:216:SER:O    | 2.39                     | 0.54              |
| 3:E:166:SER:O     | 3:E:167:ASN:C     | 2.49                     | 0.54              |
| 5:K:72:MET:O      | 5:K:76:GLN:HG2    | 2.06                     | 0.54              |
| 1:UL:51:TYR:OH    | 1:UL:76:PRO:HB2   | 2.05                     | 0.54              |
| 1:UL:102:GLN:HG2  | 1:UL:193:ALA:HB2  | 1.88                     | 0.54              |
| 1:UN:211:THR:HG23 | 1:UN:219:LEU:HD11 | 1.89                     | 0.54              |
| 1:WA:200:SER:O    | 1:WB:158:ALA:HB2  | 2.08                     | 0.54              |
| 1:WM:200:SER:HG   | 1:WN:175:SER:HB2  | 1.68                     | 0.54              |
| 1:WO:197:LEU:HA   | 1:WP:175:SER:OG   | 2.07                     | 0.54              |
| 4:F:37:SER:HA     | 4:F:123:MET:HE2   | 1.89                     | 0.54              |
| 1:z:409:MET:HE2   | 1:z:409:MET:HA    | 1.89                     | 0.54              |
| 1:7:409:MET:HE2   | 1:7:409:MET:HA    | 1.89                     | 0.54              |
| 1:AQ:409:MET:HE2  | 1:AQ:409:MET:HA   | 1.89                     | 0.54              |
| 1:UP:126:PHE:CD1  | 1:UP:130:VAL:CG2  | 2.90                     | 0.54              |
| 1:WH:186:LEU:HD22 | 1:WH:190:GLN:CD   | 2.32                     | 0.54              |
| 1:WS:145:GLU:O    | 1:WS:147:LEU:N    | 2.39                     | 0.54              |
| 1:WU:130:VAL:O    | 1:WU:134:ARG:HG3  | 2.07                     | 0.54              |
| 5:N:21:ALA:CB     | 1:4:278:THR:CG2   | 2.74                     | 0.54              |
| 6:R:90:PRO:HB3    | 6:R:99:THR:HB     | 1.88                     | 0.54              |
| 7:V:113:GLN:O     | 7:V:117:GLU:HG2   | 2.07                     | 0.54              |
| 1:1:264:ALA:HB2   | 1:1:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:1:409:MET:HA    | 1:1:409:MET:HE2   | 1.89                     | 0.54              |
| 1:3:264:ALA:HB2   | 1:3:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:0:264:ALA:HB2   | 1:0:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:AJ:409:MET:HA   | 1:AJ:409:MET:HE2  | 1.89                     | 0.54              |
| 1:UK:102:GLN:HG2  | 1:UK:193:ALA:HB2  | 1.88                     | 0.54              |
| 1:UL:55:PHE:HB2   | 1:UL:58:LEU:HD11  | 1.88                     | 0.54              |
| 1:UL:211:THR:HG23 | 1:UL:219:LEU:HD11 | 1.89                     | 0.54              |
| 1:WH:167:ARG:HH22 | 4:J:162:PRO:HG3   | 1.72                     | 0.54              |
| 1:WK:171:SER:HB3  | 1:WK:206:PRO:HG3  | 1.89                     | 0.54              |
| 1:WV:128:GLU:HG3  | 1:WW:126:PHE:CD2  | 2.43                     | 0.54              |
| 4:F:83:ALA:HB3    | 4:F:84:PRO:HD3    | 1.89                     | 0.54              |
| 5:O:77:LYS:HE3    | 6:U:13:GLN:HE22   | 1.73                     | 0.54              |
| 1:9:409:MET:HA    | 1:9:409:MET:HE2   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:409:MET:HE2  | 1:AB:409:MET:HA   | 1.89                     | 0.54              |
| 1:UK:55:PHE:HB2   | 1:UK:58:LEU:HD11  | 1.88                     | 0.54              |
| 1:UK:98:LEU:CD1   | 1:UK:146:THR:HG1  | 2.20                     | 0.54              |
| 1:UM:55:PHE:HB2   | 1:UM:58:LEU:HD11  | 1.88                     | 0.54              |
| 6:S:36:PRO:HB3    | 6:S:96:ASP:HB2    | 1.89                     | 0.54              |
| 1:4:264:ALA:HB2   | 1:4:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:7:264:ALA:HB2   | 1:7:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:WM:193:ALA:CB   | 1:WN:213:VAL:HG11 | 2.27                     | 0.54              |
| 1:WV:113:PHE:O    | 1:WV:116:LEU:HB3  | 2.07                     | 0.54              |
| 2:B:36:SER:HB3    | 2:C:44:ILE:HG23   | 1.89                     | 0.54              |
| 1:z:264:ALA:HB2   | 1:z:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:AD:409:MET:HA   | 1:AD:409:MET:HE2  | 1.89                     | 0.54              |
| 1:AI:409:MET:HE2  | 1:AI:409:MET:HA   | 1.89                     | 0.54              |
| 1:UJ:260:THR:HG23 | 1:UJ:268:LEU:HD11 | 1.89                     | 0.54              |
| 1:UK:211:THR:HG23 | 1:UK:219:LEU:HD11 | 1.89                     | 0.54              |
| 1:UM:103:GLN:NE2  | 1:WQ:182:PRO:CB   | 2.71                     | 0.54              |
| 1:UM:126:PHE:CD1  | 1:UM:130:VAL:CG2  | 2.90                     | 0.54              |
| 1:WS:186:LEU:HA   | 1:WS:190:GLN:OE1  | 2.08                     | 0.54              |
| 2:C:54:LYS:HZ3    | 2:D:48:THR:HG21   | 1.72                     | 0.54              |
| 3:E:38:ILE:HB     | 3:E:43:LYS:HE2    | 1.90                     | 0.54              |
| 3:E:236:ILE:O     | 3:E:240:CYS:N     | 2.36                     | 0.54              |
| 5:N:11:ILE:HG22   | 1:6:372:ILE:HB    | 1.88                     | 0.54              |
| 5:O:77:LYS:HE3    | 6:U:13:GLN:NE2    | 2.23                     | 0.54              |
| 1:t:264:ALA:HB2   | 1:t:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:w:264:ALA:HB2   | 1:w:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:2:409:MET:HE2   | 1:2:409:MET:HA    | 1.89                     | 0.54              |
| 1:0:409:MET:HE2   | 1:0:409:MET:HA    | 1.89                     | 0.54              |
| 1:AC:264:ALA:HB2  | 1:AC:389:VAL:HG13 | 1.89                     | 0.54              |
| 1:AD:264:ALA:HB2  | 1:AD:389:VAL:HG13 | 1.89                     | 0.54              |
| 1:UL:88:VAL:HB    | 1:UL:89:PRO:HD2   | 1.90                     | 0.54              |
| 1:WI:145:GLU:O    | 1:WI:147:LEU:N    | 2.41                     | 0.54              |
| 1:WS:118:GLN:O    | 1:WS:119:GLU:C    | 2.49                     | 0.54              |
| 1:WT:166:VAL:HG21 | 4:G:158:PRO:CB    | 2.38                     | 0.54              |
| 1:WU:114:GLU:O    | 1:WU:117:ASP:N    | 2.41                     | 0.54              |
| 2:D:51:PHE:HB3    | 4:I:205:MET:HE3   | 1.90                     | 0.54              |
| 1:f:319:GLN:CB    | 1:AG:303:GLN:HE22 | 2.18                     | 0.54              |
| 1:AF:282:TYR:HB3  | 1:AG:292:THR:HG21 | 1.90                     | 0.54              |
| 1:AK:264:ALA:HB2  | 1:AK:389:VAL:HG13 | 1.89                     | 0.54              |
| 1:UK:88:VAL:HB    | 1:UK:89:PRO:HD2   | 1.90                     | 0.54              |
| 1:UL:167:ARG:O    | 1:UL:168:GLU:C    | 2.49                     | 0.54              |
| 1:WE:196:HIS:HB3  | 1:WF:211:THR:HG21 | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WN:145:GLU:C    | 1:WN:147:LEU:H    | 2.15                     | 0.54              |
| 1:WT:145:GLU:O    | 1:WT:147:LEU:N    | 2.40                     | 0.54              |
| 4:F:126:ALA:O     | 4:F:127:LEU:C     | 2.48                     | 0.54              |
| 1:AD:282:TYR:HB3  | 1:AE:292:THR:HG21 | 1.90                     | 0.54              |
| 1:AE:282:TYR:HB3  | 1:AF:292:THR:HG21 | 1.90                     | 0.54              |
| 1:AH:409:MET:HE2  | 1:AH:409:MET:HA   | 1.89                     | 0.54              |
| 1:AO:264:ALA:HB2  | 1:AO:389:VAL:HG13 | 1.89                     | 0.54              |
| 1:WF:193:ALA:HB1  | 1:WG:213:VAL:CG1  | 2.38                     | 0.54              |
| 1:WF:212:LEU:HB3  | 1:WF:221:THR:HG23 | 1.90                     | 0.54              |
| 1:WK:196:HIS:CG   | 1:WL:211:THR:HG21 | 2.42                     | 0.54              |
| 1:WQ:124:SER:O    | 1:WQ:125:GLN:C    | 2.50                     | 0.54              |
| 5:N:76:GLN:NE2    | 7:Y:132:LEU:O     | 2.41                     | 0.54              |
| 1:AF:264:ALA:HB2  | 1:AF:389:VAL:HG13 | 1.89                     | 0.54              |
| 1:WD:186:LEU:HD22 | 1:WD:190:GLN:CD   | 2.32                     | 0.53              |
| 5:N:7:ILE:CG2     | 1:6:278:THR:CG2   | 2.80                     | 0.53              |
| 5:P:4:ILE:HD11    | 1:u:374:HIS:HB2   | 1.90                     | 0.53              |
| 6:S:65:LEU:HD13   | 1:AD:365:ASN:ND2  | 2.23                     | 0.53              |
| 7:a:85:ALA:HB1    | 7:a:89:GLY:HA2    | 1.89                     | 0.53              |
| 1:AB:282:TYR:HB3  | 1:AC:292:THR:HG21 | 1.90                     | 0.53              |
| 1:AC:282:TYR:HB3  | 1:AD:292:THR:HG21 | 1.90                     | 0.53              |
| 1:AG:282:TYR:HB3  | 1:AH:292:THR:HG21 | 1.90                     | 0.53              |
| 1:AG:409:MET:HA   | 1:AG:409:MET:HE2  | 1.89                     | 0.53              |
| 1:AI:264:ALA:HB2  | 1:AI:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:UN:80:ALA:HB3   | 1:UN:83:SER:HB3   | 1.91                     | 0.53              |
| 1:WP:145:GLU:HG2  | 1:WP:152:SER:HA   | 1.91                     | 0.53              |
| 1:WU:196:HIS:HB3  | 1:WV:211:THR:HG21 | 1.89                     | 0.53              |
| 3:E:186:LEU:HD21  | 3:E:236:ILE:HG22  | 1.90                     | 0.53              |
| 3:E:188:LEU:O     | 3:E:190:VAL:N     | 2.39                     | 0.53              |
| 4:I:139:LEU:HG    | 4:I:170:LEU:HD21  | 1.90                     | 0.53              |
| 6:U:103:ASP:OD1   | 7:a:112:TYR:OH    | 2.26                     | 0.53              |
| 1:v:282:TYR:HB3   | 1:w:292:THR:HG21  | 1.90                     | 0.53              |
| 1:x:282:TYR:HB3   | 1:y:292:THR:HG21  | 1.90                     | 0.53              |
| 1:3:409:MET:HE2   | 1:3:409:MET:HA    | 1.89                     | 0.53              |
| 1:AB:264:ALA:HB2  | 1:AB:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:AH:264:ALA:HB2  | 1:AH:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:AM:264:ALA:HB2  | 1:AM:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:WE:200:SER:O    | 1:WF:158:ALA:HB2  | 2.09                     | 0.53              |
| 1:WS:145:GLU:HG2  | 1:WS:152:SER:HA   | 1.91                     | 0.53              |
| 1:WT:145:GLU:HG2  | 1:WT:152:SER:HA   | 1.91                     | 0.53              |
| 4:F:211:MET:SD    | 4:G:211:MET:HE3   | 2.49                     | 0.53              |
| 1:AA:409:MET:HE2  | 1:AA:409:MET:HA   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AE:409:MET:HE2  | 1:AE:409:MET:HA   | 1.89                     | 0.53              |
| 1:AL:264:ALA:HB2  | 1:AL:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:UP:80:ALA:HB3   | 1:UP:83:SER:HB3   | 1.91                     | 0.53              |
| 1:WA:166:VAL:HG11 | 4:H:160:GLN:HE22  | 1.74                     | 0.53              |
| 1:WD:200:SER:OG   | 1:WE:175:SER:CB   | 2.47                     | 0.53              |
| 1:WI:164:LEU:HD22 | 4:J:148:ALA:CA    | 2.39                     | 0.53              |
| 1:WJ:190:GLN:NE2  | 1:WK:216:SER:O    | 2.41                     | 0.53              |
| 1:WU:145:GLU:HG2  | 1:WU:152:SER:HA   | 1.91                     | 0.53              |
| 2:D:42:THR:HG22   | 2:D:44:ILE:HG12   | 1.91                     | 0.53              |
| 4:I:163:GLU:N     | 4:I:163:GLU:OE2   | 2.39                     | 0.53              |
| 6:R:65:LEU:HB3    | 1:AJ:295:SER:HB2  | 1.90                     | 0.53              |
| 1:z:282:TYR:HB3   | 1:1:292:THR:HG21  | 1.90                     | 0.53              |
| 1:1:282:TYR:HB3   | 1:2:292:THR:HG21  | 1.90                     | 0.53              |
| 1:AA:282:TYR:HB3  | 1:AB:292:THR:HG21 | 1.90                     | 0.53              |
| 1:AG:264:ALA:HB2  | 1:AG:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:AH:282:TYR:HB3  | 1:AI:292:THR:HG21 | 1.90                     | 0.53              |
| 1:UO:126:PHE:CD1  | 1:UO:130:VAL:CG2  | 2.90                     | 0.53              |
| 1:UP:88:VAL:HB    | 1:UP:89:PRO:HD2   | 1.90                     | 0.53              |
| 1:WD:168:GLU:CD   | 1:WD:170:LYS:NZ   | 2.67                     | 0.53              |
| 1:WO:145:GLU:HG2  | 1:WO:152:SER:HA   | 1.91                     | 0.53              |
| 1:WQ:145:GLU:HG2  | 1:WQ:152:SER:HA   | 1.91                     | 0.53              |
| 4:F:75:ARG:HD2    | 4:F:84:PRO:HD2    | 1.89                     | 0.53              |
| 4:I:59:LEU:HD11   | 5:N:102:MET:HE1   | 1.90                     | 0.53              |
| 5:M:4:ILE:HG12    | 1:AC:372:ILE:CG2  | 2.37                     | 0.53              |
| 1:t:292:THR:HG21  | 1:AQ:282:TYR:HB3  | 1.90                     | 0.53              |
| 1:u:282:TYR:HB3   | 1:v:292:THR:HG21  | 1.90                     | 0.53              |
| 1:3:282:TYR:HB3   | 1:4:292:THR:HG21  | 1.90                     | 0.53              |
| 1:4:409:MET:HE2   | 1:4:409:MET:HA    | 1.89                     | 0.53              |
| 1:UN:88:VAL:HB    | 1:UN:89:PRO:HD2   | 1.90                     | 0.53              |
| 1:UO:80:ALA:HB3   | 1:UO:83:SER:HB3   | 1.91                     | 0.53              |
| 1:WO:149:PRO:HB3  | 1:WO:184:ARG:HB3  | 1.90                     | 0.53              |
| 1:WV:145:GLU:HG2  | 1:WV:152:SER:HA   | 1.91                     | 0.53              |
| 2:D:9:MET:HE1     | 4:J:188:THR:HA    | 1.90                     | 0.53              |
| 1:0:282:TYR:HB3   | 1:AA:292:THR:HG21 | 1.90                     | 0.53              |
| 1:AF:409:MET:HE2  | 1:AF:409:MET:HA   | 1.89                     | 0.53              |
| 1:AI:282:TYR:HB3  | 1:AJ:292:THR:HG21 | 1.90                     | 0.53              |
| 1:AJ:264:ALA:HB2  | 1:AJ:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:UI:159:MET:N    | 1:UI:159:MET:SD   | 2.82                     | 0.53              |
| 1:UL:80:ALA:HB3   | 1:UL:83:SER:HB3   | 1.91                     | 0.53              |
| 1:WQ:212:LEU:HB3  | 1:WQ:221:THR:HG23 | 1.90                     | 0.53              |
| 1:WR:145:GLU:HG2  | 1:WR:152:SER:HA   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WW:145:GLU:HG2  | 1:WW:152:SER:HA   | 1.90                     | 0.53              |
| 2:B:77:VAL:HG21   | 4:H:225:LEU:HD11  | 1.91                     | 0.53              |
| 4:F:207:LEU:HD23  | 4:F:209:MET:HE1   | 1.91                     | 0.53              |
| 5:M:11:ILE:HG21   | 1:AB:372:ILE:HG22 | 1.91                     | 0.53              |
| 5:O:10:VAL:HG12   | 1:z:372:ILE:CD1   | 2.39                     | 0.53              |
| 1:5:409:MET:HE2   | 1:5:409:MET:HA    | 1.89                     | 0.53              |
| 1:AJ:282:TYR:HB3  | 1:AK:292:THR:HG21 | 1.90                     | 0.53              |
| 1:UK:80:ALA:HB3   | 1:UK:83:SER:HB3   | 1.91                     | 0.53              |
| 1:UM:80:ALA:HB3   | 1:UM:83:SER:HB3   | 1.91                     | 0.53              |
| 1:WK:163:SER:O    | 3:E:252:ALA:CB    | 2.57                     | 0.53              |
| 1:WU:160:PRO:HG2  | 1:WU:170:LYS:O    | 2.08                     | 0.53              |
| 1:WV:193:ALA:HB1  | 1:WW:213:VAL:HG11 | 1.91                     | 0.53              |
| 2:B:62:ILE:O      | 2:B:66:GLY:N      | 2.39                     | 0.53              |
| 3:E:54:ILE:HD11   | 4:J:153:LEU:HB3   | 1.91                     | 0.53              |
| 3:E:101:PHE:CE2   | 4:F:223:LEU:HD11  | 2.43                     | 0.53              |
| 3:E:127:ARG:O     | 3:E:131:MET:HE3   | 2.08                     | 0.53              |
| 5:N:11:ILE:CG2    | 1:6:372:ILE:CG2   | 2.87                     | 0.53              |
| 6:Q:50:LYS:O      | 6:Q:54:VAL:HG22   | 2.09                     | 0.53              |
| 1:1:293:LEU:HD21  | 1:1:364:SER:HB3   | 1.91                     | 0.53              |
| 1:3:293:LEU:HD21  | 1:3:364:SER:HB3   | 1.91                     | 0.53              |
| 1:8:409:MET:HE2   | 1:8:409:MET:HA    | 1.89                     | 0.53              |
| 1:9:282:TYR:HB3   | 1:0:292:THR:HG21  | 1.90                     | 0.53              |
| 1:0:293:LEU:HD21  | 1:0:364:SER:HB3   | 1.91                     | 0.53              |
| 1:AE:264:ALA:HB2  | 1:AE:389:VAL:HG13 | 1.89                     | 0.53              |
| 1:AK:282:TYR:HB3  | 1:AL:292:THR:HG21 | 1.90                     | 0.53              |
| 7:W:23:VAL:HG21   | 7:W:47:VAL:HG13   | 1.91                     | 0.53              |
| 7:Z:57:GLN:O      | 7:Z:59:THR:N      | 2.40                     | 0.53              |
| 1:z:293:LEU:HD21  | 1:z:364:SER:HB3   | 1.91                     | 0.53              |
| 1:6:409:MET:HA    | 1:6:409:MET:HE2   | 1.89                     | 0.53              |
| 1:AC:409:MET:HE2  | 1:AC:409:MET:HA   | 1.89                     | 0.53              |
| 1:UK:127:SER:O    | 1:UK:131:ASN:CG   | 2.52                     | 0.53              |
| 1:UL:127:SER:O    | 1:UL:131:ASN:CG   | 2.52                     | 0.53              |
| 1:UN:127:SER:O    | 1:UN:131:ASN:CG   | 2.52                     | 0.53              |
| 1:UO:159:MET:N    | 1:UO:159:MET:SD   | 2.82                     | 0.53              |
| 1:WO:200:SER:O    | 1:WP:158:ALA:CB   | 2.56                     | 0.53              |
| 5:O:7:ILE:HG22    | 1:z:278:THR:CG2   | 2.32                     | 0.53              |
| 1:y:282:TYR:HB3   | 1:z:292:THR:HG21  | 1.90                     | 0.53              |
| 1:8:293:LEU:HD21  | 1:8:364:SER:HB3   | 1.91                     | 0.53              |
| 1:AA:293:LEU:HD21 | 1:AA:364:SER:HB3  | 1.91                     | 0.53              |
| 1:AC:293:LEU:HD21 | 1:AC:364:SER:HB3  | 1.91                     | 0.53              |
| 1:UJ:88:VAL:HB    | 1:UJ:89:PRO:HD2   | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WB:145:GLU:HG2  | 1:WB:152:SER:HA   | 1.91                     | 0.52              |
| 1:WN:145:GLU:HG2  | 1:WN:152:SER:HA   | 1.90                     | 0.52              |
| 4:H:194:LEU:HD11  | 4:I:217:ILE:HA    | 1.91                     | 0.52              |
| 4:I:180:LYS:O     | 4:I:184:GLN:HG3   | 2.09                     | 0.52              |
| 7:Y:10:ALA:HB3    | 7:Y:119:LEU:HD13  | 1.89                     | 0.52              |
| 1:5:293:LEU:HD21  | 1:5:364:SER:HB3   | 1.91                     | 0.52              |
| 1:AE:293:LEU:HD21 | 1:AE:364:SER:HB3  | 1.91                     | 0.52              |
| 1:UJ:127:SER:O    | 1:UJ:131:ASN:CG   | 2.52                     | 0.52              |
| 1:UM:88:VAL:HB    | 1:UM:89:PRO:HD2   | 1.90                     | 0.52              |
| 1:WA:145:GLU:HG2  | 1:WA:152:SER:HA   | 1.90                     | 0.52              |
| 1:WD:145:GLU:HG2  | 1:WD:152:SER:HA   | 1.91                     | 0.52              |
| 1:WG:165:PHE:CE1  | 4:J:240:ALA:CB    | 2.89                     | 0.52              |
| 1:WR:111:VAL:HB   | 1:WR:114:GLU:HB3  | 1.92                     | 0.52              |
| 3:E:188:LEU:HB3   | 3:E:189:PRO:HD2   | 1.91                     | 0.52              |
| 4:H:232:TRP:O     | 4:H:236:MET:HG3   | 2.10                     | 0.52              |
| 4:J:41:SER:HB3    | 6:U:133:VAL:HG21  | 1.91                     | 0.52              |
| 5:P:76:GLN:NE2    | 7:V:123:LYS:HB2   | 2.24                     | 0.52              |
| 1:y:293:LEU:HD21  | 1:y:364:SER:HB3   | 1.91                     | 0.52              |
| 1:4:293:LEU:HD21  | 1:4:364:SER:HB3   | 1.91                     | 0.52              |
| 1:6:282:TYR:HB3   | 1:7:292:THR:HG21  | 1.90                     | 0.52              |
| 1:6:293:LEU:HD21  | 1:6:364:SER:HB3   | 1.91                     | 0.52              |
| 1:AB:293:LEU:HD21 | 1:AB:364:SER:HB3  | 1.92                     | 0.52              |
| 1:AL:282:TYR:HB3  | 1:AM:292:THR:HG21 | 1.90                     | 0.52              |
| 1:UO:127:SER:O    | 1:UO:131:ASN:CG   | 2.52                     | 0.52              |
| 1:WB:164:LEU:O    | 4:H:152:ARG:CD    | 2.54                     | 0.52              |
| 1:WJ:125:GLN:HB2  | 3:E:242:HIS:HB2   | 1.92                     | 0.52              |
| 1:WP:163:SER:C    | 1:WP:165:PHE:H    | 2.17                     | 0.52              |
| 1:WT:124:SER:CB   | 2:A:4:GLU:OE2     | 2.57                     | 0.52              |
| 4:G:205:MET:HE3   | 4:H:209:MET:HA    | 1.91                     | 0.52              |
| 4:I:116:PHE:O     | 6:T:4:ARG:NH2     | 2.42                     | 0.52              |
| 7:V:80:PRO:HB3    | 7:V:89:GLY:HA3    | 1.90                     | 0.52              |
| 1:w:282:TYR:HB3   | 1:x:292:THR:HG21  | 1.90                     | 0.52              |
| 1:x:293:LEU:HD21  | 1:x:364:SER:HB3   | 1.91                     | 0.52              |
| 1:2:282:TYR:HB3   | 1:3:292:THR:HG21  | 1.90                     | 0.52              |
| 1:2:293:LEU:HD21  | 1:2:364:SER:HB3   | 1.91                     | 0.52              |
| 1:5:282:TYR:HB3   | 1:6:292:THR:HG21  | 1.90                     | 0.52              |
| 1:AD:293:LEU:HD21 | 1:AD:364:SER:HB3  | 1.91                     | 0.52              |
| 1:AM:282:TYR:HB3  | 1:AN:292:THR:HG21 | 1.90                     | 0.52              |
| 1:UM:159:MET:N    | 1:UM:159:MET:SD   | 2.82                     | 0.52              |
| 1:WJ:141:ALA:O    | 1:WJ:145:GLU:HG3  | 2.09                     | 0.52              |
| 1:WP:145:GLU:O    | 1:WP:147:LEU:N    | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WQ:168:GLU:O    | 1:WQ:169:GLN:C    | 2.52                     | 0.52              |
| 1:WV:142:ARG:O    | 1:WV:146:THR:HG23 | 2.10                     | 0.52              |
| 1:WV:164:LEU:HD23 | 4:G:152:ARG:HH12  | 1.75                     | 0.52              |
| 4:F:149:LEU:HD22  | 4:G:233:GLN:HG3   | 1.92                     | 0.52              |
| 4:J:52:THR:OG1    | 5:O:91:LYS:NZ     | 2.32                     | 0.52              |
| 5:O:73:ALA:HB1    | 6:U:13:GLN:HE21   | 1.74                     | 0.52              |
| 6:T:72:HIS:HD2    | 1:7:365:ASN:CG    | 2.16                     | 0.52              |
| 1:u:235:LEU:HB3   | 1:v:244:ARG:HH22  | 1.75                     | 0.52              |
| 1:4:282:TYR:HB3   | 1:5:292:THR:HG21  | 1.90                     | 0.52              |
| 1:8:282:TYR:HB3   | 1:9:292:THR:HG21  | 1.90                     | 0.52              |
| 1:AG:293:LEU:HD21 | 1:AG:364:SER:HB3  | 1.91                     | 0.52              |
| 1:UO:88:VAL:HB    | 1:UO:89:PRO:HD2   | 1.90                     | 0.52              |
| 1:UP:127:SER:O    | 1:UP:131:ASN:CG   | 2.52                     | 0.52              |
| 1:WF:116:LEU:HD21 | 1:WF:134:ARG:CZ   | 2.38                     | 0.52              |
| 1:WI:145:GLU:HG2  | 1:WI:152:SER:HA   | 1.91                     | 0.52              |
| 1:WK:145:GLU:HG2  | 1:WK:152:SER:HA   | 1.90                     | 0.52              |
| 5:N:7:ILE:HG21    | 1:6:278:THR:HG22  | 1.91                     | 0.52              |
| 1:t:282:TYR:HB3   | 1:u:292:THR:HG21  | 1.90                     | 0.52              |
| 1:7:293:LEU:HD21  | 1:7:364:SER:HB3   | 1.92                     | 0.52              |
| 1:9:293:LEU:HD21  | 1:9:364:SER:HB3   | 1.91                     | 0.52              |
| 1:UJ:159:MET:N    | 1:UJ:159:MET:SD   | 2.82                     | 0.52              |
| 1:UK:207:PRO:CG   | 1:WE:187:ASP:OD2  | 2.57                     | 0.52              |
| 1:WP:200:SER:O    | 1:WQ:158:ALA:HB3  | 2.09                     | 0.52              |
| 7:V:131:THR:O     | 7:V:131:THR:HG22  | 2.09                     | 0.52              |
| 1:1:235:LEU:HB3   | 1:2:244:ARG:HH22  | 1.75                     | 0.52              |
| 1:AF:293:LEU:HD21 | 1:AF:364:SER:HB3  | 1.91                     | 0.52              |
| 1:AO:282:TYR:HB3  | 1:AP:292:THR:HG21 | 1.90                     | 0.52              |
| 1:UI:80:ALA:HB3   | 1:UI:83:SER:HB3   | 1.91                     | 0.52              |
| 1:WD:142:ARG:O    | 1:WD:146:THR:HG23 | 2.10                     | 0.52              |
| 1:WU:186:LEU:HA   | 1:WU:190:GLN:OE1  | 2.10                     | 0.52              |
| 2:B:3:PRO:O       | 2:B:7:MET:HG2     | 2.09                     | 0.52              |
| 7:Y:20:ARG:NH2    | 7:Y:107:SER:HB2   | 2.24                     | 0.52              |
| 1:w:293:LEU:HD21  | 1:w:364:SER:HB3   | 1.91                     | 0.52              |
| 1:AM:235:LEU:HB3  | 1:AN:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:UJ:80:ALA:HB3   | 1:UJ:83:SER:HB3   | 1.91                     | 0.52              |
| 1:UK:159:MET:N    | 1:UK:159:MET:SD   | 2.82                     | 0.52              |
| 1:WK:162:PRO:CB   | 3:E:249:ASN:HB2   | 2.35                     | 0.52              |
| 1:WL:145:GLU:HG2  | 1:WL:152:SER:HA   | 1.91                     | 0.52              |
| 1:WQ:145:GLU:O    | 1:WQ:147:LEU:N    | 2.43                     | 0.52              |
| 1:WU:113:PHE:HB3  | 1:WV:134:ARG:CZ   | 2.39                     | 0.52              |
| 2:D:35:ILE:HG21   | 2:D:50:SER:HA     | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:77:VAL:HG11   | 4:J:229:VAL:HG21  | 1.90                     | 0.52              |
| 4:F:199:VAL:O     | 4:F:203:VAL:HG23  | 2.10                     | 0.52              |
| 5:O:48:ARG:NH1    | 6:U:3:ASP:OD2     | 2.43                     | 0.52              |
| 1:4:235:LEU:HB3   | 1:5:244:ARG:HH22  | 1.75                     | 0.52              |
| 1:AH:235:LEU:HB3  | 1:AI:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:UI:88:VAL:HB    | 1:UI:89:PRO:HD2   | 1.90                     | 0.52              |
| 1:WF:125:GLN:O    | 1:WF:128:GLU:N    | 2.43                     | 0.52              |
| 1:WV:186:LEU:HA   | 1:WV:190:GLN:OE1  | 2.10                     | 0.52              |
| 6:S:46:ALA:O      | 6:S:50:LYS:HG3    | 2.09                     | 0.52              |
| 1:v:293:LEU:HD21  | 1:v:364:SER:HB3   | 1.91                     | 0.52              |
| 1:x:235:LEU:HB3   | 1:y:244:ARG:HH22  | 1.75                     | 0.52              |
| 1:AN:282:TYR:HB3  | 1:AO:292:THR:HG21 | 1.90                     | 0.52              |
| 1:AP:282:TYR:HB3  | 1:AQ:292:THR:HG21 | 1.90                     | 0.52              |
| 1:WD:149:PRO:CG   | 1:WD:190:GLN:HE22 | 2.23                     | 0.52              |
| 1:WD:168:GLU:OE1  | 1:WD:170:LYS:NZ   | 2.42                     | 0.52              |
| 1:WD:197:LEU:HA   | 1:WE:175:SER:CB   | 2.40                     | 0.52              |
| 1:WM:132:TYR:CD1  | 1:WN:130:VAL:HG22 | 2.45                     | 0.52              |
| 1:WN:200:SER:HB2  | 1:WO:173:SER:HB2  | 1.92                     | 0.52              |
| 1:WS:190:GLN:HG2  | 1:WT:217:GLY:HA3  | 1.91                     | 0.52              |
| 1:WW:118:GLN:O    | 1:WW:119:GLU:C    | 2.49                     | 0.52              |
| 4:G:74:LEU:HD22   | 4:G:235:LEU:HD22  | 1.91                     | 0.52              |
| 4:H:80:THR:O      | 4:H:80:THR:OG1    | 2.26                     | 0.52              |
| 4:I:73:LEU:HD13   | 4:I:186:GLY:HA3   | 1.92                     | 0.52              |
| 1:j:325:GLU:OE1   | 1:j:325:GLU:N     | 2.43                     | 0.52              |
| 1:v:235:LEU:HB3   | 1:w:244:ARG:HH22  | 1.75                     | 0.52              |
| 1:y:235:LEU:HB3   | 1:z:244:ARG:HH22  | 1.75                     | 0.52              |
| 1:AE:235:LEU:HB3  | 1:AF:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:AJ:235:LEU:HB3  | 1:AK:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:AL:235:LEU:HB3  | 1:AM:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:AO:235:LEU:HB3  | 1:AP:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:AP:235:LEU:HB3  | 1:AQ:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:UM:127:SER:O    | 1:UM:131:ASN:CG   | 2.52                     | 0.51              |
| 1:WG:145:GLU:HG2  | 1:WG:152:SER:HA   | 1.91                     | 0.51              |
| 1:WT:160:PRO:HD3  | 1:WT:172:PRO:CA   | 2.38                     | 0.51              |
| 1:WT:161:LYS:HB3  | 1:WT:162:PRO:HD2  | 1.91                     | 0.51              |
| 2:A:65:ALA:O      | 2:A:69:MET:HG3    | 2.09                     | 0.51              |
| 4:G:83:ALA:HB1    | 4:G:84:PRO:HD2    | 1.92                     | 0.51              |
| 6:R:67:LEU:HG     | 6:R:72:HIS:HB3    | 1.92                     | 0.51              |
| 1:7:282:TYR:HB3   | 1:8:292:THR:HG21  | 1.90                     | 0.51              |
| 1:AH:293:LEU:HD21 | 1:AH:364:SER:HB3  | 1.91                     | 0.51              |
| 1:AI:293:LEU:HD21 | 1:AI:364:SER:HB3  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UI:127:SER:O    | 1:UI:131:ASN:CG   | 2.52                     | 0.51              |
| 1:WF:197:LEU:HA   | 1:WG:175:SER:OG   | 2.10                     | 0.51              |
| 1:WH:145:GLU:HG2  | 1:WH:152:SER:HA   | 1.91                     | 0.51              |
| 1:WP:166:VAL:HA   | 1:WP:169:GLN:HB2  | 1.91                     | 0.51              |
| 1:WQ:125:GLN:O    | 1:WQ:128:GLU:N    | 2.43                     | 0.51              |
| 3:E:227:MET:SD    | 3:E:228:LEU:N     | 2.82                     | 0.51              |
| 7:Z:23:VAL:HG21   | 7:Z:47:VAL:HG13   | 1.91                     | 0.51              |
| 7:a:72:ALA:HB3    | 7:a:95:ASN:HD22   | 1.74                     | 0.51              |
| 1:t:235:LEU:HB3   | 1:u:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:2:235:LEU:HB3   | 1:3:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:AC:235:LEU:HB3  | 1:AD:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:AK:235:LEU:HB3  | 1:AL:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:UL:98:LEU:CD1   | 1:UL:146:THR:HG1  | 2.23                     | 0.51              |
| 1:WC:145:GLU:HG2  | 1:WC:152:SER:HA   | 1.91                     | 0.51              |
| 1:WC:197:LEU:HA   | 1:WD:175:SER:OG   | 2.11                     | 0.51              |
| 1:WF:125:GLN:O    | 1:WF:126:PHE:C    | 2.53                     | 0.51              |
| 1:WM:145:GLU:HG2  | 1:WM:152:SER:HA   | 1.91                     | 0.51              |
| 1:WR:165:PHE:C    | 1:WR:167:ARG:H    | 2.18                     | 0.51              |
| 1:WR:190:GLN:NE2  | 1:WS:216:SER:O    | 2.43                     | 0.51              |
| 1:WS:165:PHE:HE1  | 2:A:89:GLY:C      | 2.17                     | 0.51              |
| 6:Q:29:ASN:ND2    | 6:Q:41:ARG:O      | 2.36                     | 0.51              |
| 1:5:256:ILE:HG13  | 1:5:257:VAL:N     | 2.26                     | 0.51              |
| 1:0:235:LEU:HB3   | 1:AA:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:AO:293:LEU:HD21 | 1:AO:364:SER:HB3  | 1.91                     | 0.51              |
| 1:UP:204:GLY:O    | 1:UP:206:PRO:HD3  | 2.11                     | 0.51              |
| 1:WC:197:LEU:CD1  | 1:WD:175:SER:OG   | 2.58                     | 0.51              |
| 1:WJ:128:GLU:HG3  | 1:WK:126:PHE:CD2  | 2.43                     | 0.51              |
| 2:D:78:ARG:HG3    | 4:J:234:LEU:HD11  | 1.91                     | 0.51              |
| 4:F:67:ILE:H      | 4:F:67:ILE:HD12   | 1.75                     | 0.51              |
| 6:Q:62:GLY:HA2    | 6:Q:79:SER:HB3    | 1.91                     | 0.51              |
| 6:R:68:THR:HG21   | 1:AJ:294:ARG:HD2  | 1.92                     | 0.51              |
| 7:W:7:PHE:HZ      | 7:W:123:LYS:HB2   | 1.76                     | 0.51              |
| 7:Z:28:LEU:HD21   | 7:Z:101:GLU:HB2   | 1.91                     | 0.51              |
| 1:u:293:LEU:HD21  | 1:u:364:SER:HB3   | 1.91                     | 0.51              |
| 1:3:235:LEU:HB3   | 1:4:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:6:235:LEU:HB3   | 1:7:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:7:235:LEU:HB3   | 1:8:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:UO:204:GLY:O    | 1:UO:206:PRO:HD3  | 2.11                     | 0.51              |
| 1:WA:132:TYR:HB2  | 1:WB:126:PHE:HZ   | 1.76                     | 0.51              |
| 1:WQ:125:GLN:O    | 1:WQ:126:PHE:C    | 2.53                     | 0.51              |
| 2:B:59:PHE:HZ     | 4:G:198:LEU:HD21  | 1.75                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:4:GLU:C       | 2:C:6:VAL:N       | 2.67                     | 0.51              |
| 3:E:130:ASP:O     | 3:E:134:MET:HG2   | 2.10                     | 0.51              |
| 4:H:42:VAL:HG13   | 5:N:42:LEU:HD22   | 1.93                     | 0.51              |
| 5:M:8:GLU:O       | 5:M:11:ILE:HG13   | 2.09                     | 0.51              |
| 5:O:53:ARG:O      | 5:O:57:GLU:HG2    | 2.11                     | 0.51              |
| 6:U:65:LEU:CB     | 1:1:295:SER:HB2   | 2.39                     | 0.51              |
| 1:7:256:ILE:HG13  | 1:7:257:VAL:N     | 2.26                     | 0.51              |
| 1:AG:235:LEU:HB3  | 1:AH:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:AJ:256:ILE:HG13 | 1:AJ:257:VAL:N    | 2.26                     | 0.51              |
| 1:UJ:253:GLY:O    | 1:UJ:255:PRO:HD3  | 2.11                     | 0.51              |
| 1:UL:159:MET:SD   | 1:UL:159:MET:N    | 2.82                     | 0.51              |
| 1:WK:200:SER:CA   | 1:WL:173:SER:OG   | 2.59                     | 0.51              |
| 1:WN:203:ALA:HB1  | 1:WO:160:PRO:HB3  | 1.93                     | 0.51              |
| 2:D:17:ALA:HB2    | 4:J:195:ILE:HG23  | 1.92                     | 0.51              |
| 6:S:67:LEU:HA     | 6:S:72:HIS:HE2    | 1.74                     | 0.51              |
| 1:9:235:LEU:HB3   | 1:0:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:9:256:ILE:HG13  | 1:9:257:VAL:N     | 2.26                     | 0.51              |
| 1:AB:235:LEU:HB3  | 1:AC:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:AL:293:LEU:HD21 | 1:AL:364:SER:HB3  | 1.91                     | 0.51              |
| 5:L:7:ILE:CD1     | 1:AI:370:ARG:HE   | 2.24                     | 0.51              |
| 1:t:293:LEU:HD21  | 1:t:364:SER:HB3   | 1.91                     | 0.51              |
| 1:w:235:LEU:HB3   | 1:x:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:AH:256:ILE:HG13 | 1:AH:257:VAL:N    | 2.26                     | 0.51              |
| 1:AL:256:ILE:HG13 | 1:AL:257:VAL:N    | 2.26                     | 0.51              |
| 1:AM:256:ILE:HG13 | 1:AM:257:VAL:N    | 2.26                     | 0.51              |
| 1:UI:98:LEU:HD22  | 1:UI:147:LEU:CD2  | 2.39                     | 0.51              |
| 1:UN:204:GLY:O    | 1:UN:206:PRO:HD3  | 2.11                     | 0.51              |
| 1:WF:116:LEU:CD2  | 1:WF:134:ARG:HD3  | 2.41                     | 0.51              |
| 1:WR:115:LEU:HD22 | 1:WR:134:ARG:HH11 | 1.75                     | 0.51              |
| 3:E:88:MET:HG2    | 3:E:146:LEU:HD11  | 1.93                     | 0.51              |
| 4:F:135:ARG:NH2   | 4:F:165:VAL:O     | 2.44                     | 0.51              |
| 4:I:75:ARG:NH1    | 4:I:86:ASN:OD1    | 2.36                     | 0.51              |
| 1:8:256:ILE:HG13  | 1:8:257:VAL:N     | 2.26                     | 0.51              |
| 1:AF:235:LEU:HB3  | 1:AG:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:AJ:293:LEU:HD21 | 1:AJ:364:SER:HB3  | 1.91                     | 0.51              |
| 1:AK:293:LEU:HD21 | 1:AK:364:SER:HB3  | 1.91                     | 0.51              |
| 1:AN:293:LEU:HD21 | 1:AN:364:SER:HB3  | 1.92                     | 0.51              |
| 1:AQ:293:LEU:HD21 | 1:AQ:364:SER:HB3  | 1.91                     | 0.51              |
| 1:UI:204:GLY:O    | 1:UI:206:PRO:HD3  | 2.11                     | 0.51              |
| 1:WP:128:GLU:CG   | 1:WQ:126:PHE:CE2  | 2.93                     | 0.51              |
| 1:WQ:147:LEU:O    | 1:WQ:148:GLY:C    | 2.54                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2:THR:HG23    | 2:D:5:SER:H       | 1.76                     | 0.51              |
| 3:E:86:PHE:CZ     | 4:F:91:GLY:HA3    | 2.45                     | 0.51              |
| 4:G:193:PHE:HB3   | 4:G:222:LYS:HD3   | 1.92                     | 0.51              |
| 6:U:92:GLN:HE21   | 7:a:19:LYS:HG2    | 1.76                     | 0.51              |
| 1:2:256:ILE:HG13  | 1:2:257:VAL:N     | 2.26                     | 0.51              |
| 1:3:256:ILE:HG13  | 1:3:257:VAL:N     | 2.26                     | 0.51              |
| 1:AF:256:ILE:HG13 | 1:AF:257:VAL:N    | 2.26                     | 0.51              |
| 1:AO:256:ILE:HG13 | 1:AO:257:VAL:N    | 2.26                     | 0.51              |
| 1:UM:204:GLY:O    | 1:UM:206:PRO:HD3  | 2.11                     | 0.51              |
| 1:UO:98:LEU:HD22  | 1:UO:147:LEU:CD2  | 2.39                     | 0.51              |
| 1:WB:190:GLN:NE2  | 1:WC:216:SER:O    | 2.44                     | 0.51              |
| 1:WI:193:ALA:HB1  | 1:WJ:213:VAL:HG21 | 1.93                     | 0.51              |
| 2:B:10:GLY:O      | 2:B:14:MET:HE2    | 2.11                     | 0.51              |
| 1:t:244:ARG:HH22  | 1:AQ:235:LEU:HB3  | 1.75                     | 0.51              |
| 1:4:256:ILE:HG13  | 1:4:257:VAL:N     | 2.26                     | 0.51              |
| 1:UO:98:LEU:CD1   | 1:UO:146:THR:HG1  | 2.24                     | 0.50              |
| 1:WQ:190:GLN:HG2  | 1:WR:216:SER:O    | 2.11                     | 0.50              |
| 2:D:58:VAL:O      | 2:D:62:ILE:HD12   | 2.11                     | 0.50              |
| 1:t:256:ILE:HG13  | 1:t:257:VAL:N     | 2.26                     | 0.50              |
| 1:AM:293:LEU:HD21 | 1:AM:364:SER:HB3  | 1.91                     | 0.50              |
| 1:AP:256:ILE:HG13 | 1:AP:257:VAL:N    | 2.26                     | 0.50              |
| 1:UL:204:GLY:O    | 1:UL:206:PRO:HD3  | 2.11                     | 0.50              |
| 1:WG:200:SER:OG   | 1:WH:175:SER:CB   | 2.45                     | 0.50              |
| 1:WJ:139:GLU:HB3  | 1:WK:156:HIS:HE1  | 1.76                     | 0.50              |
| 1:WK:160:PRO:HB3  | 1:WK:170:LYS:HB2  | 1.94                     | 0.50              |
| 2:D:2:THR:OG1     | 2:D:4:GLU:OE1     | 2.29                     | 0.50              |
| 3:E:205:ASN:ND2   | 4:F:211:MET:HB2   | 2.25                     | 0.50              |
| 4:H:65:THR:O      | 4:H:68:ILE:HG22   | 2.12                     | 0.50              |
| 5:O:84:MET:O      | 5:O:88:VAL:HG23   | 2.11                     | 0.50              |
| 7:Z:56:GLY:HA3    | 1:1:303:GLN:HE22  | 1.76                     | 0.50              |
| 1:5:235:LEU:HB3   | 1:6:244:ARG:HH22  | 1.75                     | 0.50              |
| 1:AD:256:ILE:HG13 | 1:AD:257:VAL:N    | 2.26                     | 0.50              |
| 1:AI:256:ILE:HG13 | 1:AI:257:VAL:N    | 2.26                     | 0.50              |
| 1:WE:167:ARG:HH21 | 4:I:162:PRO:HD2   | 1.75                     | 0.50              |
| 1:WF:116:LEU:HD21 | 1:WF:134:ARG:HD3  | 1.93                     | 0.50              |
| 1:WM:145:GLU:O    | 1:WM:146:THR:C    | 2.54                     | 0.50              |
| 4:I:119:GLN:HG3   | 6:T:4:ARG:HE      | 1.76                     | 0.50              |
| 4:I:161:GLY:C     | 4:I:163:GLU:N     | 2.69                     | 0.50              |
| 5:N:11:ILE:HG22   | 1:6:372:ILE:CB    | 2.40                     | 0.50              |
| 1:AA:235:LEU:HB3  | 1:AB:244:ARG:HH22 | 1.75                     | 0.50              |
| 1:AN:235:LEU:HB3  | 1:AO:244:ARG:HH22 | 1.75                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AP:293:LEU:HD21 | 1:AP:364:SER:HB3  | 1.92                     | 0.50              |
| 1:UK:204:GLY:O    | 1:UK:206:PRO:HD3  | 2.11                     | 0.50              |
| 1:WT:162:PRO:O    | 1:WT:163:SER:HB3  | 2.11                     | 0.50              |
| 1:WV:120:LYS:HZ3  | 1:WV:123:ILE:CD1  | 2.13                     | 0.50              |
| 2:D:2:THR:O       | 2:D:5:SER:OG      | 2.24                     | 0.50              |
| 4:I:204:LEU:HD11  | 4:I:217:ILE:HD12  | 1.93                     | 0.50              |
| 1:6:256:ILE:HG13  | 1:6:257:VAL:N     | 2.26                     | 0.50              |
| 1:AI:235:LEU:HB3  | 1:AJ:244:ARG:HH22 | 1.75                     | 0.50              |
| 1:UK:98:LEU:HD22  | 1:UK:147:LEU:CD2  | 2.39                     | 0.50              |
| 1:UO:162:PRO:O    | 1:UO:163:SER:C    | 2.55                     | 0.50              |
| 1:UP:162:PRO:O    | 1:UP:163:SER:C    | 2.55                     | 0.50              |
| 1:WG:115:LEU:HG   | 1:WG:116:LEU:N    | 2.25                     | 0.50              |
| 1:WH:200:SER:HG   | 1:WI:175:SER:HB2  | 1.74                     | 0.50              |
| 1:WV:196:HIS:HB3  | 1:WW:211:THR:HG21 | 1.93                     | 0.50              |
| 3:E:106:MET:HE1   | 3:E:226:ILE:HG13  | 1.93                     | 0.50              |
| 7:W:54:ALA:HB3    | 7:W:55:PRO:HD3    | 1.93                     | 0.50              |
| 1:AB:256:ILE:HG13 | 1:AB:257:VAL:N    | 2.26                     | 0.50              |
| 1:AD:235:LEU:HB3  | 1:AE:244:ARG:HH22 | 1.75                     | 0.50              |
| 1:WD:197:LEU:CD1  | 1:WE:175:SER:OG   | 2.59                     | 0.50              |
| 1:WT:166:VAL:HG21 | 4:G:158:PRO:HB2   | 1.93                     | 0.50              |
| 1:WU:114:GLU:O    | 1:WU:115:LEU:C    | 2.54                     | 0.50              |
| 1:WW:145:GLU:C    | 1:WW:147:LEU:H    | 2.19                     | 0.50              |
| 4:G:180:LYS:NZ    | 4:H:230:ASP:OD1   | 2.27                     | 0.50              |
| 5:K:86:ILE:HG12   | 5:P:102:MET:HE2   | 1.93                     | 0.50              |
| 5:N:57:GLU:HG2    | 6:S:11:PHE:CE2    | 2.47                     | 0.50              |
| 7:Y:10:ALA:O      | 7:Y:14:LEU:HG     | 2.12                     | 0.50              |
| 1:y:256:ILE:HG13  | 1:y:257:VAL:N     | 2.26                     | 0.50              |
| 1:z:235:LEU:HB3   | 1:1:244:ARG:HH22  | 1.75                     | 0.50              |
| 1:AA:256:ILE:HG13 | 1:AA:257:VAL:N    | 2.26                     | 0.50              |
| 1:UI:162:PRO:O    | 1:UI:163:SER:C    | 2.55                     | 0.50              |
| 1:WA:112:GLY:O    | 1:WA:115:LEU:HB3  | 2.12                     | 0.50              |
| 1:WC:181:GLU:O    | 1:WC:182:PRO:C    | 2.54                     | 0.50              |
| 1:WP:165:PHE:HA   | 4:F:160:GLN:O     | 2.12                     | 0.50              |
| 3:E:229:MET:O     | 3:E:233:MET:HG2   | 2.12                     | 0.50              |
| 4:F:143:ARG:HH21  | 4:F:180:LYS:HB3   | 1.77                     | 0.50              |
| 4:F:224:MET:O     | 4:F:228:LEU:HB2   | 2.11                     | 0.50              |
| 5:P:11:ILE:HG22   | 1:t:372:ILE:CG2   | 2.41                     | 0.50              |
| 6:T:123:LEU:HD23  | 7:Y:132:LEU:HD11  | 1.92                     | 0.50              |
| 1:w:256:ILE:HG13  | 1:w:257:VAL:N     | 2.26                     | 0.50              |
| 1:UK:162:PRO:O    | 1:UK:163:SER:C    | 2.55                     | 0.50              |
| 1:UL:162:PRO:O    | 1:UL:163:SER:C    | 2.55                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UN:98:LEU:CD1   | 1:UN:146:THR:HG1  | 2.25                     | 0.50              |
| 1:WC:143:THR:OG1  | 1:WD:154:ARG:HG2  | 2.12                     | 0.50              |
| 4:G:75:ARG:NH2    | 4:G:84:PRO:O      | 2.44                     | 0.50              |
| 4:G:86:ASN:HD21   | 5:L:103:GLN:HA    | 1.77                     | 0.50              |
| 1:z:256:ILE:HG13  | 1:z:257:VAL:N     | 2.26                     | 0.50              |
| 1:UP:159:MET:SD   | 1:UP:159:MET:N    | 2.82                     | 0.50              |
| 1:WQ:163:SER:HB3  | 1:WQ:166:VAL:HG23 | 1.94                     | 0.50              |
| 1:WS:166:VAL:HG22 | 4:G:144:GLU:HG2   | 1.94                     | 0.50              |
| 1:WU:202:VAL:HB   | 1:WU:205:LEU:HB2  | 1.94                     | 0.50              |
| 1:WV:200:SER:OG   | 1:WW:175:SER:HB2  | 2.11                     | 0.50              |
| 4:J:167:MET:HG3   | 4:J:171:LEU:HG    | 1.93                     | 0.50              |
| 7:Y:106:MET:O     | 7:Y:110:ARG:HG2   | 2.12                     | 0.50              |
| 1:v:256:ILE:HG13  | 1:v:257:VAL:N     | 2.26                     | 0.50              |
| 1:2:294:ARG:HD2   | 1:2:367:GLU:OE1   | 2.12                     | 0.50              |
| 1:8:235:LEU:HB3   | 1:9:244:ARG:HH22  | 1.75                     | 0.50              |
| 1:0:256:ILE:HG13  | 1:0:257:VAL:N     | 2.26                     | 0.50              |
| 1:UN:159:MET:N    | 1:UN:159:MET:SD   | 2.82                     | 0.49              |
| 1:WQ:142:ARG:O    | 1:WQ:146:THR:HG23 | 2.13                     | 0.49              |
| 1:WQ:202:VAL:HB   | 1:WQ:205:LEU:HB2  | 1.94                     | 0.49              |
| 1:WS:197:LEU:HA   | 1:WT:175:SER:OG   | 2.11                     | 0.49              |
| 3:E:185:MET:HE3   | 3:E:188:LEU:HD22  | 1.94                     | 0.49              |
| 1:t:294:ARG:HD2   | 1:t:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:u:294:ARG:HD2   | 1:u:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:w:294:ARG:HD2   | 1:w:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:x:294:ARG:HD2   | 1:x:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:y:294:ARG:HD2   | 1:y:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:z:294:ARG:HD2   | 1:z:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:1:294:ARG:HD2   | 1:1:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:AO:294:ARG:HD2  | 1:AO:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:AP:294:ARG:HD2  | 1:AP:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:UJ:162:PRO:O    | 1:UJ:163:SER:C    | 2.55                     | 0.49              |
| 1:UM:162:PRO:O    | 1:UM:163:SER:C    | 2.55                     | 0.49              |
| 1:UN:162:PRO:O    | 1:UN:163:SER:C    | 2.55                     | 0.49              |
| 1:UP:98:LEU:HD22  | 1:UP:147:LEU:CD2  | 2.39                     | 0.49              |
| 1:WB:187:ASP:OD1  | 1:WB:190:GLN:HG3  | 2.12                     | 0.49              |
| 1:WD:149:PRO:HG2  | 1:WD:190:GLN:NE2  | 2.23                     | 0.49              |
| 1:WL:145:GLU:O    | 1:WL:146:THR:C    | 2.53                     | 0.49              |
| 1:WO:206:PRO:O    | 1:WO:207:PRO:C    | 2.56                     | 0.49              |
| 4:I:161:GLY:C     | 4:I:163:GLU:H     | 2.20                     | 0.49              |
| 5:P:55:GLN:HG2    | 5:P:71:VAL:HG22   | 1.94                     | 0.49              |
| 6:U:46:ALA:O      | 6:U:50:LYS:HG2    | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:U:66:THR:HG23   | 1:z:365:ASN:ND2   | 2.27                     | 0.49              |
| 1:AE:256:ILE:HG13 | 1:AE:257:VAL:N    | 2.26                     | 0.49              |
| 1:AK:256:ILE:HG13 | 1:AK:257:VAL:N    | 2.26                     | 0.49              |
| 1:AM:294:ARG:HD2  | 1:AM:367:GLU:OE1  | 2.13                     | 0.49              |
| 1:AN:294:ARG:HD2  | 1:AN:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:AQ:256:ILE:HG13 | 1:AQ:257:VAL:N    | 2.26                     | 0.49              |
| 1:AQ:294:ARG:HD2  | 1:AQ:367:GLU:OE1  | 2.13                     | 0.49              |
| 1:UM:98:LEU:HD22  | 1:UM:147:LEU:CD2  | 2.39                     | 0.49              |
| 1:UN:69:GLN:HE22  | 1:WS:182:PRO:HG2  | 1.77                     | 0.49              |
| 1:WB:114:GLU:O    | 1:WB:115:LEU:C    | 2.55                     | 0.49              |
| 1:WG:206:PRO:O    | 1:WG:207:PRO:C    | 2.56                     | 0.49              |
| 1:WH:202:VAL:HB   | 1:WH:205:LEU:HB2  | 1.95                     | 0.49              |
| 1:WN:202:VAL:HB   | 1:WN:205:LEU:HB2  | 1.94                     | 0.49              |
| 6:S:66:THR:OG1    | 1:AD:294:ARG:HG2  | 2.11                     | 0.49              |
| 1:u:256:ILE:HG13  | 1:u:257:VAL:N     | 2.26                     | 0.49              |
| 1:v:294:ARG:HD2   | 1:v:367:GLU:OE1   | 2.13                     | 0.49              |
| 1:3:294:ARG:HD2   | 1:3:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:AN:256:ILE:HG13 | 1:AN:257:VAL:N    | 2.26                     | 0.49              |
| 1:UN:73:MET:HE1   | 1:UN:99:ARG:HD2   | 1.95                     | 0.49              |
| 1:UN:208:GLY:CA   | 1:WR:187:ASP:OD1  | 2.60                     | 0.49              |
| 1:UO:103:GLN:CG   | 1:WU:182:PRO:HB3  | 2.42                     | 0.49              |
| 1:WC:121:PHE:CE1  | 2:C:15:LYS:NZ     | 2.67                     | 0.49              |
| 1:WE:206:PRO:O    | 1:WE:207:PRO:C    | 2.56                     | 0.49              |
| 1:WN:145:GLU:O    | 1:WN:147:LEU:N    | 2.46                     | 0.49              |
| 1:1:256:ILE:HG13  | 1:1:257:VAL:N     | 2.26                     | 0.49              |
| 1:WA:112:GLY:HA2  | 1:WA:135:ALA:CA   | 2.27                     | 0.49              |
| 1:WD:200:SER:O    | 1:WE:158:ALA:HB3  | 2.10                     | 0.49              |
| 1:WE:202:VAL:HB   | 1:WE:205:LEU:HB2  | 1.95                     | 0.49              |
| 1:WG:219:LEU:HD21 | 1:WG:222:GLN:O    | 2.13                     | 0.49              |
| 1:WO:142:ARG:O    | 1:WO:146:THR:HG23 | 2.11                     | 0.49              |
| 1:WP:164:LEU:HD11 | 4:F:151:ALA:HB3   | 1.93                     | 0.49              |
| 1:WQ:206:PRO:O    | 1:WQ:207:PRO:C    | 2.56                     | 0.49              |
| 4:F:101:MET:HE1   | 4:F:137:PHE:CZ    | 2.47                     | 0.49              |
| 4:F:232:TRP:NE1   | 4:F:236:MET:HE3   | 2.27                     | 0.49              |
| 4:I:59:LEU:O      | 4:I:65:THR:OG1    | 2.28                     | 0.49              |
| 4:J:40:LEU:HD23   | 6:U:130:MET:HE1   | 1.94                     | 0.49              |
| 6:S:76:GLN:N      | 1:AD:297:GLN:HE22 | 2.08                     | 0.49              |
| 1:AL:294:ARG:HD2  | 1:AL:367:GLU:OE1  | 2.13                     | 0.49              |
| 1:WC:128:GLU:HG2  | 1:WC:129:GLN:N    | 2.28                     | 0.49              |
| 1:WD:145:GLU:O    | 1:WD:147:LEU:N    | 2.46                     | 0.49              |
| 1:WF:202:VAL:HB   | 1:WF:205:LEU:HB2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WK:202:VAL:HB   | 1:WK:205:LEU:HB2  | 1.95                     | 0.49              |
| 1:WM:197:LEU:HA   | 1:WN:175:SER:CB   | 2.42                     | 0.49              |
| 1:WS:202:VAL:HB   | 1:WS:205:LEU:HB2  | 1.94                     | 0.49              |
| 2:D:77:VAL:CG1    | 4:J:229:VAL:HG21  | 2.42                     | 0.49              |
| 4:G:66:ARG:NH2    | 4:G:178:GLU:OE1   | 2.45                     | 0.49              |
| 1:x:256:ILE:HG13  | 1:x:257:VAL:N     | 2.26                     | 0.49              |
| 1:AC:256:ILE:HG13 | 1:AC:257:VAL:N    | 2.26                     | 0.49              |
| 1:UI:129:GLN:O    | 1:UI:133:GLN:N    | 2.29                     | 0.49              |
| 1:UJ:73:MET:HE3   | 1:UJ:99:ARG:CD    | 2.41                     | 0.49              |
| 1:UK:73:MET:HE3   | 1:UK:99:ARG:CD    | 2.41                     | 0.49              |
| 1:UN:80:ALA:CB    | 1:UN:83:SER:HB3   | 2.43                     | 0.49              |
| 1:WA:213:VAL:CG2  | 1:WW:193:ALA:HB1  | 2.42                     | 0.49              |
| 1:WF:193:ALA:HB1  | 1:WG:213:VAL:HG11 | 1.94                     | 0.49              |
| 1:WH:206:PRO:O    | 1:WH:207:PRO:C    | 2.55                     | 0.49              |
| 3:E:12:TRP:CZ3    | 5:P:34:PHE:HB2    | 2.48                     | 0.49              |
| 6:T:68:THR:CG2    | 1:7:294:ARG:CD    | 2.91                     | 0.49              |
| 1:w:266:VAL:HG22  | 1:w:387:VAL:HG22  | 1.95                     | 0.49              |
| 1:4:294:ARG:HD2   | 1:4:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:UJ:98:LEU:HD22  | 1:UJ:147:LEU:CD2  | 2.39                     | 0.49              |
| 1:UK:80:ALA:CB    | 1:UK:83:SER:HB3   | 2.43                     | 0.49              |
| 1:WA:167:ARG:HH21 | 4:H:162:PRO:HD2   | 1.78                     | 0.49              |
| 1:WE:112:GLY:O    | 1:WE:115:LEU:HB3  | 2.12                     | 0.49              |
| 1:WF:116:LEU:HD22 | 1:WF:131:ASN:HA   | 1.94                     | 0.49              |
| 1:WG:164:LEU:O    | 4:J:241:GLN:CG    | 2.47                     | 0.49              |
| 1:WL:202:VAL:HB   | 1:WL:205:LEU:HB2  | 1.95                     | 0.49              |
| 1:WP:144:ILE:O    | 1:WP:147:LEU:HB2  | 2.13                     | 0.49              |
| 1:WS:206:PRO:O    | 1:WS:207:PRO:C    | 2.56                     | 0.49              |
| 1:WU:206:PRO:O    | 1:WU:207:PRO:C    | 2.55                     | 0.49              |
| 2:C:36:SER:OG     | 2:D:44:ILE:HG23   | 2.12                     | 0.49              |
| 5:L:82:MET:HE3    | 6:Q:133:VAL:CG2   | 2.43                     | 0.49              |
| 6:Q:17:ASN:HD22   | 6:Q:57:ARG:NH1    | 2.10                     | 0.49              |
| 6:T:102:MET:HB3   | 6:T:106:ARG:HH21  | 1.77                     | 0.49              |
| 1:AG:256:ILE:HG13 | 1:AG:257:VAL:N    | 2.26                     | 0.49              |
| 1:AK:294:ARG:HD2  | 1:AK:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:UJ:80:ALA:CB    | 1:UJ:83:SER:HB3   | 2.43                     | 0.49              |
| 1:UL:80:ALA:CB    | 1:UL:83:SER:HB3   | 2.43                     | 0.49              |
| 1:UP:80:ALA:CB    | 1:UP:83:SER:HB3   | 2.43                     | 0.49              |
| 1:WC:197:LEU:HD11 | 1:WD:156:HIS:HD2  | 1.78                     | 0.49              |
| 1:WF:145:GLU:HG2  | 1:WF:152:SER:HA   | 1.95                     | 0.49              |
| 1:WF:206:PRO:O    | 1:WF:207:PRO:C    | 2.56                     | 0.49              |
| 1:WH:193:ALA:CB   | 1:WI:213:VAL:CG1  | 2.88                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WI:206:PRO:O    | 1:WI:207:PRO:C    | 2.56                     | 0.49              |
| 6:R:68:THR:HG21   | 1:AJ:294:ARG:CD   | 2.42                     | 0.49              |
| 1:d:319:GLN:OE1   | 1:AM:303:GLN:CD   | 2.56                     | 0.49              |
| 1:v:266:VAL:HG22  | 1:v:387:VAL:HG22  | 1.95                     | 0.49              |
| 1:AB:266:VAL:HG22 | 1:AB:387:VAL:HG22 | 1.95                     | 0.49              |
| 1:UN:98:LEU:HD22  | 1:UN:147:LEU:CD2  | 2.39                     | 0.49              |
| 1:UP:73:MET:HE1   | 1:UP:99:ARG:HD2   | 1.95                     | 0.49              |
| 1:WK:143:THR:OG1  | 1:WL:156:HIS:NE2  | 1.94                     | 0.49              |
| 1:WS:197:LEU:HD11 | 1:WT:156:HIS:HD2  | 1.78                     | 0.49              |
| 1:WW:115:LEU:HA   | 1:WW:118:GLN:OE1  | 2.13                     | 0.49              |
| 5:K:7:ILE:HG21    | 1:AM:278:THR:HG22 | 1.81                     | 0.49              |
| 5:L:11:ILE:CG2    | 1:AH:372:ILE:HD12 | 2.28                     | 0.49              |
| 1:x:266:VAL:HG22  | 1:x:387:VAL:HG22  | 1.95                     | 0.49              |
| 1:AA:266:VAL:HG22 | 1:AA:387:VAL:HG22 | 1.95                     | 0.49              |
| 1:AC:266:VAL:HG22 | 1:AC:387:VAL:HG22 | 1.95                     | 0.49              |
| 1:UM:80:ALA:CB    | 1:UM:83:SER:HB3   | 2.43                     | 0.48              |
| 1:WB:202:VAL:HB   | 1:WB:205:LEU:HB2  | 1.94                     | 0.48              |
| 4:F:179:LEU:HD22  | 4:G:84:PRO:HG3    | 1.95                     | 0.48              |
| 1:4:266:VAL:HG22  | 1:4:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:5:294:ARG:HD2   | 1:5:367:GLU:OE1   | 2.13                     | 0.48              |
| 1:AJ:294:ARG:HD2  | 1:AJ:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:WA:206:PRO:O    | 1:WA:207:PRO:C    | 2.56                     | 0.48              |
| 1:WB:145:GLU:C    | 1:WB:147:LEU:H    | 2.22                     | 0.48              |
| 1:WJ:200:SER:OG   | 1:WK:175:SER:HB2  | 2.13                     | 0.48              |
| 2:A:48:THR:HG21   | 4:F:208:GLY:HA2   | 1.95                     | 0.48              |
| 4:F:92:LEU:HD13   | 4:F:232:TRP:HZ2   | 1.77                     | 0.48              |
| 4:F:130:GLY:O     | 4:F:133:PRO:HD2   | 2.13                     | 0.48              |
| 4:J:73:LEU:HD13   | 4:J:186:GLY:HA3   | 1.94                     | 0.48              |
| 5:N:4:ILE:HG12    | 1:7:372:ILE:CG2   | 2.43                     | 0.48              |
| 6:R:68:THR:HG21   | 1:AJ:294:ARG:HH11 | 1.78                     | 0.48              |
| 6:S:72:HIS:ND1    | 1:AD:365:ASN:CG   | 2.70                     | 0.48              |
| 6:T:49:LEU:O      | 6:T:53:MET:HG2    | 2.13                     | 0.48              |
| 6:T:67:LEU:HD21   | 6:T:74:PRO:HB3    | 1.94                     | 0.48              |
| 7:X:94:PRO:HB2    | 7:X:96:VAL:HG23   | 1.94                     | 0.48              |
| 1:AA:294:ARG:HD2  | 1:AA:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:AB:294:ARG:HD2  | 1:AB:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:AC:294:ARG:HD2  | 1:AC:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:UI:127:SER:O    | 1:UI:131:ASN:HB2  | 2.14                     | 0.48              |
| 1:UL:98:LEU:HD22  | 1:UL:147:LEU:CD2  | 2.39                     | 0.48              |
| 1:WJ:206:PRO:O    | 1:WJ:207:PRO:C    | 2.56                     | 0.48              |
| 1:WR:165:PHE:HZ   | 4:G:240:ALA:HB1   | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WS:200:SER:O    | 1:WT:158:ALA:HB3  | 2.05                     | 0.48              |
| 4:I:42:VAL:HG13   | 5:O:42:LEU:HD22   | 1.95                     | 0.48              |
| 7:V:37:PRO:HD3    | 7:a:51:VAL:HG13   | 1.95                     | 0.48              |
| 7:X:97:ASP:O      | 7:X:101:GLU:HG2   | 2.13                     | 0.48              |
| 1:f:319:GLN:HB3   | 1:AG:303:GLN:NE2  | 2.25                     | 0.48              |
| 1:9:294:ARG:HD2   | 1:9:367:GLU:OE1   | 2.12                     | 0.48              |
| 1:0:294:ARG:HD2   | 1:0:367:GLU:OE1   | 2.12                     | 0.48              |
| 1:AD:294:ARG:HD2  | 1:AD:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:AE:294:ARG:HD2  | 1:AE:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:AG:266:VAL:HG22 | 1:AG:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:AH:266:VAL:HG22 | 1:AH:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:UI:80:ALA:CB    | 1:UI:83:SER:HB3   | 2.43                     | 0.48              |
| 1:WJ:202:VAL:HB   | 1:WJ:205:LEU:HB2  | 1.95                     | 0.48              |
| 1:WK:132:TYR:CB   | 1:WL:126:PHE:HZ   | 2.19                     | 0.48              |
| 1:WK:206:PRO:O    | 1:WK:207:PRO:C    | 2.55                     | 0.48              |
| 1:WM:202:VAL:HB   | 1:WM:205:LEU:HB2  | 1.94                     | 0.48              |
| 1:WP:202:VAL:HB   | 1:WP:205:LEU:HB2  | 1.95                     | 0.48              |
| 3:E:114:VAL:HG21  | 4:I:211:MET:HE1   | 1.96                     | 0.48              |
| 5:N:99:VAL:O      | 5:N:102:MET:HG2   | 2.13                     | 0.48              |
| 5:P:11:ILE:HD11   | 1:AQ:276:GLU:CD   | 2.38                     | 0.48              |
| 6:S:32:ASN:ND2    | 7:X:51:VAL:HG12   | 2.28                     | 0.48              |
| 6:S:65:LEU:HD11   | 1:AD:365:ASN:HD21 | 1.78                     | 0.48              |
| 1:3:266:VAL:HG22  | 1:3:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:5:266:VAL:HG22  | 1:5:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:8:294:ARG:HD2   | 1:8:367:GLU:OE1   | 2.13                     | 0.48              |
| 1:AD:266:VAL:HG22 | 1:AD:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:AG:294:ARG:HD2  | 1:AG:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:UJ:256:PRO:HD2  | 1:WC:187:ASP:HB3  | 1.94                     | 0.48              |
| 1:UK:127:SER:O    | 1:UK:131:ASN:HB2  | 2.14                     | 0.48              |
| 1:UO:73:MET:HE3   | 1:UO:99:ARG:CD    | 2.41                     | 0.48              |
| 1:WC:164:LEU:O    | 4:I:241:GLN:HG3   | 2.08                     | 0.48              |
| 1:WK:193:ALA:CB   | 1:WL:213:VAL:HG11 | 2.44                     | 0.48              |
| 1:WM:206:PRO:O    | 1:WM:207:PRO:C    | 2.56                     | 0.48              |
| 1:WW:202:VAL:HB   | 1:WW:205:LEU:HB2  | 1.95                     | 0.48              |
| 2:D:36:SER:OG     | 3:E:211:LEU:O     | 2.24                     | 0.48              |
| 1:y:266:VAL:HG22  | 1:y:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:6:266:VAL:HG22  | 1:6:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:7:294:ARG:HD2   | 1:7:367:GLU:OE1   | 2.13                     | 0.48              |
| 1:0:266:VAL:HG22  | 1:0:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:UJ:127:SER:O    | 1:UJ:131:ASN:HB2  | 2.14                     | 0.48              |
| 1:WA:142:ARG:O    | 1:WA:146:THR:HG23 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WA:196:HIS:CD2  | 1:WB:219:LEU:HD22 | 2.49                     | 0.48              |
| 1:WB:206:PRO:O    | 1:WB:207:PRO:C    | 2.56                     | 0.48              |
| 1:WI:202:VAL:HB   | 1:WI:205:LEU:HB2  | 1.94                     | 0.48              |
| 1:WV:164:LEU:CB   | 4:G:152:ARG:HH12  | 2.27                     | 0.48              |
| 3:E:178:LEU:HD13  | 3:E:181:LEU:HD23  | 1.95                     | 0.48              |
| 4:J:150:PHE:CE1   | 4:J:172:PRO:HB2   | 2.48                     | 0.48              |
| 5:O:4:ILE:HG12    | 1:1:372:ILE:CG2   | 2.42                     | 0.48              |
| 1:u:266:VAL:HG22  | 1:u:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:6:294:ARG:HD2   | 1:6:367:GLU:OE1   | 2.13                     | 0.48              |
| 1:AI:294:ARG:HD2  | 1:AI:367:GLU:OE1  | 2.12                     | 0.48              |
| 1:AP:266:VAL:HG22 | 1:AP:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:UO:80:ALA:CB    | 1:UO:83:SER:HB3   | 2.43                     | 0.48              |
| 1:WA:193:ALA:HB1  | 1:WB:213:VAL:CG1  | 2.43                     | 0.48              |
| 1:WC:202:VAL:HB   | 1:WC:205:LEU:HB2  | 1.95                     | 0.48              |
| 1:WC:206:PRO:O    | 1:WC:207:PRO:C    | 2.56                     | 0.48              |
| 1:WD:167:ARG:HH21 | 1:WD:168:GLU:HA   | 1.77                     | 0.48              |
| 1:WF:124:SER:O    | 1:WF:127:SER:N    | 2.46                     | 0.48              |
| 1:WG:142:ARG:O    | 1:WG:146:THR:HG23 | 2.14                     | 0.48              |
| 1:WR:202:VAL:HB   | 1:WR:205:LEU:HB2  | 1.95                     | 0.48              |
| 1:WT:206:PRO:O    | 1:WT:207:PRO:C    | 2.56                     | 0.48              |
| 1:WV:192:SER:O    | 1:WV:195:VAL:N    | 2.47                     | 0.48              |
| 1:WW:206:PRO:O    | 1:WW:207:PRO:C    | 2.56                     | 0.48              |
| 3:E:101:PHE:CE2   | 4:F:80:THR:HG21   | 2.48                     | 0.48              |
| 4:I:159:LEU:O     | 4:I:160:GLN:HB2   | 2.14                     | 0.48              |
| 4:J:71:PHE:CZ     | 4:J:236:MET:HE1   | 2.49                     | 0.48              |
| 6:T:55:ARG:CZ     | 1:5:299:ASN:HD22  | 2.16                     | 0.48              |
| 7:X:27:ASN:OD1    | 7:X:42:TYR:OH     | 2.27                     | 0.48              |
| 1:2:266:VAL:HG22  | 1:2:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:AF:266:VAL:HG22 | 1:AF:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:UP:167:ARG:NH1  | 1:8:236:LYS:CE    | 2.76                     | 0.48              |
| 1:WB:128:GLU:HG2  | 1:WC:126:PHE:HD2  | 1.79                     | 0.48              |
| 1:WB:197:LEU:HA   | 1:WC:175:SER:OG   | 2.13                     | 0.48              |
| 1:WC:187:ASP:O    | 1:WC:190:GLN:HB3  | 2.14                     | 0.48              |
| 1:WQ:164:LEU:HD23 | 4:F:149:LEU:HB2   | 1.95                     | 0.48              |
| 1:WR:206:PRO:O    | 1:WR:207:PRO:C    | 2.56                     | 0.48              |
| 5:L:55:GLN:HG2    | 5:L:71:VAL:HG22   | 1.95                     | 0.48              |
| 6:T:11:PHE:CD1    | 6:T:53:MET:HE2    | 2.48                     | 0.48              |
| 1:AF:294:ARG:HD2  | 1:AF:367:GLU:OE1  | 2.13                     | 0.48              |
| 1:AH:294:ARG:HD2  | 1:AH:367:GLU:OE1  | 2.13                     | 0.48              |
| 1:AI:266:VAL:HG22 | 1:AI:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:AQ:266:VAL:HG22 | 1:AQ:387:VAL:HG22 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UI:73:MET:HE3   | 1:UI:99:ARG:CD    | 2.41                     | 0.48              |
| 1:WA:202:VAL:HB   | 1:WA:205:LEU:HB2  | 1.94                     | 0.48              |
| 1:WJ:171:SER:HB3  | 1:WJ:206:PRO:HG3  | 1.96                     | 0.48              |
| 1:WV:202:VAL:HB   | 1:WV:205:LEU:HB2  | 1.95                     | 0.48              |
| 2:C:14:MET:HE3    | 2:D:63:ILE:HD11   | 1.96                     | 0.48              |
| 3:E:86:PHE:CZ     | 4:F:88:VAL:HA     | 2.48                     | 0.48              |
| 4:F:99:PHE:C      | 4:F:99:PHE:CD2    | 2.91                     | 0.48              |
| 5:M:11:ILE:HG23   | 1:AB:372:ILE:HG21 | 1.89                     | 0.48              |
| 1:AO:266:VAL:HG22 | 1:AO:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:UJ:103:GLN:HB3  | 1:WD:182:PRO:HA   | 1.91                     | 0.48              |
| 1:WN:200:SER:CB   | 1:WO:173:SER:HB2  | 2.44                     | 0.48              |
| 1:WN:206:PRO:O    | 1:WN:207:PRO:C    | 2.56                     | 0.48              |
| 1:WT:145:GLU:C    | 1:WT:147:LEU:N    | 2.72                     | 0.48              |
| 1:WV:206:PRO:O    | 1:WV:207:PRO:C    | 2.56                     | 0.48              |
| 2:C:54:LYS:NZ     | 2:D:48:THR:HG21   | 2.29                     | 0.48              |
| 2:D:60:ILE:HA     | 2:D:63:ILE:HG12   | 1.96                     | 0.48              |
| 3:E:158:PRO:HG2   | 3:E:162:ASN:ND2   | 2.16                     | 0.48              |
| 7:V:27:ASN:ND2    | 7:V:45:LYS:O      | 2.33                     | 0.48              |
| 1:AK:296:ARG:HH11 | 1:AK:296:ARG:HG2  | 1.79                     | 0.48              |
| 1:UJ:129:GLN:O    | 1:UJ:133:GLN:N    | 2.29                     | 0.47              |
| 1:WA:216:SER:O    | 1:WW:190:GLN:HG2  | 2.14                     | 0.47              |
| 1:WH:187:ASP:OD2  | 1:WH:190:GLN:HB2  | 2.14                     | 0.47              |
| 1:WI:193:ALA:HB1  | 1:WJ:213:VAL:HG11 | 1.94                     | 0.47              |
| 1:WN:142:ARG:O    | 1:WN:146:THR:HG23 | 2.14                     | 0.47              |
| 1:WO:202:VAL:HB   | 1:WO:205:LEU:HB2  | 1.95                     | 0.47              |
| 1:WU:113:PHE:CE2  | 1:WU:139:GLU:HG3  | 2.48                     | 0.47              |
| 2:B:44:ILE:HD13   | 2:B:44:ILE:HA     | 1.75                     | 0.47              |
| 3:E:94:ALA:HB2    | 3:E:179:ILE:HA    | 1.96                     | 0.47              |
| 5:K:7:ILE:CD1     | 1:AM:278:THR:HG21 | 2.44                     | 0.47              |
| 5:K:11:ILE:CD1    | 1:AL:276:GLU:CD   | 2.87                     | 0.47              |
| 6:R:29:ASN:HD21   | 6:R:41:ARG:H      | 1.61                     | 0.47              |
| 7:W:44:ALA:HB2    | 7:W:96:VAL:HG22   | 1.96                     | 0.47              |
| 7:Z:42:TYR:O      | 7:Z:94:PRO:HB3    | 2.14                     | 0.47              |
| 1:u:296:ARG:HG2   | 1:u:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:9:296:ARG:HG2   | 1:9:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:AE:266:VAL:HG22 | 1:AE:387:VAL:HG22 | 1.95                     | 0.47              |
| 1:WB:187:ASP:OD1  | 1:WB:190:GLN:N    | 2.41                     | 0.47              |
| 1:WG:202:VAL:HB   | 1:WG:205:LEU:HB2  | 1.95                     | 0.47              |
| 2:B:11:THR:HA     | 2:B:14:MET:HE3    | 1.96                     | 0.47              |
| 5:P:7:ILE:CB      | 1:t:278:THR:HG21  | 2.41                     | 0.47              |
| 7:Y:28:LEU:HD21   | 7:Y:102:MET:HE2   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AD:296:ARG:HG2  | 1:AD:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:AG:296:ARG:HG2  | 1:AG:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:AL:266:VAL:HG22 | 1:AL:387:VAL:HG22 | 1.95                     | 0.47              |
| 1:AN:296:ARG:HG2  | 1:AN:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:AQ:296:ARG:HG2  | 1:AQ:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:UL:73:MET:HE3   | 1:UL:99:ARG:CD    | 2.41                     | 0.47              |
| 1:UL:180:LEU:HB2  | 1:UL:215:GLN:HE22 | 1.79                     | 0.47              |
| 1:WA:167:ARG:NH2  | 4:H:162:PRO:HD3   | 2.26                     | 0.47              |
| 1:WA:190:GLN:O    | 1:WA:191:ILE:C    | 2.57                     | 0.47              |
| 1:WH:165:PHE:O    | 4:J:144:GLU:HG2   | 2.14                     | 0.47              |
| 1:WI:201:ALA:C    | 1:WJ:158:ALA:HB2  | 2.39                     | 0.47              |
| 1:WL:206:PRO:O    | 1:WL:207:PRO:C    | 2.56                     | 0.47              |
| 1:WP:206:PRO:O    | 1:WP:207:PRO:C    | 2.56                     | 0.47              |
| 1:WT:202:VAL:HB   | 1:WT:205:LEU:HB2  | 1.95                     | 0.47              |
| 1:WU:115:LEU:HD21 | 1:WU:134:ARG:HD3  | 1.95                     | 0.47              |
| 1:WW:142:ARG:O    | 1:WW:146:THR:HG23 | 2.14                     | 0.47              |
| 4:G:82:SER:HA     | 5:K:103:GLN:HE21  | 1.79                     | 0.47              |
| 1:t:266:VAL:HG22  | 1:t:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:7:266:VAL:HG22  | 1:7:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:UM:127:SER:O    | 1:UM:131:ASN:HB2  | 2.14                     | 0.47              |
| 1:WA:196:HIS:HB3  | 1:WB:211:THR:CG2  | 2.36                     | 0.47              |
| 1:WC:145:GLU:O    | 1:WC:146:THR:C    | 2.56                     | 0.47              |
| 1:WD:202:VAL:HB   | 1:WD:205:LEU:HB2  | 1.95                     | 0.47              |
| 1:WI:193:ALA:HB1  | 1:WJ:213:VAL:CG2  | 2.45                     | 0.47              |
| 1:WV:112:GLY:HA2  | 1:WV:135:ALA:CA   | 2.28                     | 0.47              |
| 2:B:70:LEU:O      | 2:B:74:LEU:HG     | 2.14                     | 0.47              |
| 4:H:190:PHE:CD1   | 4:I:220:PRO:HG3   | 2.49                     | 0.47              |
| 6:R:24:GLU:OE1    | 7:W:5:ASN:HB2     | 2.15                     | 0.47              |
| 1:4:296:ARG:HG2   | 1:4:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:7:296:ARG:HG2   | 1:7:296:ARG:HH11  | 1.80                     | 0.47              |
| 1:AB:296:ARG:HG2  | 1:AB:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:AP:296:ARG:HG2  | 1:AP:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:UI:98:LEU:CD1   | 1:UI:146:THR:HG1  | 2.27                     | 0.47              |
| 1:UL:103:GLN:CG   | 1:WH:182:PRO:HB3  | 2.43                     | 0.47              |
| 1:WU:142:ARG:O    | 1:WU:146:THR:HG23 | 2.14                     | 0.47              |
| 5:L:99:VAL:HA     | 5:L:102:MET:HE3   | 1.96                     | 0.47              |
| 7:Y:52:ASP:OD1    | 7:Y:63:LYS:HD3    | 2.13                     | 0.47              |
| 1:1:266:VAL:HG22  | 1:1:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:6:296:ARG:HG2   | 1:6:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:AH:296:ARG:HG2  | 1:AH:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:AK:266:VAL:HG22 | 1:AK:387:VAL:HG22 | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:266:VAL:HG22 | 1:AM:387:VAL:HG22 | 1.95                     | 0.47              |
| 1:UN:127:SER:O    | 1:UN:131:ASN:HB2  | 2.14                     | 0.47              |
| 1:WG:122:GLY:O    | 1:WG:123:ILE:C    | 2.58                     | 0.47              |
| 2:B:7:MET:SD      | 2:C:70:LEU:HD22   | 2.54                     | 0.47              |
| 5:M:4:ILE:HG13    | 1:AC:372:ILE:HG22 | 1.92                     | 0.47              |
| 6:S:10:ARG:HE     | 6:S:53:MET:HE1    | 1.79                     | 0.47              |
| 6:T:11:PHE:HD1    | 6:T:53:MET:HE2    | 1.80                     | 0.47              |
| 1:z:266:VAL:HG22  | 1:z:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:9:266:VAL:HG22  | 1:9:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:0:296:ARG:HG2   | 1:0:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:AA:296:ARG:HG2  | 1:AA:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:AJ:266:VAL:HG22 | 1:AJ:387:VAL:HG22 | 1.95                     | 0.47              |
| 1:AJ:296:ARG:HG2  | 1:AJ:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:WD:206:PRO:O    | 1:WD:207:PRO:C    | 2.56                     | 0.47              |
| 1:WF:147:LEU:HA   | 1:WG:215:GLN:O    | 2.14                     | 0.47              |
| 1:WI:196:HIS:HB3  | 1:WJ:211:THR:CG2  | 2.32                     | 0.47              |
| 1:WI:197:LEU:HA   | 1:WJ:175:SER:OG   | 2.15                     | 0.47              |
| 1:WS:200:SER:HG   | 1:WT:175:SER:HB2  | 1.77                     | 0.47              |
| 1:WT:186:LEU:HA   | 1:WT:190:GLN:OE1  | 2.15                     | 0.47              |
| 1:WW:115:LEU:O    | 1:WW:116:LEU:C    | 2.57                     | 0.47              |
| 1:WW:145:GLU:O    | 1:WW:147:LEU:N    | 2.48                     | 0.47              |
| 3:E:9:TRP:CD1     | 3:E:9:TRP:H       | 2.31                     | 0.47              |
| 4:F:189:ILE:O     | 4:F:192:PRO:HD2   | 2.15                     | 0.47              |
| 5:K:80:VAL:HG22   | 6:Q:131:MET:SD    | 2.54                     | 0.47              |
| 6:R:96:ASP:OD1    | 6:R:96:ASP:N      | 2.39                     | 0.47              |
| 6:T:55:ARG:HH22   | 1:5:299:ASN:HD22  | 1.59                     | 0.47              |
| 6:T:73:ILE:HD12   | 6:T:74:PRO:HD2    | 1.95                     | 0.47              |
| 6:T:102:MET:HE3   | 6:T:106:ARG:HE    | 1.78                     | 0.47              |
| 1:b:318:ASN:O     | 1:b:319:GLN:C     | 2.58                     | 0.47              |
| 1:v:296:ARG:HG2   | 1:v:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:x:296:ARG:HH11  | 1:x:296:ARG:HG2   | 1.80                     | 0.47              |
| 1:z:296:ARG:HG2   | 1:z:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:1:296:ARG:HG2   | 1:1:296:ARG:HH11  | 1.80                     | 0.47              |
| 1:AC:296:ARG:HG2  | 1:AC:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:UL:127:SER:O    | 1:UL:131:ASN:HB2  | 2.14                     | 0.47              |
| 3:E:72:TRP:HE1    | 3:E:161:SER:HB2   | 1.80                     | 0.47              |
| 5:N:4:ILE:HG12    | 1:7:372:ILE:HB    | 1.96                     | 0.47              |
| 6:S:72:HIS:CA     | 1:AE:295:SER:CB   | 2.93                     | 0.47              |
| 6:U:72:HIS:CE1    | 1:2:294:ARG:CG    | 2.96                     | 0.47              |
| 1:AN:266:VAL:HG22 | 1:AN:387:VAL:HG22 | 1.95                     | 0.47              |
| 1:UL:167:ARG:HA   | 1:UL:167:ARG:HD3  | 1.74                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UO:127:SER:O    | 1:UO:131:ASN:HB2  | 2.14                     | 0.47              |
| 1:WJ:164:LEU:HD23 | 3:E:144:LEU:CB    | 2.43                     | 0.47              |
| 6:S:73:ILE:HG22   | 6:S:75:ALA:H      | 1.80                     | 0.47              |
| 1:d:319:GLN:HG2   | 1:d:320:PRO:HD2   | 1.95                     | 0.47              |
| 1:8:266:VAL:HG22  | 1:8:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:AE:296:ARG:HG2  | 1:AE:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:AL:296:ARG:HG2  | 1:AL:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:UM:73:MET:HE3   | 1:UM:99:ARG:CD    | 2.41                     | 0.47              |
| 1:UM:136:LEU:HD23 | 1:UM:157:LEU:CD1  | 2.45                     | 0.47              |
| 1:UO:129:GLN:O    | 1:UO:133:GLN:N    | 2.29                     | 0.47              |
| 1:WB:145:GLU:O    | 1:WB:147:LEU:N    | 2.48                     | 0.47              |
| 1:WJ:125:GLN:HB2  | 3:E:242:HIS:CG    | 2.50                     | 0.47              |
| 1:WL:159:MET:HB2  | 1:WL:159:MET:HE3  | 1.69                     | 0.47              |
| 2:C:31:THR:O      | 2:C:35:ILE:HG12   | 2.14                     | 0.47              |
| 5:L:48:ARG:HH22   | 6:R:6:ASP:CG      | 2.22                     | 0.47              |
| 5:M:48:ARG:NH2    | 6:S:6:ASP:OD2     | 2.48                     | 0.47              |
| 5:N:59:PHE:CD2    | 6:S:118:MET:HE1   | 2.50                     | 0.47              |
| 6:Q:22:ARG:NH2    | 6:Q:108:GLN:OE1   | 2.47                     | 0.47              |
| 7:a:86:ASP:OD1    | 7:a:86:ASP:N      | 2.38                     | 0.47              |
| 1:w:296:ARG:HG2   | 1:w:296:ARG:HH11  | 1.79                     | 0.47              |
| 1:AI:296:ARG:HG2  | 1:AI:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:AM:296:ARG:HG2  | 1:AM:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:AO:296:ARG:HG2  | 1:AO:296:ARG:HH11 | 1.80                     | 0.47              |
| 1:WF:187:ASP:H    | 1:WF:190:GLN:CD   | 2.22                     | 0.46              |
| 1:WI:193:ALA:HB1  | 1:WJ:213:VAL:CG1  | 2.45                     | 0.46              |
| 1:WP:145:GLU:C    | 1:WP:147:LEU:N    | 2.72                     | 0.46              |
| 1:WW:147:LEU:O    | 1:WW:148:GLY:C    | 2.59                     | 0.46              |
| 3:E:103:GLY:O     | 3:E:106:MET:HB2   | 2.16                     | 0.46              |
| 5:M:7:ILE:O       | 5:M:11:ILE:HG23   | 2.16                     | 0.46              |
| 5:N:4:ILE:CG1     | 1:7:372:ILE:HG21  | 2.45                     | 0.46              |
| 6:U:67:LEU:HD11   | 6:U:74:PRO:HA     | 1.97                     | 0.46              |
| 7:V:22:ASN:HD21   | 7:a:5:ASN:ND2     | 2.13                     | 0.46              |
| 7:W:14:LEU:HD21   | 7:W:116:ILE:HG13  | 1.97                     | 0.46              |
| 1:y:296:ARG:HG2   | 1:y:296:ARG:HH11  | 1.79                     | 0.46              |
| 1:UO:136:LEU:HD23 | 1:UO:157:LEU:CD1  | 2.45                     | 0.46              |
| 1:WE:134:ARG:HB3  | 1:WE:134:ARG:NH2  | 2.27                     | 0.46              |
| 1:WG:112:GLY:HA3  | 1:WG:139:GLU:OE1  | 2.15                     | 0.46              |
| 1:WG:149:PRO:HG2  | 1:WG:190:GLN:HE22 | 1.79                     | 0.46              |
| 1:WK:145:GLU:O    | 1:WK:146:THR:C    | 2.58                     | 0.46              |
| 1:WN:145:GLU:C    | 1:WN:147:LEU:N    | 2.74                     | 0.46              |
| 1:WP:164:LEU:HD21 | 4:F:151:ALA:CB    | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WU:190:GLN:NE2  | 1:WV:216:SER:O    | 2.47                     | 0.46              |
| 2:A:17:ALA:HB2    | 4:G:195:ILE:HD12  | 1.96                     | 0.46              |
| 2:B:29:LEU:HD23   | 2:B:30:ILE:HD13   | 1.96                     | 0.46              |
| 4:H:138:MET:HE2   | 4:H:170:LEU:HG    | 1.98                     | 0.46              |
| 5:K:21:ALA:HB3    | 1:AK:278:THR:CG2  | 2.39                     | 0.46              |
| 6:S:65:LEU:HD13   | 1:AD:295:SER:OG   | 2.14                     | 0.46              |
| 6:S:114:LEU:HD21  | 7:Y:126:MET:CE    | 2.45                     | 0.46              |
| 7:a:88:ASN:HB2    | 7:a:90:TYR:CD2    | 2.50                     | 0.46              |
| 1:3:296:ARG:HG2   | 1:3:296:ARG:HH11  | 1.80                     | 0.46              |
| 1:UJ:73:MET:HE1   | 1:UJ:99:ARG:HD2   | 1.95                     | 0.46              |
| 1:WA:170:LYS:H    | 1:WA:170:LYS:HD2  | 1.80                     | 0.46              |
| 1:WD:187:ASP:OD1  | 1:WD:190:GLN:N    | 2.46                     | 0.46              |
| 1:WJ:164:LEU:HD11 | 3:E:145:TRP:HA    | 1.97                     | 0.46              |
| 1:WK:201:ALA:HA   | 1:WL:158:ALA:HB2  | 1.98                     | 0.46              |
| 1:WN:197:LEU:CD1  | 1:WO:175:SER:HB3  | 2.42                     | 0.46              |
| 1:WU:190:GLN:HG2  | 1:WV:216:SER:O    | 2.15                     | 0.46              |
| 4:F:230:ASP:O     | 4:F:234:LEU:HG    | 2.15                     | 0.46              |
| 4:J:105:ILE:HD13  | 5:O:34:PHE:HZ     | 1.80                     | 0.46              |
| 1:2:296:ARG:HH11  | 1:2:296:ARG:HG2   | 1.79                     | 0.46              |
| 1:UJ:136:LEU:HD23 | 1:UJ:157:LEU:CD1  | 2.46                     | 0.46              |
| 1:UL:73:MET:HE1   | 1:UL:99:ARG:HD2   | 1.95                     | 0.46              |
| 1:UN:73:MET:HE3   | 1:UN:99:ARG:CD    | 2.41                     | 0.46              |
| 1:UP:127:SER:O    | 1:UP:131:ASN:HB2  | 2.14                     | 0.46              |
| 1:WF:143:THR:OG1  | 1:WG:154:ARG:HG2  | 2.14                     | 0.46              |
| 1:WJ:200:SER:O    | 1:WK:158:ALA:HB2  | 2.15                     | 0.46              |
| 1:WN:135:ALA:O    | 1:WN:139:GLU:HG2  | 2.16                     | 0.46              |
| 1:WR:145:GLU:O    | 1:WR:146:THR:C    | 2.59                     | 0.46              |
| 4:J:83:ALA:HB3    | 4:J:84:PRO:CD     | 2.38                     | 0.46              |
| 5:L:15:GLN:HG3    | 5:L:16:ALA:N      | 2.30                     | 0.46              |
| 1:5:296:ARG:HG2   | 1:5:296:ARG:HH11  | 1.79                     | 0.46              |
| 1:WD:190:GLN:NE2  | 1:WE:216:SER:O    | 2.49                     | 0.46              |
| 1:WE:143:THR:HA   | 1:WE:146:THR:HG23 | 1.97                     | 0.46              |
| 1:WI:145:GLU:C    | 1:WI:147:LEU:N    | 2.74                     | 0.46              |
| 4:F:75:ARG:HD3    | 4:F:89:LEU:HD11   | 1.97                     | 0.46              |
| 4:F:100:ILE:HG23  | 4:F:101:MET:HE2   | 1.98                     | 0.46              |
| 5:O:48:ARG:NH2    | 6:U:6:ASP:OD1     | 2.48                     | 0.46              |
| 6:S:76:GLN:H      | 1:AD:297:GLN:NE2  | 2.12                     | 0.46              |
| 7:X:114:ALA:O     | 7:X:118:VAL:HG23  | 2.16                     | 0.46              |
| 7:Z:47:VAL:HG12   | 7:Z:67:VAL:HG22   | 1.96                     | 0.46              |
| 1:AF:296:ARG:HG2  | 1:AF:296:ARG:HH11 | 1.80                     | 0.46              |
| 1:UN:136:LEU:HD23 | 1:UN:157:LEU:CD1  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WK:135:ALA:O    | 1:WK:139:GLU:HG2  | 2.16                     | 0.46              |
| 1:WO:135:ALA:O    | 1:WO:139:GLU:HG2  | 2.16                     | 0.46              |
| 4:J:159:LEU:HD13  | 4:J:165:VAL:HG22  | 1.98                     | 0.46              |
| 5:P:7:ILE:HG21    | 1:t:278:THR:HG22  | 1.89                     | 0.46              |
| 6:R:51:LYS:O      | 6:R:55:ARG:HG2    | 2.16                     | 0.46              |
| 1:8:235:LEU:HD13  | 1:9:244:ARG:HH22  | 1.81                     | 0.46              |
| 1:UP:136:LEU:HD23 | 1:UP:157:LEU:CD1  | 2.45                     | 0.46              |
| 1:WB:147:LEU:O    | 1:WB:148:GLY:C    | 2.58                     | 0.46              |
| 1:WC:135:ALA:O    | 1:WC:139:GLU:HG2  | 2.16                     | 0.46              |
| 1:WD:135:ALA:O    | 1:WD:139:GLU:HG2  | 2.16                     | 0.46              |
| 4:G:59:LEU:O      | 4:G:65:THR:OG1    | 2.21                     | 0.46              |
| 1:x:235:LEU:HD13  | 1:y:244:ARG:HH22  | 1.81                     | 0.46              |
| 1:8:296:ARG:HG2   | 1:8:296:ARG:HH11  | 1.80                     | 0.46              |
| 1:0:235:LEU:HD13  | 1:AA:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:AH:235:LEU:HD13 | 1:AI:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:AK:235:LEU:HD13 | 1:AL:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:UJ:98:LEU:HD11  | 1:UJ:143:THR:O    | 2.16                     | 0.46              |
| 1:UK:73:MET:HE1   | 1:UK:99:ARG:HD2   | 1.95                     | 0.46              |
| 1:UM:98:LEU:HD12  | 1:UM:146:THR:HG1  | 1.80                     | 0.46              |
| 1:UO:73:MET:HE1   | 1:UO:99:ARG:HD2   | 1.95                     | 0.46              |
| 1:WT:197:LEU:HA   | 1:WU:175:SER:OG   | 2.16                     | 0.46              |
| 4:I:138:MET:O     | 4:I:142:THR:OG1   | 2.28                     | 0.46              |
| 5:N:11:ILE:CG2    | 1:6:372:ILE:HB    | 2.45                     | 0.46              |
| 6:Q:113:SER:O     | 6:Q:117:GLN:HG3   | 2.15                     | 0.46              |
| 6:U:76:GLN:OE1    | 1:2:297:GLN:OE1   | 2.33                     | 0.46              |
| 7:X:43:ARG:HD2    | 7:X:69:GLU:OE2    | 2.14                     | 0.46              |
| 1:t:244:ARG:HH22  | 1:AQ:235:LEU:HD13 | 1.81                     | 0.46              |
| 1:t:296:ARG:HG2   | 1:t:296:ARG:HH11  | 1.80                     | 0.46              |
| 1:3:235:LEU:HD13  | 1:4:244:ARG:HH22  | 1.81                     | 0.46              |
| 1:AN:235:LEU:HD13 | 1:AO:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:UM:73:MET:HE1   | 1:UM:99:ARG:HD2   | 1.95                     | 0.46              |
| 1:WH:197:LEU:HA   | 1:WI:175:SER:CB   | 2.46                     | 0.46              |
| 1:WK:197:LEU:HD13 | 1:WL:175:SER:OG   | 2.16                     | 0.46              |
| 1:WQ:124:SER:OG   | 2:A:75:ASP:OD1    | 2.33                     | 0.46              |
| 1:WU:167:ARG:NH1  | 4:G:158:PRO:HD3   | 2.30                     | 0.46              |
| 1:WW:187:ASP:N    | 1:WW:190:GLN:HB2  | 2.31                     | 0.46              |
| 2:C:85:PRO:HG3    | 4:I:238:SER:HA    | 1.97                     | 0.46              |
| 3:E:86:PHE:HZ     | 4:F:87:GLN:O      | 1.97                     | 0.46              |
| 4:F:150:PHE:CZ    | 4:F:172:PRO:HB2   | 2.51                     | 0.46              |
| 4:G:97:THR:O      | 4:G:101:MET:HG2   | 2.16                     | 0.46              |
| 4:G:171:LEU:HB3   | 4:G:172:PRO:HD3   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:U:65:LEU:HG     | 6:U:75:ALA:CA     | 2.46                     | 0.46              |
| 1:z:235:LEU:HD13  | 1:1:244:ARG:HH22  | 1.81                     | 0.46              |
| 1:1:235:LEU:HD13  | 1:2:244:ARG:HH22  | 1.81                     | 0.46              |
| 1:5:235:LEU:HD13  | 1:6:244:ARG:HH22  | 1.81                     | 0.46              |
| 1:AO:235:LEU:HD13 | 1:AP:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:UK:136:LEU:HD23 | 1:UK:157:LEU:CD1  | 2.45                     | 0.46              |
| 1:UL:98:LEU:HD11  | 1:UL:143:THR:O    | 2.16                     | 0.46              |
| 1:UL:136:LEU:HD23 | 1:UL:157:LEU:CD1  | 2.45                     | 0.46              |
| 1:UN:103:GLN:CG   | 1:WS:182:PRO:HB3  | 2.43                     | 0.46              |
| 1:WF:196:HIS:CD2  | 1:WG:219:LEU:HD22 | 2.51                     | 0.46              |
| 1:WF:200:SER:O    | 1:WG:158:ALA:HB2  | 2.16                     | 0.46              |
| 1:WI:165:PHE:HB2  | 4:J:159:LEU:O     | 2.16                     | 0.46              |
| 1:WW:135:ALA:O    | 1:WW:139:GLU:HG2  | 2.16                     | 0.46              |
| 2:C:15:LYS:HB2    | 2:C:15:LYS:HE2    | 1.70                     | 0.46              |
| 2:C:24:LEU:HD11   | 2:C:62:ILE:HD11   | 1.96                     | 0.46              |
| 6:R:66:THR:OG1    | 1:AJ:294:ARG:CG   | 2.64                     | 0.46              |
| 7:a:3:LEU:HB2     | 1:b:319:GLN:HE21  | 1.80                     | 0.46              |
| 1:AC:235:LEU:HD13 | 1:AD:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:WI:147:LEU:O    | 1:WI:148:GLY:C    | 2.60                     | 0.45              |
| 1:WP:142:ARG:O    | 1:WP:146:THR:HG23 | 2.16                     | 0.45              |
| 1:WP:197:LEU:CD1  | 1:WQ:175:SER:OG   | 2.58                     | 0.45              |
| 2:A:84:LEU:HD21   | 4:G:185:ILE:HG23  | 1.97                     | 0.45              |
| 5:O:14:LEU:CD2    | 1:y:278:THR:HG21  | 2.46                     | 0.45              |
| 1:t:235:LEU:HD13  | 1:u:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:AB:235:LEU:HD13 | 1:AC:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:AE:235:LEU:HD13 | 1:AF:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:WE:135:ALA:O    | 1:WE:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WG:135:ALA:O    | 1:WG:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WK:145:GLU:O    | 1:WK:147:LEU:N    | 2.49                     | 0.45              |
| 1:WN:200:SER:HB2  | 1:WO:173:SER:CB   | 2.45                     | 0.45              |
| 1:WP:135:ALA:O    | 1:WP:139:GLU:HG2  | 2.16                     | 0.45              |
| 3:E:108:LEU:HA    | 3:E:108:LEU:HD23  | 1.76                     | 0.45              |
| 4:H:109:TYR:HA    | 4:H:113:TYR:HB3   | 1.98                     | 0.45              |
| 4:I:48:ILE:HD11   | 5:O:89:ARG:HH12   | 1.81                     | 0.45              |
| 6:T:115:LYS:HE2   | 7:Z:4:LEU:HD21    | 1.97                     | 0.45              |
| 6:U:130:MET:HE2   | 6:U:130:MET:HB2   | 1.87                     | 0.45              |
| 1:6:235:LEU:HD13  | 1:7:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:UI:94:HIS:HB2   | 1:UI:146:THR:HG21 | 1.97                     | 0.45              |
| 1:UO:94:HIS:HB2   | 1:UO:146:THR:HG21 | 1.97                     | 0.45              |
| 1:UP:98:LEU:HD11  | 1:UP:143:THR:O    | 2.16                     | 0.45              |
| 1:WH:145:GLU:O    | 1:WH:146:THR:C    | 2.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WP:190:GLN:C    | 1:WP:192:SER:N    | 2.73                     | 0.45              |
| 1:WU:112:GLY:HA2  | 1:WU:139:GLU:OE1  | 2.17                     | 0.45              |
| 2:D:7:MET:HA      | 2:D:7:MET:HE3     | 1.97                     | 0.45              |
| 4:G:205:MET:CE    | 4:H:209:MET:HA    | 2.45                     | 0.45              |
| 4:I:190:PHE:CD1   | 4:J:220:PRO:HG3   | 2.52                     | 0.45              |
| 5:N:7:ILE:HD11    | 1:7:370:ARG:NH2   | 2.30                     | 0.45              |
| 5:N:69:ASN:HB2    | 6:T:16:LEU:HD23   | 1.98                     | 0.45              |
| 1:AA:235:LEU:HD13 | 1:AB:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:AI:235:LEU:HD13 | 1:AJ:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:UK:98:LEU:HD11  | 1:UK:143:THR:O    | 2.16                     | 0.45              |
| 1:WA:217:GLY:HA3  | 1:WW:190:GLN:HG2  | 1.98                     | 0.45              |
| 1:WH:139:GLU:HB3  | 1:WI:154:ARG:HH21 | 1.80                     | 0.45              |
| 1:WJ:181:GLU:O    | 1:WJ:182:PRO:C    | 2.60                     | 0.45              |
| 1:WM:135:ALA:O    | 1:WM:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WM:181:GLU:O    | 1:WM:182:PRO:C    | 2.60                     | 0.45              |
| 1:WQ:160:PRO:HG2  | 1:WQ:170:LYS:O    | 2.16                     | 0.45              |
| 1:WS:124:SER:HB2  | 2:A:8:MET:HE3     | 1.95                     | 0.45              |
| 1:WU:181:GLU:O    | 1:WU:182:PRO:C    | 2.60                     | 0.45              |
| 1:WV:190:GLN:HG2  | 1:WW:217:GLY:HA3  | 1.97                     | 0.45              |
| 2:D:14:MET:HE2    | 3:E:229:MET:SD    | 2.56                     | 0.45              |
| 3:E:158:PRO:HD2   | 3:E:162:ASN:ND2   | 2.32                     | 0.45              |
| 4:H:66:ARG:HB2    | 4:H:178:GLU:OE1   | 2.17                     | 0.45              |
| 5:K:86:ILE:HG12   | 5:P:102:MET:CE    | 2.46                     | 0.45              |
| 6:Q:104:ARG:O     | 6:Q:108:GLN:HG2   | 2.17                     | 0.45              |
| 6:S:33:ALA:O      | 6:S:98:ASN:ND2    | 2.50                     | 0.45              |
| 1:AL:235:LEU:HD13 | 1:AM:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:UI:136:LEU:HD23 | 1:UI:157:LEU:CD1  | 2.45                     | 0.45              |
| 1:UJ:88:VAL:O     | 1:UJ:89:PRO:C     | 2.60                     | 0.45              |
| 1:UK:207:PRO:HG2  | 1:WE:187:ASP:OD1  | 2.10                     | 0.45              |
| 1:UL:164:LEU:HD22 | 1:UL:164:LEU:H    | 1.81                     | 0.45              |
| 1:UM:164:LEU:HD22 | 1:UM:164:LEU:H    | 1.82                     | 0.45              |
| 1:WC:164:LEU:HB3  | 4:H:152:ARG:NH2   | 2.30                     | 0.45              |
| 1:WC:193:ALA:HB1  | 1:WD:213:VAL:HG21 | 1.98                     | 0.45              |
| 1:WD:145:GLU:C    | 1:WD:147:LEU:N    | 2.74                     | 0.45              |
| 1:WL:181:GLU:O    | 1:WL:182:PRO:C    | 2.60                     | 0.45              |
| 1:WP:147:LEU:O    | 1:WP:148:GLY:C    | 2.58                     | 0.45              |
| 1:WP:200:SER:HG   | 1:WQ:175:SER:HB2  | 1.79                     | 0.45              |
| 1:WQ:135:ALA:O    | 1:WQ:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WT:135:ALA:O    | 1:WT:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WT:190:GLN:HG2  | 1:WU:217:GLY:HA3  | 1.99                     | 0.45              |
| 2:A:58:VAL:HG21   | 4:G:207:LEU:HD21  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:9:MET:HE1     | 4:J:188:THR:HB    | 1.99                     | 0.45              |
| 6:S:128:LYS:HE2   | 7:X:134:GLN:HG2   | 1.98                     | 0.45              |
| 1:v:235:LEU:HD13  | 1:w:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:2:235:LEU:HD13  | 1:3:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:7:235:LEU:HD13  | 1:8:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:AG:235:LEU:HD13 | 1:AH:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:AJ:235:LEU:HD13 | 1:AK:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:UI:88:VAL:O     | 1:UI:89:PRO:C     | 2.60                     | 0.45              |
| 1:UK:80:ALA:N     | 1:UK:85:ALA:O     | 2.49                     | 0.45              |
| 1:WB:164:LEU:HD23 | 1:WB:164:LEU:HA   | 1.75                     | 0.45              |
| 1:WC:131:ASN:O    | 1:WC:132:TYR:C    | 2.60                     | 0.45              |
| 1:WF:114:GLU:HA   | 1:WF:117:ASP:HB2  | 1.99                     | 0.45              |
| 1:WG:190:GLN:HG3  | 1:WH:217:GLY:HA3  | 1.99                     | 0.45              |
| 1:WI:197:LEU:HD13 | 1:WJ:175:SER:OG   | 2.09                     | 0.45              |
| 1:WR:181:GLU:O    | 1:WR:182:PRO:C    | 2.60                     | 0.45              |
| 1:WV:135:ALA:O    | 1:WV:139:GLU:HG2  | 2.16                     | 0.45              |
| 5:N:15:GLN:HG3    | 5:N:16:ALA:N      | 2.30                     | 0.45              |
| 5:O:15:GLN:HG3    | 5:O:16:ALA:N      | 2.30                     | 0.45              |
| 5:P:15:GLN:HG3    | 5:P:16:ALA:N      | 2.30                     | 0.45              |
| 5:P:61:LEU:HD21   | 6:U:50:LYS:NZ     | 2.31                     | 0.45              |
| 6:Q:11:PHE:HD1    | 6:Q:53:MET:HE2    | 1.82                     | 0.45              |
| 6:T:78:VAL:CG1    | 1:6:361:ASN:ND2   | 2.78                     | 0.45              |
| 1:UM:94:HIS:HB2   | 1:UM:146:THR:HG21 | 1.97                     | 0.45              |
| 1:UN:52:ARG:O     | 1:UN:88:VAL:N     | 2.38                     | 0.45              |
| 1:WA:187:ASP:OD2  | 1:WA:190:GLN:HG3  | 2.16                     | 0.45              |
| 1:WD:129:GLN:O    | 1:WD:130:VAL:C    | 2.60                     | 0.45              |
| 1:WF:124:SER:O    | 1:WF:125:GLN:C    | 2.59                     | 0.45              |
| 1:WF:128:GLU:CG   | 1:WG:126:PHE:CD2  | 2.98                     | 0.45              |
| 1:WJ:135:ALA:O    | 1:WJ:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WP:181:GLU:O    | 1:WP:182:PRO:C    | 2.60                     | 0.45              |
| 1:WS:137:GLU:HG3  | 1:WS:155:VAL:O    | 2.16                     | 0.45              |
| 1:WT:167:ARG:HG2  | 1:WT:168:GLU:N    | 2.31                     | 0.45              |
| 1:WT:181:GLU:O    | 1:WT:182:PRO:C    | 2.60                     | 0.45              |
| 1:WW:219:LEU:HG   | 1:WW:221:THR:H    | 1.82                     | 0.45              |
| 4:G:59:LEU:HD11   | 5:L:102:MET:HE1   | 1.99                     | 0.45              |
| 4:G:204:LEU:HD12  | 4:G:214:PRO:HB3   | 1.99                     | 0.45              |
| 1:u:235:LEU:HD13  | 1:v:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:WB:112:GLY:HA2  | 1:WB:139:GLU:OE1  | 2.17                     | 0.45              |
| 1:WC:169:GLN:NE2  | 1:WC:170:LYS:O    | 2.44                     | 0.45              |
| 1:WG:181:GLU:O    | 1:WG:182:PRO:C    | 2.60                     | 0.45              |
| 1:WH:167:ARG:HH22 | 4:J:162:PRO:HG2   | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WH:181:GLU:O    | 1:WH:182:PRO:C    | 2.60                     | 0.45              |
| 1:WK:193:ALA:HB1  | 1:WL:213:VAL:HG11 | 1.98                     | 0.45              |
| 1:WN:181:GLU:O    | 1:WN:182:PRO:C    | 2.60                     | 0.45              |
| 1:WQ:145:GLU:C    | 1:WQ:147:LEU:N    | 2.75                     | 0.45              |
| 1:WS:219:LEU:HG   | 1:WS:221:THR:H    | 1.82                     | 0.45              |
| 1:WV:164:LEU:HB3  | 4:G:152:ARG:HH12  | 1.82                     | 0.45              |
| 1:WW:181:GLU:O    | 1:WW:182:PRO:C    | 2.60                     | 0.45              |
| 2:D:60:ILE:O      | 2:D:64:VAL:HG22   | 2.17                     | 0.45              |
| 4:J:239:LEU:HD12  | 4:J:239:LEU:HA    | 1.84                     | 0.45              |
| 5:P:64:PRO:CG     | 1:b:322:PRO:HB3   | 2.47                     | 0.45              |
| 1:w:235:LEU:HD13  | 1:x:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:9:235:LEU:HD13  | 1:0:244:ARG:HH22  | 1.81                     | 0.45              |
| 1:UL:129:GLN:O    | 1:UL:133:GLN:N    | 2.29                     | 0.45              |
| 1:UM:80:ALA:N     | 1:UM:85:ALA:O     | 2.49                     | 0.45              |
| 1:UP:167:ARG:HH11 | 1:8:236:LYS:CE    | 2.29                     | 0.45              |
| 1:WB:113:PHE:CE2  | 1:WB:139:GLU:HG3  | 2.52                     | 0.45              |
| 1:WD:147:LEU:O    | 1:WD:148:GLY:C    | 2.59                     | 0.45              |
| 1:WE:164:LEU:CD2  | 4:I:159:LEU:HD22  | 2.46                     | 0.45              |
| 1:WI:181:GLU:O    | 1:WI:182:PRO:C    | 2.60                     | 0.45              |
| 1:WU:164:LEU:CA   | 4:G:152:ARG:HG3   | 2.47                     | 0.45              |
| 2:A:10:GLY:O      | 2:A:14:MET:HG2    | 2.16                     | 0.45              |
| 4:H:90:LEU:HG     | 5:M:104:VAL:CG2   | 2.47                     | 0.45              |
| 4:J:221:PHE:O     | 4:J:224:MET:HE2   | 2.17                     | 0.45              |
| 7:a:128:LYS:O     | 7:a:131:THR:HG22  | 2.17                     | 0.45              |
| 1:AF:235:LEU:HD13 | 1:AG:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:UK:88:VAL:O     | 1:UK:89:PRO:C     | 2.60                     | 0.45              |
| 1:UL:216:SER:C    | 1:UL:218:HIS:N    | 2.75                     | 0.45              |
| 1:UM:98:LEU:HD11  | 1:UM:143:THR:O    | 2.16                     | 0.45              |
| 1:UN:80:ALA:N     | 1:UN:85:ALA:O     | 2.49                     | 0.45              |
| 1:UO:164:LEU:HD22 | 1:UO:164:LEU:H    | 1.82                     | 0.45              |
| 1:WD:167:ARG:C    | 1:WD:167:ARG:HE   | 2.25                     | 0.45              |
| 1:WE:181:GLU:O    | 1:WE:182:PRO:C    | 2.60                     | 0.45              |
| 1:WF:135:ALA:O    | 1:WF:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:WO:219:LEU:HG   | 1:WO:221:THR:H    | 1.82                     | 0.45              |
| 3:E:8:GLN:O       | 3:E:12:TRP:HD1    | 2.00                     | 0.45              |
| 3:E:144:LEU:HB3   | 4:J:149:LEU:HD22  | 1.98                     | 0.45              |
| 4:J:114:GLN:HB3   | 4:J:115:PRO:HD3   | 1.99                     | 0.45              |
| 5:P:7:ILE:HD11    | 1:u:370:ARG:HH21  | 1.82                     | 0.45              |
| 7:V:112:TYR:CD1   | 7:a:125:MET:HG3   | 2.51                     | 0.45              |
| 1:AM:235:LEU:HD13 | 1:AN:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:WH:135:ALA:O    | 1:WH:139:GLU:HG2  | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WI:165:PHE:CE2  | 4:J:162:PRO:HA    | 2.53                     | 0.44              |
| 1:WR:143:THR:O    | 1:WR:146:THR:OG1  | 2.30                     | 0.44              |
| 1:WU:135:ALA:O    | 1:WU:139:GLU:HG2  | 2.16                     | 0.44              |
| 1:WW:192:SER:O    | 1:WW:195:VAL:HB   | 2.17                     | 0.44              |
| 2:C:27:VAL:HG22   | 2:C:57:ALA:HB1    | 1.99                     | 0.44              |
| 6:S:31:ALA:HB1    | 7:X:13:ALA:HB2    | 1.98                     | 0.44              |
| 6:S:73:ILE:HD12   | 1:AD:363:THR:HG23 | 1.98                     | 0.44              |
| 7:W:20:ARG:HD3    | 1:e:313:PRO:HG2   | 1.99                     | 0.44              |
| 7:W:86:ASP:OD1    | 7:W:86:ASP:N      | 2.41                     | 0.44              |
| 1:y:235:LEU:HD13  | 1:z:244:ARG:HH22  | 1.81                     | 0.44              |
| 1:UI:103:GLN:NE2  | 1:WB:182:PRO:HB3  | 2.32                     | 0.44              |
| 1:UJ:55:PHE:O     | 1:UJ:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UJ:103:GLN:OE1  | 1:WD:182:PRO:CG   | 2.65                     | 0.44              |
| 1:UL:88:VAL:O     | 1:UL:89:PRO:C     | 2.60                     | 0.44              |
| 1:UN:88:VAL:O     | 1:UN:89:PRO:C     | 2.60                     | 0.44              |
| 1:UN:98:LEU:HD11  | 1:UN:143:THR:O    | 2.16                     | 0.44              |
| 1:WB:166:VAL:O    | 4:H:152:ARG:CD    | 2.63                     | 0.44              |
| 1:WC:131:ASN:O    | 1:WC:134:ARG:N    | 2.51                     | 0.44              |
| 1:WC:190:GLN:C    | 1:WC:192:SER:H    | 2.23                     | 0.44              |
| 1:WE:161:LYS:H    | 1:WE:161:LYS:HD3  | 1.82                     | 0.44              |
| 1:WV:187:ASP:N    | 1:WV:190:GLN:HB2  | 2.31                     | 0.44              |
| 2:B:2:THR:HG23    | 2:B:5:SER:H       | 1.82                     | 0.44              |
| 2:B:20:LEU:HD11   | 2:B:73:LEU:HD13   | 2.00                     | 0.44              |
| 4:H:101:MET:HE3   | 4:H:101:MET:HB3   | 1.77                     | 0.44              |
| 5:K:15:GLN:HG3    | 5:K:16:ALA:N      | 2.30                     | 0.44              |
| 5:L:7:ILE:CG1     | 1:AI:370:ARG:HH21 | 2.26                     | 0.44              |
| 5:M:3:ALA:C       | 1:AC:372:ILE:HD12 | 2.42                     | 0.44              |
| 5:M:70:ASP:OD1    | 6:S:13:GLN:NE2    | 2.50                     | 0.44              |
| 6:S:65:LEU:HD11   | 1:AD:365:ASN:ND2  | 2.32                     | 0.44              |
| 6:S:73:ILE:HD13   | 1:AE:297:GLN:CB   | 2.35                     | 0.44              |
| 6:S:109:PHE:CZ    | 7:X:118:VAL:HG13  | 2.53                     | 0.44              |
| 1:4:235:LEU:HD13  | 1:5:244:ARG:HH22  | 1.81                     | 0.44              |
| 1:AP:235:LEU:HD13 | 1:AQ:244:ARG:HH22 | 1.81                     | 0.44              |
| 1:UI:98:LEU:HD11  | 1:UI:143:THR:O    | 2.16                     | 0.44              |
| 1:UK:164:LEU:H    | 1:UK:164:LEU:HD22 | 1.82                     | 0.44              |
| 1:UL:55:PHE:O     | 1:UL:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UM:75:ILE:HG21  | 1:UM:96:LEU:HD11  | 2.00                     | 0.44              |
| 1:UN:164:LEU:H    | 1:UN:164:LEU:HD22 | 1.82                     | 0.44              |
| 1:WN:200:SER:C    | 1:WO:173:SER:OG   | 2.60                     | 0.44              |
| 1:WP:186:LEU:HA   | 1:WP:190:GLN:OE1  | 2.17                     | 0.44              |
| 1:WQ:181:GLU:O    | 1:WQ:182:PRO:C    | 2.60                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WR:142:ARG:O    | 1:WR:146:THR:HG23 | 2.16                     | 0.44              |
| 3:E:75:MET:O      | 3:E:79:LEU:HG     | 2.17                     | 0.44              |
| 4:G:57:ILE:O      | 4:G:61:MET:HB2    | 2.17                     | 0.44              |
| 4:J:204:LEU:HD11  | 4:J:217:ILE:HD12  | 1.99                     | 0.44              |
| 7:X:49:PHE:CG     | 1:g:313:PRO:HG3   | 2.52                     | 0.44              |
| 1:UJ:94:HIS:HB2   | 1:UJ:146:THR:HG21 | 1.97                     | 0.44              |
| 1:UO:88:VAL:O     | 1:UO:89:PRO:C     | 2.60                     | 0.44              |
| 1:WF:166:VAL:HG22 | 1:WF:168:GLU:H    | 1.82                     | 0.44              |
| 1:WO:190:GLN:NE2  | 1:WP:216:SER:O    | 2.50                     | 0.44              |
| 1:WQ:187:ASP:OD1  | 1:WQ:188:GLU:N    | 2.51                     | 0.44              |
| 1:WR:135:ALA:O    | 1:WR:139:GLU:HG2  | 2.16                     | 0.44              |
| 1:WS:145:GLU:C    | 1:WS:147:LEU:N    | 2.75                     | 0.44              |
| 1:WT:134:ARG:HH21 | 1:WT:134:ARG:HB3  | 1.83                     | 0.44              |
| 1:WU:158:ALA:O    | 1:WU:160:PRO:HD3  | 2.18                     | 0.44              |
| 2:D:7:MET:HE2     | 3:E:233:MET:O     | 2.17                     | 0.44              |
| 5:P:14:LEU:HD21   | 1:t:370:ARG:HH21  | 1.83                     | 0.44              |
| 6:S:72:HIS:CA     | 1:AE:295:SER:HB3  | 2.45                     | 0.44              |
| 1:UM:160:PRO:HG2  | 1:UM:170:LYS:HB3  | 2.00                     | 0.44              |
| 1:WA:160:PRO:O    | 1:WA:161:LYS:C    | 2.61                     | 0.44              |
| 1:WA:196:HIS:NE2  | 1:WB:219:LEU:HD22 | 2.33                     | 0.44              |
| 1:WQ:171:SER:HB3  | 1:WQ:206:PRO:HD3  | 2.00                     | 0.44              |
| 1:WS:197:LEU:CD1  | 1:WT:175:SER:OG   | 2.64                     | 0.44              |
| 1:WT:128:GLU:CG   | 1:WU:126:PHE:CD2  | 2.99                     | 0.44              |
| 4:F:100:ILE:HG23  | 4:F:101:MET:CE    | 2.47                     | 0.44              |
| 4:H:127:LEU:HD23  | 4:H:127:LEU:HA    | 1.88                     | 0.44              |
| 5:L:75:MET:HE3    | 5:L:75:MET:HB3    | 1.83                     | 0.44              |
| 5:M:21:ALA:HB3    | 1:O:278:THR:HG21  | 1.97                     | 0.44              |
| 1:AD:235:LEU:HD13 | 1:AE:244:ARG:HH22 | 1.81                     | 0.44              |
| 1:UI:55:PHE:O     | 1:UI:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UJ:100:LEU:HD23 | 1:UJ:103:GLN:HE21 | 1.83                     | 0.44              |
| 1:UK:55:PHE:O     | 1:UK:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UN:75:ILE:HG21  | 1:UN:96:LEU:HD11  | 2.00                     | 0.44              |
| 1:UP:80:ALA:N     | 1:UP:85:ALA:O     | 2.49                     | 0.44              |
| 1:WF:148:GLY:N    | 1:WG:215:GLN:O    | 2.39                     | 0.44              |
| 1:WI:167:ARG:CG   | 4:J:160:GLN:O     | 2.65                     | 0.44              |
| 1:WK:181:GLU:O    | 1:WK:182:PRO:C    | 2.60                     | 0.44              |
| 1:WV:181:GLU:O    | 1:WV:182:PRO:C    | 2.60                     | 0.44              |
| 3:E:123:PRO:HB2   | 3:E:126:ALA:HB3   | 1.99                     | 0.44              |
| 4:F:213:PRO:HA    | 4:F:214:PRO:HD3   | 1.91                     | 0.44              |
| 4:I:147:LEU:HD21  | 4:I:165:VAL:HG11  | 2.00                     | 0.44              |
| 6:Q:49:LEU:O      | 6:Q:53:MET:HG2    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:z:429:THR:OG1   | 1:1:418:GLU:OE2   | 2.36                     | 0.44              |
| 1:UL:160:PRO:HG2  | 1:UL:170:LYS:HB3  | 2.00                     | 0.44              |
| 1:WB:113:PHE:HB3  | 1:WC:134:ARG:CZ   | 2.48                     | 0.44              |
| 1:WB:142:ARG:O    | 1:WB:146:THR:HG23 | 2.17                     | 0.44              |
| 1:WD:191:ILE:O    | 1:WD:195:VAL:HG23 | 2.17                     | 0.44              |
| 1:WE:200:SER:O    | 1:WF:158:ALA:HB3  | 2.18                     | 0.44              |
| 1:WF:181:GLU:O    | 1:WF:182:PRO:C    | 2.60                     | 0.44              |
| 1:WH:219:LEU:HG   | 1:WH:221:THR:H    | 1.82                     | 0.44              |
| 1:WJ:145:GLU:HG2  | 1:WJ:153:ALA:N    | 2.33                     | 0.44              |
| 1:WJ:164:LEU:HD21 | 3:E:144:LEU:C     | 2.42                     | 0.44              |
| 1:WN:219:LEU:HG   | 1:WN:221:THR:H    | 1.82                     | 0.44              |
| 1:WP:196:HIS:CD2  | 1:WQ:219:LEU:HD13 | 2.52                     | 0.44              |
| 1:WS:168:GLU:O    | 1:WS:169:GLN:HB3  | 2.18                     | 0.44              |
| 5:O:11:ILE:HG22   | 1:z:372:ILE:CG2   | 2.47                     | 0.44              |
| 7:a:3:LEU:H       | 1:b:319:GLN:HE21  | 1.66                     | 0.44              |
| 1:u:429:THR:OG1   | 1:v:418:GLU:OE2   | 2.36                     | 0.44              |
| 1:w:429:THR:OG1   | 1:x:418:GLU:OE2   | 2.36                     | 0.44              |
| 1:UL:94:HIS:HB2   | 1:UL:146:THR:HG21 | 1.97                     | 0.44              |
| 1:UO:55:PHE:O     | 1:UO:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UO:75:ILE:HG21  | 1:UO:96:LEU:HD11  | 2.00                     | 0.44              |
| 1:WB:190:GLN:O    | 1:WB:191:ILE:C    | 2.61                     | 0.44              |
| 1:WC:130:VAL:HG12 | 1:WC:134:ARG:HD2  | 1.99                     | 0.44              |
| 1:WC:200:SER:O    | 1:WD:158:ALA:HB3  | 2.14                     | 0.44              |
| 1:WE:164:LEU:HD13 | 1:WE:165:PHE:H    | 1.82                     | 0.44              |
| 1:WG:164:LEU:HD13 | 1:WG:164:LEU:HA   | 1.80                     | 0.44              |
| 1:WO:200:SER:HG   | 1:WP:175:SER:HB2  | 1.76                     | 0.44              |
| 1:WS:125:GLN:CB   | 2:A:4:GLU:HB2     | 2.40                     | 0.44              |
| 1:WW:134:ARG:HH21 | 1:WW:134:ARG:CB   | 2.30                     | 0.44              |
| 3:E:193:LEU:O     | 3:E:196:THR:OG1   | 2.26                     | 0.44              |
| 4:I:212:VAL:HG21  | 4:I:217:ILE:HD11  | 2.00                     | 0.44              |
| 5:N:21:ALA:HB3    | 1:4:278:THR:CG2   | 2.31                     | 0.44              |
| 1:AP:429:THR:OG1  | 1:AQ:418:GLU:OE2  | 2.36                     | 0.44              |
| 1:UI:80:ALA:N     | 1:UI:85:ALA:O     | 2.49                     | 0.44              |
| 1:UK:160:PRO:HG2  | 1:UK:170:LYS:HB3  | 2.00                     | 0.44              |
| 1:UM:55:PHE:O     | 1:UM:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UO:160:PRO:HG2  | 1:UO:170:LYS:HB3  | 2.00                     | 0.44              |
| 1:UP:55:PHE:O     | 1:UP:85:ALA:HA    | 2.18                     | 0.44              |
| 1:UP:88:VAL:O     | 1:UP:89:PRO:C     | 2.60                     | 0.44              |
| 1:WB:167:ARG:C    | 1:WB:169:GLN:H    | 2.25                     | 0.44              |
| 1:WC:190:GLN:C    | 1:WC:192:SER:N    | 2.72                     | 0.44              |
| 1:WJ:125:GLN:HB3  | 3:E:242:HIS:HB2   | 1.97                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WL:219:LEU:HG   | 1:WL:221:THR:H    | 1.82                     | 0.44              |
| 1:WM:187:ASP:OD1  | 1:WM:190:GLN:N    | 2.44                     | 0.44              |
| 1:WO:181:GLU:O    | 1:WO:182:PRO:C    | 2.60                     | 0.44              |
| 1:WP:190:GLN:C    | 1:WP:192:SER:H    | 2.24                     | 0.44              |
| 1:WR:190:GLN:HG2  | 1:WS:217:GLY:HA3  | 2.00                     | 0.44              |
| 1:WS:193:ALA:HB1  | 1:WT:213:VAL:CG1  | 2.48                     | 0.44              |
| 4:F:123:MET:HE3   | 4:F:123:MET:HB3   | 1.84                     | 0.44              |
| 6:S:67:LEU:HD21   | 6:S:74:PRO:HA     | 2.00                     | 0.44              |
| 7:Z:97:ASP:O      | 7:Z:101:GLU:HG2   | 2.18                     | 0.44              |
| 1:3:429:THR:OG1   | 1:4:418:GLU:OE2   | 2.36                     | 0.44              |
| 1:AC:429:THR:OG1  | 1:AD:418:GLU:OE2  | 2.36                     | 0.44              |
| 1:UI:160:PRO:HG2  | 1:UI:170:LYS:HB3  | 2.00                     | 0.43              |
| 1:UI:164:LEU:HD22 | 1:UI:164:LEU:H    | 1.82                     | 0.43              |
| 1:UP:75:ILE:HG21  | 1:UP:96:LEU:HD11  | 2.00                     | 0.43              |
| 1:UP:164:LEU:H    | 1:UP:164:LEU:HD22 | 1.81                     | 0.43              |
| 1:WE:167:ARG:HH21 | 4:I:162:PRO:CD    | 2.30                     | 0.43              |
| 1:WM:219:LEU:HG   | 1:WM:221:THR:H    | 1.82                     | 0.43              |
| 1:WS:181:GLU:O    | 1:WS:182:PRO:C    | 2.60                     | 0.43              |
| 1:WT:192:SER:O    | 1:WT:195:VAL:HB   | 2.18                     | 0.43              |
| 1:WV:117:ASP:OD1  | 1:WW:120:LYS:NZ   | 2.51                     | 0.43              |
| 1:WV:192:SER:O    | 1:WV:195:VAL:HB   | 2.18                     | 0.43              |
| 3:E:251:LEU:HD23  | 3:E:251:LEU:HA    | 1.84                     | 0.43              |
| 4:J:80:THR:CB     | 4:J:83:ALA:HB2    | 2.48                     | 0.43              |
| 5:N:14:LEU:HD11   | 1:6:370:ARG:NH2   | 2.32                     | 0.43              |
| 6:S:88:ARG:HH12   | 6:S:108:GLN:HG3   | 1.83                     | 0.43              |
| 6:U:73:ILE:HG13   | 1:2:295:SER:CB    | 2.43                     | 0.43              |
| 1:UJ:98:LEU:CD1   | 1:UJ:146:THR:HG1  | 2.31                     | 0.43              |
| 1:UJ:160:PRO:HG2  | 1:UJ:170:LYS:HB3  | 2.00                     | 0.43              |
| 1:UN:160:PRO:HG2  | 1:UN:170:LYS:HB3  | 2.00                     | 0.43              |
| 1:UP:73:MET:HE3   | 1:UP:99:ARG:CD    | 2.41                     | 0.43              |
| 1:WD:181:GLU:O    | 1:WD:182:PRO:C    | 2.60                     | 0.43              |
| 1:WH:139:GLU:HB3  | 1:WI:154:ARG:NH2  | 2.33                     | 0.43              |
| 1:WH:168:GLU:CD   | 1:WH:168:GLU:H    | 2.26                     | 0.43              |
| 2:D:52:ILE:HD13   | 2:D:52:ILE:HA     | 1.83                     | 0.43              |
| 4:J:195:ILE:O     | 4:J:199:VAL:HG13  | 2.18                     | 0.43              |
| 7:a:3:LEU:O       | 1:b:319:GLN:HG3   | 2.18                     | 0.43              |
| 1:UJ:103:GLN:CB   | 1:WD:182:PRO:HA   | 2.48                     | 0.43              |
| 1:UJ:167:ARG:NH1  | 1:2:236:LYS:NZ    | 2.60                     | 0.43              |
| 1:UM:88:VAL:O     | 1:UM:89:PRO:C     | 2.60                     | 0.43              |
| 1:UM:129:GLN:O    | 1:UM:133:GLN:N    | 2.29                     | 0.43              |
| 1:UN:218:HIS:NE2  | 1:AB:265:GLN:NE2  | 2.65                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:UO:98:LEU:HD11  | 1:UO:143:THR:O    | 2.16                     | 0.43              |
| 1:UP:125:GLN:C    | 1:UP:128:GLU:H    | 2.27                     | 0.43              |
| 1:UP:129:GLN:O    | 1:UP:133:GLN:N    | 2.29                     | 0.43              |
| 1:WM:142:ARG:O    | 1:WM:146:THR:HG23 | 2.18                     | 0.43              |
| 1:WS:113:PHE:HB3  | 1:WT:134:ARG:CZ   | 2.49                     | 0.43              |
| 2:A:37:ILE:HD13   | 2:B:44:ILE:HD11   | 2.00                     | 0.43              |
| 4:G:211:MET:HE1   | 4:H:210:MET:CE    | 2.48                     | 0.43              |
| 4:J:124:GLN:H     | 4:J:124:GLN:HG2   | 1.67                     | 0.43              |
| 6:R:68:THR:CG2    | 1:AJ:294:ARG:HD2  | 2.49                     | 0.43              |
| 7:a:6:ILE:HG22    | 1:b:315:ALA:O     | 2.18                     | 0.43              |
| 1:t:429:THR:OG1   | 1:u:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:x:429:THR:OG1   | 1:y:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:2:429:THR:OG1   | 1:3:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:AA:429:THR:OG1  | 1:AB:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:AE:429:THR:OG1  | 1:AF:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:AF:429:THR:OG1  | 1:AG:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:UI:73:MET:HE1   | 1:UI:99:ARG:HD2   | 1.95                     | 0.43              |
| 1:UK:129:GLN:O    | 1:UK:133:GLN:N    | 2.29                     | 0.43              |
| 1:UO:80:ALA:N     | 1:UO:85:ALA:O     | 2.49                     | 0.43              |
| 1:WD:172:PRO:HD2  | 1:WD:204:GLY:O    | 2.18                     | 0.43              |
| 1:WN:147:LEU:O    | 1:WN:148:GLY:C    | 2.60                     | 0.43              |
| 2:C:77:VAL:HG12   | 4:I:229:VAL:HG11  | 2.00                     | 0.43              |
| 3:E:179:ILE:H     | 3:E:179:ILE:HG13  | 1.69                     | 0.43              |
| 3:E:205:ASN:HB3   | 4:F:209:MET:HG3   | 2.00                     | 0.43              |
| 5:N:7:ILE:HD11    | 1:7:370:ARG:NE    | 2.32                     | 0.43              |
| 1:UJ:164:LEU:HD22 | 1:UJ:164:LEU:H    | 1.81                     | 0.43              |
| 1:UP:160:PRO:HG2  | 1:UP:170:LYS:HB3  | 2.00                     | 0.43              |
| 1:WD:193:ALA:HB1  | 1:WE:213:VAL:HG21 | 2.00                     | 0.43              |
| 1:WE:132:TYR:HB2  | 1:WF:126:PHE:HZ   | 1.83                     | 0.43              |
| 1:WL:172:PRO:HD2  | 1:WL:204:GLY:O    | 2.19                     | 0.43              |
| 1:WT:131:ASN:HA   | 1:WT:134:ARG:HD3  | 1.99                     | 0.43              |
| 1:WU:128:GLU:HG2  | 1:WV:126:PHE:CD2  | 2.48                     | 0.43              |
| 1:WW:187:ASP:H    | 1:WW:190:GLN:CD   | 2.26                     | 0.43              |
| 4:H:143:ARG:HH22  | 4:H:177:SER:HA    | 1.83                     | 0.43              |
| 5:K:84:MET:HE2    | 6:Q:134:LEU:HD21  | 2.00                     | 0.43              |
| 6:T:19:ARG:NH2    | 6:T:115:LYS:HD3   | 2.33                     | 0.43              |
| 6:T:117:GLN:HE22  | 7:Y:125:MET:CG    | 2.32                     | 0.43              |
| 1:d:319:GLN:OE1   | 1:AM:357:SER:OG   | 2.23                     | 0.43              |
| 1:t:418:GLU:OE2   | 1:AQ:429:THR:OG1  | 2.36                     | 0.43              |
| 1:y:429:THR:OG1   | 1:z:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:AH:429:THR:OG1  | 1:AI:418:GLU:OE2  | 2.36                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:429:THR:OG1  | 1:AN:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:UL:75:ILE:HG21  | 1:UL:96:LEU:HD11  | 2.00                     | 0.43              |
| 1:UN:129:GLN:O    | 1:UN:133:GLN:N    | 2.29                     | 0.43              |
| 1:WD:197:LEU:HD11 | 1:WE:156:HIS:HD2  | 1.84                     | 0.43              |
| 1:WI:136:LEU:O    | 1:WI:137:GLU:C    | 2.62                     | 0.43              |
| 1:WV:113:PHE:HB3  | 1:WW:134:ARG:NH1  | 2.33                     | 0.43              |
| 1:WV:200:SER:O    | 1:WW:158:ALA:HB3  | 2.16                     | 0.43              |
| 2:D:29:LEU:HD12   | 3:E:216:ILE:HG13  | 2.01                     | 0.43              |
| 4:F:63:SER:HB2    | 4:F:66:ARG:HH21   | 1.84                     | 0.43              |
| 4:G:119:GLN:HE22  | 6:R:4:ARG:HG2     | 1.84                     | 0.43              |
| 4:G:217:ILE:O     | 4:G:220:PRO:HD2   | 2.18                     | 0.43              |
| 4:H:121:ILE:HD12  | 4:H:121:ILE:HA    | 1.89                     | 0.43              |
| 4:I:59:LEU:HD21   | 5:N:102:MET:HE1   | 2.01                     | 0.43              |
| 5:N:59:PHE:CD2    | 5:N:59:PHE:C      | 2.97                     | 0.43              |
| 6:U:63:VAL:H      | 1:z:297:GLN:NE2   | 2.16                     | 0.43              |
| 1:AN:429:THR:OG1  | 1:AO:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:UI:75:ILE:HG21  | 1:UI:96:LEU:HD11  | 2.00                     | 0.43              |
| 1:UN:55:PHE:O     | 1:UN:85:ALA:HA    | 2.18                     | 0.43              |
| 1:WG:166:VAL:HG12 | 1:WG:168:GLU:H    | 1.83                     | 0.43              |
| 1:WH:166:VAL:HG12 | 4:J:147:LEU:HD12  | 2.00                     | 0.43              |
| 1:WP:166:VAL:HG21 | 4:F:160:GLN:HB3   | 1.82                     | 0.43              |
| 1:WR:192:SER:O    | 1:WR:195:VAL:HB   | 2.19                     | 0.43              |
| 3:E:224:VAL:O     | 3:E:228:LEU:HB2   | 2.18                     | 0.43              |
| 4:H:114:GLN:O     | 4:H:118:GLU:HG2   | 2.19                     | 0.43              |
| 1:1:429:THR:OG1   | 1:2:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:UI:125:GLN:C    | 1:UI:128:GLU:H    | 2.27                     | 0.43              |
| 1:UJ:102:GLN:CG   | 1:UJ:193:ALA:HB2  | 2.49                     | 0.43              |
| 1:UJ:125:GLN:C    | 1:UJ:128:GLU:H    | 2.27                     | 0.43              |
| 1:UL:103:GLN:HG2  | 1:WH:182:PRO:CB   | 2.46                     | 0.43              |
| 1:WE:164:LEU:HD21 | 4:I:159:LEU:HD22  | 2.00                     | 0.43              |
| 1:WH:186:LEU:HD22 | 1:WH:190:GLN:HG2  | 2.00                     | 0.43              |
| 1:WH:200:SER:O    | 1:WI:158:ALA:HB3  | 2.13                     | 0.43              |
| 1:WM:172:PRO:HD2  | 1:WM:204:GLY:O    | 2.18                     | 0.43              |
| 1:WS:142:ARG:O    | 1:WS:146:THR:HG23 | 2.17                     | 0.43              |
| 3:E:166:SER:C     | 3:E:168:ALA:H     | 2.27                     | 0.43              |
| 4:F:147:LEU:HD23  | 4:F:147:LEU:HA    | 1.87                     | 0.43              |
| 4:G:190:PHE:CD1   | 4:H:220:PRO:HG3   | 2.54                     | 0.43              |
| 4:H:141:GLN:NE2   | 4:H:243:PHE:HA    | 2.33                     | 0.43              |
| 6:T:68:THR:HG21   | 1:7:294:ARG:HD2   | 2.01                     | 0.43              |
| 6:T:68:THR:CG2    | 1:7:294:ARG:HD2   | 2.48                     | 0.43              |
| 7:W:7:PHE:CD2     | 7:W:119:LEU:HD11  | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:W:82:ASN:HD22   | 7:W:91:VAL:HG21   | 1.83                     | 0.43              |
| 1:5:429:THR:OG1   | 1:6:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:0:429:THR:OG1   | 1:AA:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:AJ:429:THR:OG1  | 1:AK:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:AO:429:THR:OG1  | 1:AP:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:UJ:80:ALA:N     | 1:UJ:85:ALA:O     | 2.49                     | 0.43              |
| 1:WA:187:ASP:OD1  | 1:WA:190:GLN:N    | 2.42                     | 0.43              |
| 1:WB:166:VAL:CG2  | 1:WB:169:GLN:HA   | 2.49                     | 0.43              |
| 1:WG:165:PHE:HE1  | 4:J:240:ALA:CB    | 2.18                     | 0.43              |
| 1:WN:172:PRO:HD2  | 1:WN:204:GLY:O    | 2.18                     | 0.43              |
| 1:WT:161:LYS:CB   | 1:WT:162:PRO:HD2  | 2.49                     | 0.43              |
| 1:WV:130:VAL:HG12 | 1:WV:134:ARG:HD2  | 1.99                     | 0.43              |
| 1:WV:164:LEU:O    | 1:WV:166:VAL:N    | 2.49                     | 0.43              |
| 1:WW:112:GLY:HA3  | 1:WW:135:ALA:HA   | 2.00                     | 0.43              |
| 2:B:2:THR:O       | 2:B:5:SER:OG      | 2.35                     | 0.43              |
| 3:E:49:MET:HE1    | 4:J:175:VAL:HG21  | 2.01                     | 0.43              |
| 4:F:97:THR:HA     | 4:F:100:ILE:HG22  | 2.00                     | 0.43              |
| 4:I:106:ASP:OD2   | 5:N:32:VAL:HG23   | 2.19                     | 0.43              |
| 5:N:14:LEU:HD23   | 1:5:278:THR:CG2   | 2.49                     | 0.43              |
| 7:V:122:VAL:O     | 7:V:126:MET:HG2   | 2.18                     | 0.43              |
| 1:6:429:THR:OG1   | 1:7:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:9:429:THR:OG1   | 1:0:418:GLU:OE2   | 2.36                     | 0.43              |
| 1:AD:429:THR:OG1  | 1:AE:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:AG:429:THR:OG1  | 1:AH:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:UL:125:GLN:C    | 1:UL:128:GLU:H    | 2.27                     | 0.43              |
| 1:WJ:197:LEU:HD13 | 1:WK:175:SER:OG   | 2.09                     | 0.43              |
| 1:WL:147:LEU:O    | 1:WL:148:GLY:C    | 2.61                     | 0.43              |
| 1:WP:163:SER:C    | 1:WP:165:PHE:N    | 2.76                     | 0.43              |
| 1:WT:124:SER:OG   | 2:A:4:GLU:OE2     | 2.33                     | 0.43              |
| 3:E:88:MET:HA     | 3:E:247:ILE:HG21  | 1.99                     | 0.43              |
| 5:O:4:ILE:HG12    | 1:1:372:ILE:HB    | 2.00                     | 0.43              |
| 6:S:65:LEU:HD23   | 6:S:75:ALA:CB     | 2.49                     | 0.43              |
| 1:4:290:LYS:HE3   | 1:4:290:LYS:HB2   | 1.93                     | 0.43              |
| 1:4:421:GLY:O     | 1:4:426:ARG:NH2   | 2.51                     | 0.43              |
| 1:UJ:52:ARG:O     | 1:UJ:88:VAL:N     | 2.38                     | 0.42              |
| 1:UK:94:HIS:HB2   | 1:UK:146:THR:HG21 | 1.97                     | 0.42              |
| 1:UK:102:GLN:CG   | 1:UK:193:ALA:HB2  | 2.49                     | 0.42              |
| 1:UK:125:GLN:C    | 1:UK:128:GLU:H    | 2.27                     | 0.42              |
| 1:UL:102:GLN:CG   | 1:UL:193:ALA:HB2  | 2.49                     | 0.42              |
| 1:WC:142:ARG:O    | 1:WC:146:THR:HG23 | 2.18                     | 0.42              |
| 1:WI:161:LYS:HA   | 1:WI:162:PRO:HD3  | 1.89                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:WQ:124:SER:CB  | 2:A:75:ASP:OD1    | 2.67                     | 0.42              |
| 1:WQ:124:SER:HA  | 2:A:75:ASP:OD1    | 2.19                     | 0.42              |
| 1:WQ:193:ALA:CB  | 1:WR:217:GLY:O    | 2.67                     | 0.42              |
| 2:D:45:ASN:OD1   | 2:D:45:ASN:N      | 2.49                     | 0.42              |
| 5:P:15:GLN:HB2   | 1:AQ:374:HIS:CG   | 2.53                     | 0.42              |
| 1:3:421:GLY:O    | 1:3:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:AB:429:THR:OG1 | 1:AC:418:GLU:OE2  | 2.36                     | 0.42              |
| 1:UK:75:ILE:HG21 | 1:UK:96:LEU:HD11  | 2.00                     | 0.42              |
| 1:UO:125:GLN:C   | 1:UO:128:GLU:H    | 2.27                     | 0.42              |
| 1:WA:181:GLU:O   | 1:WA:182:PRO:C    | 2.60                     | 0.42              |
| 1:WI:191:ILE:O   | 1:WI:195:VAL:HG23 | 2.19                     | 0.42              |
| 1:WJ:160:PRO:HG2 | 1:WJ:170:LYS:O    | 2.18                     | 0.42              |
| 1:WU:192:SER:O   | 1:WU:195:VAL:HB   | 2.19                     | 0.42              |
| 4:F:63:SER:O     | 4:F:67:ILE:HD12   | 2.19                     | 0.42              |
| 4:J:82:SER:OG    | 4:J:82:SER:O      | 2.37                     | 0.42              |
| 5:K:74:ASP:OD2   | 5:K:74:ASP:N      | 2.52                     | 0.42              |
| 6:Q:77:ALA:HB3   | 1:AP:297:GLN:HE22 | 1.84                     | 0.42              |
| 6:U:31:ALA:HB1   | 7:Z:13:ALA:HB2    | 2.00                     | 0.42              |
| 7:Z:3:LEU:HD12   | 7:Z:3:LEU:HA      | 1.92                     | 0.42              |
| 1:e:322:PRO:HA   | 1:e:323:PRO:HD3   | 1.94                     | 0.42              |
| 1:2:421:GLY:O    | 1:2:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:5:421:GLY:O    | 1:5:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:8:429:THR:OG1  | 1:9:418:GLU:OE2   | 2.36                     | 0.42              |
| 1:UN:99:ARG:O    | 1:UN:103:GLN:HG3  | 2.18                     | 0.42              |
| 1:UP:98:LEU:CD1  | 1:UP:146:THR:HG1  | 2.31                     | 0.42              |
| 1:WA:113:PHE:CE2 | 1:WA:139:GLU:HG3  | 2.54                     | 0.42              |
| 1:WB:181:GLU:O   | 1:WB:182:PRO:C    | 2.60                     | 0.42              |
| 1:WF:140:LEU:O   | 1:WF:144:ILE:HG13 | 2.19                     | 0.42              |
| 1:WK:128:GLU:OE1 | 1:WL:126:PHE:CE2  | 2.73                     | 0.42              |
| 1:WS:140:LEU:O   | 1:WS:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WT:140:LEU:O   | 1:WT:144:ILE:HG13 | 2.20                     | 0.42              |
| 2:C:84:LEU:HD21  | 4:I:185:ILE:HG23  | 2.01                     | 0.42              |
| 3:E:243:LEU:HD23 | 3:E:243:LEU:HA    | 1.81                     | 0.42              |
| 4:G:114:GLN:HB3  | 4:G:115:PRO:HD3   | 2.01                     | 0.42              |
| 4:G:161:GLY:O    | 4:G:162:PRO:C     | 2.62                     | 0.42              |
| 4:H:41:SER:HB2   | 5:N:82:MET:HE3    | 2.00                     | 0.42              |
| 5:N:7:ILE:CB     | 1:6:278:THR:HG21  | 2.50                     | 0.42              |
| 5:O:4:ILE:CD1    | 1:1:374:HIS:HB2   | 2.50                     | 0.42              |
| 6:Q:114:LEU:HD21 | 7:W:123:LYS:HG3   | 2.00                     | 0.42              |
| 6:R:69:SER:OG    | 1:AK:294:ARG:HD3  | 2.19                     | 0.42              |
| 7:V:13:ALA:HA    | 7:V:62:VAL:HG12   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:v:429:THR:OG1   | 1:w:418:GLU:OE2   | 2.36                     | 0.42              |
| 1:4:429:THR:OG1   | 1:5:418:GLU:OE2   | 2.36                     | 0.42              |
| 1:6:421:GLY:O     | 1:6:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:AJ:290:LYS:HE3  | 1:AJ:290:LYS:HB2  | 1.93                     | 0.42              |
| 1:AP:296:ARG:HG2  | 1:AP:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:UL:80:ALA:N     | 1:UL:85:ALA:O     | 2.49                     | 0.42              |
| 1:UN:125:GLN:C    | 1:UN:128:GLU:H    | 2.27                     | 0.42              |
| 1:WI:142:ARG:O    | 1:WI:146:THR:HG23 | 2.19                     | 0.42              |
| 1:WI:164:LEU:HD22 | 4:J:148:ALA:HA    | 2.01                     | 0.42              |
| 1:WN:140:LEU:O    | 1:WN:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WR:165:PHE:O    | 1:WR:166:VAL:HG22 | 2.19                     | 0.42              |
| 1:WT:113:PHE:CE1  | 1:WU:134:ARG:HG2  | 2.54                     | 0.42              |
| 5:L:7:ILE:HG22    | 1:AH:278:THR:HG21 | 2.01                     | 0.42              |
| 5:P:11:ILE:HG22   | 1:t:372:ILE:CB    | 2.49                     | 0.42              |
| 6:S:103:ASP:OD1   | 7:Y:112:TYR:OH    | 2.36                     | 0.42              |
| 1:5:296:ARG:HG2   | 1:5:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:AQ:296:ARG:HG2  | 1:AQ:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:UN:69:GLN:HG3   | 1:UN:103:GLN:OE1  | 2.19                     | 0.42              |
| 1:UP:94:HIS:HB2   | 1:UP:146:THR:HG21 | 1.97                     | 0.42              |
| 1:WA:140:LEU:O    | 1:WA:144:ILE:HG13 | 2.19                     | 0.42              |
| 1:WB:135:ALA:O    | 1:WB:139:GLU:HG2  | 2.18                     | 0.42              |
| 1:WC:120:LYS:HE2  | 1:WC:120:LYS:HA   | 2.00                     | 0.42              |
| 1:WC:191:ILE:O    | 1:WC:195:VAL:HG23 | 2.20                     | 0.42              |
| 1:WD:190:GLN:HA   | 1:WE:217:GLY:O    | 2.19                     | 0.42              |
| 1:WE:140:LEU:O    | 1:WE:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WG:145:GLU:O    | 1:WG:146:THR:C    | 2.63                     | 0.42              |
| 1:WH:140:LEU:O    | 1:WH:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WK:149:PRO:HD2  | 1:WK:190:GLN:HE22 | 1.84                     | 0.42              |
| 1:WM:190:GLN:HA   | 1:WN:217:GLY:HA3  | 2.00                     | 0.42              |
| 1:WQ:140:LEU:O    | 1:WQ:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WR:140:LEU:O    | 1:WR:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WT:196:HIS:HB3  | 1:WU:211:THR:CG2  | 2.30                     | 0.42              |
| 1:WW:169:GLN:NE2  | 1:WW:170:LYS:O    | 2.53                     | 0.42              |
| 2:C:52:ILE:O      | 2:C:55:ILE:HG22   | 2.18                     | 0.42              |
| 3:E:125:LEU:O     | 3:E:129:MET:HG3   | 2.20                     | 0.42              |
| 3:E:167:ASN:ND2   | 3:E:174:ARG:HH12  | 2.18                     | 0.42              |
| 4:F:60:MET:CE     | 4:G:91:GLY:HA3    | 2.47                     | 0.42              |
| 4:F:214:PRO:HG2   | 4:G:212:VAL:HG22  | 2.01                     | 0.42              |
| 4:I:171:LEU:HB3   | 4:I:172:PRO:HD3   | 2.01                     | 0.42              |
| 5:M:7:ILE:HD11    | 1:AC:370:ARG:NE   | 2.23                     | 0.42              |
| 5:M:9:GLY:O       | 5:M:13:GLN:HG3    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:O:73:ALA:HB1    | 6:U:13:GLN:NE2    | 2.33                     | 0.42              |
| 6:U:36:PRO:HG2    | 1:k:311:GLY:H     | 1.84                     | 0.42              |
| 7:Y:112:TYR:CE2   | 7:Y:116:ILE:HD11  | 2.55                     | 0.42              |
| 1:4:296:ARG:HG2   | 1:4:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:6:296:ARG:HG2   | 1:6:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:0:296:ARG:HG2   | 1:0:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:AA:296:ARG:HG2  | 1:AA:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:AB:296:ARG:HG2  | 1:AB:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:AJ:404:LEU:HD22 | 1:AJ:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AK:429:THR:OG1  | 1:AL:418:GLU:OE2  | 2.36                     | 0.42              |
| 1:UM:125:GLN:C    | 1:UM:128:GLU:H    | 2.27                     | 0.42              |
| 1:WB:164:LEU:O    | 4:H:152:ARG:HG3   | 2.18                     | 0.42              |
| 1:WI:165:PHE:O    | 1:WI:165:PHE:CG   | 2.73                     | 0.42              |
| 1:WI:187:ASP:H    | 1:WI:190:GLN:CD   | 2.28                     | 0.42              |
| 1:WJ:140:LEU:O    | 1:WJ:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WJ:164:LEU:HD23 | 3:E:144:LEU:HB2   | 1.98                     | 0.42              |
| 1:WL:214:ASP:OD1  | 1:WL:218:HIS:N    | 2.49                     | 0.42              |
| 1:WT:142:ARG:O    | 1:WT:146:THR:HG23 | 2.20                     | 0.42              |
| 1:WV:114:GLU:O    | 1:WV:118:GLN:HG3  | 2.20                     | 0.42              |
| 1:WV:187:ASP:O    | 1:WV:190:GLN:HB2  | 2.20                     | 0.42              |
| 4:H:59:LEU:O      | 4:H:65:THR:OG1    | 2.30                     | 0.42              |
| 4:J:121:ILE:HG23  | 4:J:125:GLU:HB3   | 2.02                     | 0.42              |
| 5:M:4:ILE:CD1     | 1:AC:374:HIS:CB   | 2.93                     | 0.42              |
| 6:Q:85:LEU:HA     | 6:Q:85:LEU:HD23   | 1.81                     | 0.42              |
| 1:y:296:ARG:HG2   | 1:y:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:AH:404:LEU:HD22 | 1:AH:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AI:404:LEU:HD22 | 1:AI:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AK:404:LEU:HD22 | 1:AK:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AL:404:LEU:HD22 | 1:AL:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AL:429:THR:OG1  | 1:AM:418:GLU:OE2  | 2.36                     | 0.42              |
| 1:UJ:75:ILE:HG21  | 1:UJ:96:LEU:HD11  | 2.00                     | 0.42              |
| 1:WA:115:LEU:HD22 | 1:WA:134:ARG:HD2  | 2.01                     | 0.42              |
| 1:WA:126:PHE:HD2  | 1:WW:128:GLU:HG2  | 1.84                     | 0.42              |
| 1:WG:140:LEU:O    | 1:WG:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WJ:164:LEU:CD1  | 3:E:145:TRP:HA    | 2.50                     | 0.42              |
| 1:WK:145:GLU:C    | 1:WK:147:LEU:N    | 2.76                     | 0.42              |
| 1:WK:165:PHE:O    | 1:WK:166:VAL:HB   | 2.19                     | 0.42              |
| 1:WP:140:LEU:O    | 1:WP:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WR:192:SER:O    | 1:WR:195:VAL:N    | 2.53                     | 0.42              |
| 1:WW:172:PRO:HD2  | 1:WW:204:GLY:O    | 2.19                     | 0.42              |
| 3:E:122:MET:HG3   | 4:J:214:PRO:HG2   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:162:PRO:CD    | 4:F:163:GLU:N     | 2.82                     | 0.42              |
| 4:G:121:ILE:HG12  | 4:G:125:GLU:HB3   | 2.02                     | 0.42              |
| 4:H:86:ASN:HD22   | 5:M:103:GLN:HA    | 1.83                     | 0.42              |
| 4:J:66:ARG:HA     | 4:J:182:ALA:HB2   | 2.02                     | 0.42              |
| 6:T:68:THR:HG22   | 1:7:294:ARG:HD3   | 2.01                     | 0.42              |
| 7:a:34:VAL:HG13   | 7:a:35:THR:HG22   | 2.02                     | 0.42              |
| 7:a:123:LYS:HE2   | 7:a:123:LYS:HA    | 2.02                     | 0.42              |
| 1:t:296:ARG:HG2   | 1:t:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:z:296:ARG:HG2   | 1:z:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:1:421:GLY:O     | 1:1:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:AC:296:ARG:HG2  | 1:AC:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:AO:296:ARG:HG2  | 1:AO:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:UI:102:GLN:CG   | 1:UI:193:ALA:HB2  | 2.49                     | 0.42              |
| 1:UM:207:PRO:HD2  | 1:WP:187:ASP:HB3  | 2.02                     | 0.42              |
| 1:WE:113:PHE:CE2  | 1:WE:139:GLU:HG3  | 2.54                     | 0.42              |
| 1:WG:166:VAL:CG1  | 1:WG:168:GLU:HB3  | 2.49                     | 0.42              |
| 1:WI:129:GLN:HE22 | 1:WI:132:TYR:HD2  | 1.68                     | 0.42              |
| 1:WI:140:LEU:O    | 1:WI:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WJ:172:PRO:HD2  | 1:WJ:204:GLY:O    | 2.19                     | 0.42              |
| 1:WL:135:ALA:O    | 1:WL:136:LEU:C    | 2.63                     | 0.42              |
| 1:WO:140:LEU:O    | 1:WO:144:ILE:HG13 | 2.20                     | 0.42              |
| 1:WO:214:ASP:OD1  | 1:WO:218:HIS:N    | 2.49                     | 0.42              |
| 1:WQ:196:HIS:HB3  | 1:WR:211:THR:HG21 | 2.02                     | 0.42              |
| 1:WW:140:LEU:O    | 1:WW:144:ILE:HG13 | 2.19                     | 0.42              |
| 3:E:175:ALA:HA    | 3:E:178:LEU:HD23  | 2.02                     | 0.42              |
| 3:E:254:ILE:HD13  | 3:E:254:ILE:HA    | 1.86                     | 0.42              |
| 4:F:171:LEU:HB3   | 4:F:172:PRO:HD3   | 2.01                     | 0.42              |
| 4:J:92:LEU:HD12   | 4:J:92:LEU:HA     | 1.78                     | 0.42              |
| 5:P:75:MET:HE2    | 5:P:75:MET:HB2    | 1.81                     | 0.42              |
| 7:a:16:ALA:HB1    | 7:a:49:PHE:CE1    | 2.55                     | 0.42              |
| 1:x:296:ARG:HG2   | 1:x:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:z:421:GLY:O     | 1:z:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:2:296:ARG:HG2   | 1:2:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:7:421:GLY:O     | 1:7:426:ARG:NH2   | 2.51                     | 0.42              |
| 1:AG:404:LEU:HD22 | 1:AG:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AN:404:LEU:HD22 | 1:AN:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AP:404:LEU:HD22 | 1:AP:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AQ:404:LEU:HD22 | 1:AQ:409:MET:HE3  | 2.02                     | 0.42              |
| 1:UM:102:GLN:CG   | 1:UM:193:ALA:HB2  | 2.49                     | 0.42              |
| 1:WD:113:PHE:HB3  | 1:WE:134:ARG:NH1  | 2.34                     | 0.42              |
| 1:WD:140:LEU:O    | 1:WD:144:ILE:HG13 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WE:166:VAL:HG23 | 4:I:160:GLN:HA    | 1.84                     | 0.42              |
| 1:WH:200:SER:OG   | 1:WI:175:SER:CB   | 2.54                     | 0.42              |
| 1:WS:124:SER:CB   | 2:A:8:MET:CE      | 2.82                     | 0.42              |
| 1:WS:147:LEU:O    | 1:WS:148:GLY:C    | 2.63                     | 0.42              |
| 1:WU:140:LEU:O    | 1:WU:144:ILE:HG13 | 2.20                     | 0.42              |
| 2:C:1:MET:HE2     | 2:C:1:MET:HB3     | 1.91                     | 0.42              |
| 2:C:54:LYS:HB3    | 2:C:54:LYS:HE2    | 1.84                     | 0.42              |
| 5:O:69:ASN:OD1    | 5:O:69:ASN:N      | 2.52                     | 0.42              |
| 5:O:84:MET:SD     | 6:U:134:LEU:HD21  | 2.59                     | 0.42              |
| 1:j:319:GLN:CD    | 1:4:355:PRO:HB3   | 2.44                     | 0.42              |
| 1:t:404:LEU:HD22  | 1:t:409:MET:HE3   | 2.02                     | 0.42              |
| 1:1:296:ARG:HG2   | 1:1:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:9:296:ARG:HG2   | 1:9:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:AK:296:ARG:HG2  | 1:AK:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:AO:404:LEU:HD22 | 1:AO:409:MET:HE3  | 2.02                     | 0.42              |
| 1:WE:164:LEU:HD13 | 1:WE:165:PHE:N    | 2.35                     | 0.42              |
| 1:WP:165:PHE:CA   | 4:F:160:GLN:O     | 2.68                     | 0.42              |
| 1:WQ:121:PHE:HZ   | 2:A:15:LYS:HD3    | 1.85                     | 0.42              |
| 1:WV:140:LEU:O    | 1:WV:144:ILE:HG13 | 2.20                     | 0.42              |
| 4:I:101:MET:HE3   | 4:I:101:MET:HB3   | 1.76                     | 0.42              |
| 4:J:189:ILE:O     | 4:J:192:PRO:HD2   | 2.19                     | 0.42              |
| 5:P:7:ILE:HG22    | 1:t:278:THR:CG2   | 2.42                     | 0.42              |
| 7:W:10:ALA:HB3    | 7:W:119:LEU:HD13  | 2.02                     | 0.42              |
| 1:g:316:LEU:HD12  | 1:g:316:LEU:HA    | 1.77                     | 0.42              |
| 1:w:290:LYS:HE3   | 1:w:290:LYS:HB2   | 1.93                     | 0.42              |
| 1:w:296:ARG:HG2   | 1:w:296:ARG:NH1   | 2.35                     | 0.42              |
| 1:0:290:LYS:HE3   | 1:0:290:LYS:HB2   | 1.93                     | 0.42              |
| 1:AF:404:LEU:HD22 | 1:AF:409:MET:HE3  | 2.02                     | 0.42              |
| 1:AI:429:THR:OG1  | 1:AJ:418:GLU:OE2  | 2.36                     | 0.42              |
| 1:AO:290:LYS:HE3  | 1:AO:290:LYS:HB2  | 1.93                     | 0.42              |
| 1:UO:102:GLN:CG   | 1:UO:193:ALA:HB2  | 2.49                     | 0.41              |
| 1:UO:214:ASP:OD2  | 1:UO:218:HIS:HB2  | 2.20                     | 0.41              |
| 1:WC:140:LEU:O    | 1:WC:144:ILE:HG13 | 2.20                     | 0.41              |
| 1:WU:164:LEU:HA   | 4:G:152:ARG:NH2   | 2.35                     | 0.41              |
| 1:f:319:GLN:CG    | 1:AG:303:GLN:HE22 | 2.32                     | 0.41              |
| 1:l:312:VAL:HG12  | 1:l:315:ALA:HB2   | 2.01                     | 0.41              |
| 1:3:404:LEU:HD22  | 1:3:409:MET:HE3   | 2.02                     | 0.41              |
| 1:7:296:ARG:HG2   | 1:7:296:ARG:NH1   | 2.35                     | 0.41              |
| 1:8:421:GLY:O     | 1:8:426:ARG:NH2   | 2.51                     | 0.41              |
| 1:AD:296:ARG:HG2  | 1:AD:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:AE:404:LEU:HD22 | 1:AE:409:MET:HE3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AL:296:ARG:HG2  | 1:AL:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:AM:404:LEU:HD22 | 1:AM:409:MET:HE3  | 2.02                     | 0.41              |
| 1:WH:190:GLN:HG3  | 1:WI:217:GLY:HA3  | 2.02                     | 0.41              |
| 1:WS:125:GLN:N    | 2:A:4:GLU:HB3     | 2.34                     | 0.41              |
| 1:WS:214:ASP:OD1  | 1:WS:218:HIS:N    | 2.49                     | 0.41              |
| 1:WV:120:LYS:NZ   | 1:WV:123:ILE:CD1  | 2.74                     | 0.41              |
| 4:J:85:PRO:O      | 4:J:86:ASN:C      | 2.61                     | 0.41              |
| 4:J:129:LYS:HB3   | 4:J:129:LYS:HE3   | 1.87                     | 0.41              |
| 4:J:225:LEU:HD12  | 4:J:229:VAL:HG22  | 2.01                     | 0.41              |
| 5:L:82:MET:HE3    | 6:Q:133:VAL:HG22  | 2.02                     | 0.41              |
| 5:P:11:ILE:HG22   | 1:t:372:ILE:HB    | 2.02                     | 0.41              |
| 6:T:39:GLN:HA     | 6:T:99:THR:HB     | 2.02                     | 0.41              |
| 1:u:404:LEU:HD22  | 1:u:409:MET:HE3   | 2.02                     | 0.41              |
| 1:v:296:ARG:HG2   | 1:v:296:ARG:NH1   | 2.35                     | 0.41              |
| 1:v:404:LEU:HD22  | 1:v:409:MET:HE3   | 2.02                     | 0.41              |
| 1:3:296:ARG:HG2   | 1:3:296:ARG:NH1   | 2.35                     | 0.41              |
| 1:7:429:THR:OG1   | 1:8:418:GLU:OE2   | 2.36                     | 0.41              |
| 1:AE:296:ARG:HG2  | 1:AE:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:UP:102:GLN:CG   | 1:UP:193:ALA:HB2  | 2.49                     | 0.41              |
| 1:UP:214:ASP:OD2  | 1:UP:218:HIS:HB2  | 2.20                     | 0.41              |
| 1:WB:114:GLU:O    | 1:WB:117:ASP:N    | 2.54                     | 0.41              |
| 1:WK:140:LEU:O    | 1:WK:144:ILE:HG13 | 2.20                     | 0.41              |
| 1:WV:128:GLU:CG   | 1:WW:126:PHE:CE2  | 3.03                     | 0.41              |
| 4:I:190:PHE:CG    | 4:J:220:PRO:HG3   | 2.55                     | 0.41              |
| 4:J:217:ILE:O     | 4:J:220:PRO:HD2   | 2.20                     | 0.41              |
| 6:R:29:ASN:ND2    | 6:R:40:ALA:HA     | 2.35                     | 0.41              |
| 1:5:404:LEU:HD22  | 1:5:409:MET:HE3   | 2.02                     | 0.41              |
| 1:6:404:LEU:HD22  | 1:6:409:MET:HE3   | 2.02                     | 0.41              |
| 1:8:404:LEU:HD22  | 1:8:409:MET:HE3   | 2.02                     | 0.41              |
| 1:AF:296:ARG:HG2  | 1:AF:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:WI:162:PRO:HG2  | 1:WJ:165:PHE:HZ   | 1.86                     | 0.41              |
| 1:WP:164:LEU:O    | 4:F:159:LEU:O     | 2.38                     | 0.41              |
| 1:WR:128:GLU:HB3  | 1:WS:126:PHE:CE2  | 2.55                     | 0.41              |
| 1:WR:165:PHE:O    | 1:WR:167:ARG:N    | 2.53                     | 0.41              |
| 1:WR:197:LEU:HA   | 1:WS:175:SER:CB   | 2.50                     | 0.41              |
| 1:WT:147:LEU:O    | 1:WT:148:GLY:C    | 2.64                     | 0.41              |
| 3:E:176:GLY:HA2   | 3:E:179:ILE:CD1   | 2.49                     | 0.41              |
| 5:M:80:VAL:HG22   | 6:S:131:MET:HG2   | 2.01                     | 0.41              |
| 5:P:82:MET:HE2    | 5:P:82:MET:HA     | 2.03                     | 0.41              |
| 7:Z:119:LEU:HA    | 7:Z:119:LEU:HD23  | 1.67                     | 0.41              |
| 1:u:296:ARG:HG2   | 1:u:296:ARG:NH1   | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AD:404:LEU:HD22 | 1:AD:409:MET:HE3  | 2.02                     | 0.41              |
| 1:AG:296:ARG:HG2  | 1:AG:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:AM:296:ARG:HG2  | 1:AM:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:UI:214:ASP:OD2  | 1:UI:218:HIS:HB2  | 2.20                     | 0.41              |
| 1:UK:207:PRO:CA   | 1:WE:187:ASP:OD1  | 2.67                     | 0.41              |
| 1:WA:196:HIS:CD2  | 1:WB:219:LEU:HD13 | 2.56                     | 0.41              |
| 1:WB:140:LEU:O    | 1:WB:144:ILE:HG13 | 2.20                     | 0.41              |
| 1:WB:166:VAL:HG21 | 1:WB:169:GLN:HA   | 2.01                     | 0.41              |
| 1:WB:196:HIS:HB3  | 1:WC:211:THR:HG21 | 2.01                     | 0.41              |
| 1:WJ:125:GLN:HG3  | 3:E:242:HIS:CG    | 2.54                     | 0.41              |
| 1:WK:190:GLN:CG   | 1:WL:217:GLY:HA3  | 2.51                     | 0.41              |
| 1:WK:190:GLN:HA   | 1:WL:217:GLY:O    | 2.20                     | 0.41              |
| 2:A:18:LEU:HD12   | 2:A:18:LEU:HA     | 1.91                     | 0.41              |
| 4:F:217:ILE:HD13  | 4:F:217:ILE:HA    | 1.89                     | 0.41              |
| 4:J:83:ALA:O      | 4:J:85:PRO:N      | 2.54                     | 0.41              |
| 5:M:3:ALA:HA      | 1:AC:372:ILE:HD13 | 2.02                     | 0.41              |
| 5:N:4:ILE:HG12    | 1:7:372:ILE:HG21  | 2.02                     | 0.41              |
| 6:U:66:THR:HG23   | 1:z:365:ASN:CG    | 2.45                     | 0.41              |
| 1:k:322:PRO:HA    | 1:k:323:PRO:HD3   | 1.98                     | 0.41              |
| 1:y:421:GLY:O     | 1:y:426:ARG:NH2   | 2.51                     | 0.41              |
| 1:AJ:296:ARG:HG2  | 1:AJ:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:AN:296:ARG:HG2  | 1:AN:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:AP:421:GLY:O    | 1:AP:426:ARG:NH2  | 2.51                     | 0.41              |
| 1:UK:125:GLN:C    | 1:UK:127:SER:N    | 2.77                     | 0.41              |
| 1:UN:94:HIS:HB2   | 1:UN:146:THR:HG21 | 1.97                     | 0.41              |
| 1:WG:214:ASP:OD1  | 1:WG:218:HIS:N    | 2.51                     | 0.41              |
| 1:WI:135:ALA:O    | 1:WI:139:GLU:HG2  | 2.21                     | 0.41              |
| 1:WT:128:GLU:HG3  | 1:WU:126:PHE:CE2  | 2.55                     | 0.41              |
| 1:WV:145:GLU:C    | 1:WV:147:LEU:N    | 2.78                     | 0.41              |
| 4:G:171:LEU:HD23  | 4:H:95:PHE:CZ     | 2.55                     | 0.41              |
| 4:G:194:LEU:HD23  | 4:G:194:LEU:HA    | 1.83                     | 0.41              |
| 4:I:52:THR:HG23   | 5:O:97:GLN:HE21   | 1.85                     | 0.41              |
| 5:M:7:ILE:CD1     | 1:AC:370:ARG:HE   | 2.24                     | 0.41              |
| 6:S:16:LEU:HD11   | 6:S:120:LEU:HG    | 2.02                     | 0.41              |
| 7:V:30:ASN:ND2    | 7:a:62:VAL:HB     | 2.36                     | 0.41              |
| 7:a:98:VAL:O      | 7:a:102:MET:HG2   | 2.21                     | 0.41              |
| 1:j:319:GLN:CD    | 1:4:355:PRO:CB    | 2.94                     | 0.41              |
| 1:O:404:LEU:HD22  | 1:O:409:MET:HE3   | 2.02                     | 0.41              |
| 1:AE:290:LYS:HE3  | 1:AE:290:LYS:HB2  | 1.93                     | 0.41              |
| 1:AH:296:ARG:HG2  | 1:AH:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:UP:125:GLN:C    | 1:UP:127:SER:N    | 2.77                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WD:190:GLN:O    | 1:WD:191:ILE:C    | 2.64                     | 0.41              |
| 1:WG:193:ALA:HB1  | 1:WH:213:VAL:CG1  | 2.48                     | 0.41              |
| 1:WI:144:ILE:O    | 1:WI:147:LEU:HB2  | 2.20                     | 0.41              |
| 1:WI:181:GLU:CB   | 1:WI:184:ARG:CG   | 2.85                     | 0.41              |
| 1:WL:140:LEU:O    | 1:WL:144:ILE:HG13 | 2.20                     | 0.41              |
| 1:WL:190:GLN:HG2  | 1:WM:216:SER:O    | 2.21                     | 0.41              |
| 1:WM:140:LEU:O    | 1:WM:144:ILE:HG13 | 2.20                     | 0.41              |
| 1:WO:181:GLU:CB   | 1:WO:184:ARG:CG   | 2.85                     | 0.41              |
| 1:WT:165:PHE:HZ   | 4:G:144:GLU:HG2   | 1.86                     | 0.41              |
| 1:WW:131:ASN:HA   | 1:WW:134:ARG:HD3  | 2.01                     | 0.41              |
| 4:F:194:LEU:HD12  | 4:G:220:PRO:HG2   | 2.03                     | 0.41              |
| 1:w:404:LEU:HD22  | 1:w:409:MET:HE3   | 2.02                     | 0.41              |
| 1:7:404:LEU:HD22  | 1:7:409:MET:HE3   | 2.02                     | 0.41              |
| 1:AE:235:LEU:HB3  | 1:AF:244:ARG:NH2  | 2.36                     | 0.41              |
| 1:UN:214:ASP:OD2  | 1:UN:218:HIS:HB2  | 2.20                     | 0.41              |
| 1:WA:168:GLU:OE1  | 1:WW:169:GLN:HB2  | 2.21                     | 0.41              |
| 1:WH:166:VAL:HG11 | 4:J:147:LEU:HD11  | 2.01                     | 0.41              |
| 1:WL:196:HIS:HB3  | 1:WM:211:THR:HG21 | 2.03                     | 0.41              |
| 1:WM:181:GLU:CB   | 1:WM:184:ARG:CG   | 2.85                     | 0.41              |
| 1:WQ:186:LEU:HD23 | 1:WQ:186:LEU:HA   | 1.92                     | 0.41              |
| 1:WR:165:PHE:CE2  | 4:F:153:LEU:HD23  | 2.55                     | 0.41              |
| 1:WW:125:GLN:CD   | 2:B:2:THR:HG21    | 2.45                     | 0.41              |
| 2:A:52:ILE:N      | 2:A:52:ILE:HD12   | 2.35                     | 0.41              |
| 2:B:51:PHE:CE2    | 2:B:55:ILE:HD11   | 2.56                     | 0.41              |
| 3:E:231:ALA:O     | 3:E:234:PRO:HD2   | 2.21                     | 0.41              |
| 4:F:44:THR:HG23   | 5:K:84:MET:HE1    | 2.01                     | 0.41              |
| 4:F:175:VAL:O     | 4:F:179:LEU:HG    | 2.20                     | 0.41              |
| 4:G:234:LEU:HD12  | 4:G:234:LEU:HA    | 1.92                     | 0.41              |
| 1:8:296:ARG:HG2   | 1:8:296:ARG:NH1   | 2.35                     | 0.41              |
| 1:9:235:LEU:HB3   | 1:0:244:ARG:NH2   | 2.36                     | 0.41              |
| 1:AC:404:LEU:HD22 | 1:AC:409:MET:HE3  | 2.02                     | 0.41              |
| 1:UJ:125:GLN:C    | 1:UJ:127:SER:N    | 2.77                     | 0.41              |
| 1:UJ:263:ASP:OD2  | 1:UJ:267:HIS:HB2  | 2.20                     | 0.41              |
| 1:WA:213:VAL:HG11 | 1:WW:193:ALA:CB   | 2.48                     | 0.41              |
| 1:WB:190:GLN:CG   | 1:WC:216:SER:O    | 2.67                     | 0.41              |
| 1:WG:121:PHE:CE2  | 1:WG:123:ILE:HA   | 2.55                     | 0.41              |
| 1:WJ:159:MET:HE3  | 1:WJ:159:MET:HB3  | 1.78                     | 0.41              |
| 1:WK:181:GLU:CB   | 1:WK:184:ARG:CG   | 2.85                     | 0.41              |
| 1:WO:186:LEU:HA   | 1:WO:190:GLN:OE1  | 2.21                     | 0.41              |
| 1:WQ:164:LEU:CD2  | 4:F:149:LEU:HD13  | 2.51                     | 0.41              |
| 1:WQ:164:LEU:HD21 | 4:F:149:LEU:HD13  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WU:163:SER:O    | 1:WU:166:VAL:HG22 | 2.20                     | 0.41              |
| 1:WU:193:ALA:HB1  | 1:WV:213:VAL:HG11 | 2.03                     | 0.41              |
| 1:WV:145:GLU:O    | 1:WV:147:LEU:N    | 2.54                     | 0.41              |
| 2:B:39:GLN:NE2    | 2:B:49:LEU:HD12   | 2.31                     | 0.41              |
| 2:B:59:PHE:CZ     | 4:G:198:LEU:HD21  | 2.55                     | 0.41              |
| 4:G:171:LEU:O     | 4:G:175:VAL:HG23  | 2.21                     | 0.41              |
| 4:G:204:LEU:HD11  | 4:G:217:ILE:HD12  | 2.01                     | 0.41              |
| 4:I:187:PHE:CD2   | 4:J:224:MET:HB2   | 2.56                     | 0.41              |
| 4:J:213:PRO:HA    | 4:J:214:PRO:HD3   | 1.91                     | 0.41              |
| 5:K:11:ILE:HD13   | 1:AL:276:GLU:CD   | 2.46                     | 0.41              |
| 6:Q:60:THR:O      | 1:AO:297:GLN:NE2  | 2.52                     | 0.41              |
| 6:R:29:ASN:HD22   | 6:R:38:TYR:HE2    | 1.68                     | 0.41              |
| 6:U:72:HIS:CE1    | 1:1:366:TYR:O     | 2.74                     | 0.41              |
| 7:Y:8:ASP:C       | 7:Y:8:ASP:OD2     | 2.64                     | 0.41              |
| 7:Z:126:MET:O     | 7:Z:129:THR:HG22  | 2.21                     | 0.41              |
| 1:z:404:LEU:HD22  | 1:z:409:MET:HE3   | 2.02                     | 0.41              |
| 1:1:404:LEU:HD22  | 1:1:409:MET:HE3   | 2.02                     | 0.41              |
| 1:6:235:LEU:HB3   | 1:7:244:ARG:NH2   | 2.36                     | 0.41              |
| 1:8:235:LEU:HB3   | 1:9:244:ARG:NH2   | 2.36                     | 0.41              |
| 1:9:290:LYS:HE3   | 1:9:290:LYS:HB2   | 1.93                     | 0.41              |
| 1:9:421:GLY:O     | 1:9:426:ARG:NH2   | 2.51                     | 0.41              |
| 1:AB:235:LEU:HB3  | 1:AC:244:ARG:NH2  | 2.36                     | 0.41              |
| 1:AH:235:LEU:HB3  | 1:AI:244:ARG:NH2  | 2.36                     | 0.41              |
| 1:AI:296:ARG:HG2  | 1:AI:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:AK:235:LEU:HB3  | 1:AL:244:ARG:NH2  | 2.36                     | 0.41              |
| 1:AO:421:GLY:O    | 1:AO:426:ARG:NH2  | 2.51                     | 0.41              |
| 1:WE:197:LEU:HA   | 1:WF:175:SER:OG   | 2.21                     | 0.41              |
| 1:WH:149:PRO:CD   | 1:WH:190:GLN:HE22 | 2.33                     | 0.41              |
| 1:WJ:187:ASP:H    | 1:WJ:190:GLN:CD   | 2.29                     | 0.41              |
| 1:WK:167:ARG:CB   | 3:E:156:THR:HG22  | 2.50                     | 0.41              |
| 1:WU:145:GLU:O    | 1:WU:147:LEU:N    | 2.54                     | 0.41              |
| 2:D:35:ILE:HD13   | 2:D:35:ILE:HA     | 1.98                     | 0.41              |
| 6:U:68:THR:HG22   | 1:1:294:ARG:CD    | 2.36                     | 0.41              |
| 7:Z:45:LYS:C      | 7:Z:46:GLN:HG2    | 2.46                     | 0.41              |
| 1:x:404:LEU:HD22  | 1:x:409:MET:HE3   | 2.02                     | 0.41              |
| 1:AA:404:LEU:HD22 | 1:AA:409:MET:HE3  | 2.02                     | 0.41              |
| 1:UL:69:GLN:NE2   | 1:WH:182:PRO:CG   | 2.84                     | 0.40              |
| 1:UL:125:GLN:C    | 1:UL:127:SER:N    | 2.77                     | 0.40              |
| 1:UL:219:LEU:HD22 | 1:u:247:ARG:HH12  | 1.77                     | 0.40              |
| 1:WC:143:THR:O    | 1:WC:146:THR:OG1  | 2.36                     | 0.40              |
| 1:WJ:165:PHE:N    | 4:J:152:ARG:HH22  | 2.18                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WS:115:LEU:HA   | 1:WS:118:GLN:OE1  | 2.21                     | 0.40              |
| 1:WT:181:GLU:CB   | 1:WT:184:ARG:CG   | 2.85                     | 0.40              |
| 2:D:77:VAL:HG11   | 4:J:225:LEU:HD11  | 2.03                     | 0.40              |
| 4:F:187:PHE:CZ    | 4:F:191:ILE:HD11  | 2.56                     | 0.40              |
| 4:H:189:ILE:HD13  | 4:H:235:LEU:HD11  | 2.03                     | 0.40              |
| 4:J:64:PHE:HE2    | 5:O:102:MET:HE1   | 1.85                     | 0.40              |
| 5:O:7:ILE:O       | 5:O:11:ILE:HG23   | 2.21                     | 0.40              |
| 5:P:69:ASN:OD1    | 7:V:112:TYR:OH    | 2.11                     | 0.40              |
| 1:w:360:ARG:NH1   | 1:w:362:GLU:OE1   | 2.55                     | 0.40              |
| 1:2:404:LEU:HD22  | 1:2:409:MET:HE3   | 2.02                     | 0.40              |
| 1:3:290:LYS:HE3   | 1:3:290:LYS:HB2   | 1.93                     | 0.40              |
| 1:4:404:LEU:HD22  | 1:4:409:MET:HE3   | 2.02                     | 0.40              |
| 1:5:235:LEU:HB3   | 1:6:244:ARG:NH2   | 2.36                     | 0.40              |
| 1:AO:425:LYS:HE3  | 1:AO:425:LYS:HB3  | 1.96                     | 0.40              |
| 1:UK:214:ASP:OD2  | 1:UK:218:HIS:HB2  | 2.20                     | 0.40              |
| 1:UL:51:TYR:HB2   | 1:UL:78:ARG:CZ    | 2.51                     | 0.40              |
| 1:UN:102:GLN:CG   | 1:UN:193:ALA:HB2  | 2.49                     | 0.40              |
| 1:WC:125:GLN:O    | 1:WC:128:GLU:HG2  | 2.20                     | 0.40              |
| 1:WM:193:ALA:CB   | 1:WN:213:VAL:CG1  | 2.94                     | 0.40              |
| 1:WR:193:ALA:HB1  | 1:WS:213:VAL:HG21 | 2.03                     | 0.40              |
| 3:E:4:VAL:HB      | 5:P:44:ARG:HH12   | 1.86                     | 0.40              |
| 4:F:138:MET:O     | 4:F:142:THR:OG1   | 2.16                     | 0.40              |
| 4:G:75:ARG:HB2    | 4:G:83:ALA:CB     | 2.52                     | 0.40              |
| 5:K:68:LEU:H      | 5:K:68:LEU:HD12   | 1.85                     | 0.40              |
| 6:Q:128:LYS:HD2   | 6:Q:128:LYS:HA    | 1.62                     | 0.40              |
| 1:t:360:ARG:NH1   | 1:t:362:GLU:OE1   | 2.55                     | 0.40              |
| 1:3:235:LEU:HB3   | 1:4:244:ARG:NH2   | 2.36                     | 0.40              |
| 1:AA:235:LEU:HB3  | 1:AB:244:ARG:NH2  | 2.36                     | 0.40              |
| 1:AB:404:LEU:HD22 | 1:AB:409:MET:HE3  | 2.02                     | 0.40              |
| 1:AH:360:ARG:NH1  | 1:AH:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:AN:421:GLY:O    | 1:AN:426:ARG:NH2  | 2.51                     | 0.40              |
| 1:UI:52:ARG:O     | 1:UI:88:VAL:N     | 2.38                     | 0.40              |
| 1:UI:125:GLN:C    | 1:UI:127:SER:N    | 2.77                     | 0.40              |
| 1:UJ:51:TYR:HB2   | 1:UJ:78:ARG:CZ    | 2.51                     | 0.40              |
| 1:UJ:54:LEU:HG    | 1:UJ:55:PHE:CD2   | 2.57                     | 0.40              |
| 1:UJ:261:LEU:HG   | 1:UJ:269:LEU:HD12 | 2.04                     | 0.40              |
| 1:UM:212:LEU:HG   | 1:UM:220:LEU:HD12 | 2.04                     | 0.40              |
| 1:UM:214:ASP:OD2  | 1:UM:218:HIS:HB2  | 2.20                     | 0.40              |
| 1:UO:54:LEU:HG    | 1:UO:55:PHE:CD2   | 2.57                     | 0.40              |
| 1:WC:164:LEU:O    | 4:I:241:GLN:CD    | 2.63                     | 0.40              |
| 1:WF:143:THR:O    | 1:WF:146:THR:OG1  | 2.37                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:15:LYS:HE2    | 2:A:15:LYS:HB3    | 1.88                     | 0.40              |
| 2:A:50:SER:OG     | 2:B:46:GLU:OE2    | 2.25                     | 0.40              |
| 2:B:84:LEU:HD22   | 4:H:185:ILE:HG23  | 2.03                     | 0.40              |
| 2:C:49:LEU:HD23   | 2:C:49:LEU:HA     | 1.94                     | 0.40              |
| 4:F:153:LEU:HD23  | 4:F:153:LEU:HA    | 1.91                     | 0.40              |
| 4:H:71:PHE:HD1    | 4:H:71:PHE:HA     | 1.80                     | 0.40              |
| 4:H:189:ILE:O     | 4:H:192:PRO:HD2   | 2.21                     | 0.40              |
| 4:I:132:GLN:HB2   | 4:I:133:PRO:HD3   | 2.04                     | 0.40              |
| 5:O:103:GLN:CD    | 5:O:103:GLN:H     | 2.30                     | 0.40              |
| 1:x:421:GLY:O     | 1:x:426:ARG:NH2   | 2.51                     | 0.40              |
| 1:y:404:LEU:HD22  | 1:y:409:MET:HE3   | 2.02                     | 0.40              |
| 1:AB:360:ARG:NH1  | 1:AB:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:AG:360:ARG:NH1  | 1:AG:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:AK:360:ARG:NH1  | 1:AK:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:AO:360:ARG:NH1  | 1:AO:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:UM:51:TYR:HB2   | 1:UM:78:ARG:CZ    | 2.52                     | 0.40              |
| 1:UM:54:LEU:HG    | 1:UM:55:PHE:CD2   | 2.57                     | 0.40              |
| 1:UM:125:GLN:C    | 1:UM:127:SER:N    | 2.77                     | 0.40              |
| 1:WD:193:ALA:HB1  | 1:WE:213:VAL:CG2  | 2.50                     | 0.40              |
| 1:WG:120:LYS:HA   | 1:WG:120:LYS:HE2  | 2.03                     | 0.40              |
| 1:WQ:121:PHE:O    | 1:WQ:122:GLY:C    | 2.64                     | 0.40              |
| 1:WR:139:GLU:HB3  | 1:WS:156:HIS:HE1  | 1.87                     | 0.40              |
| 1:WR:181:GLU:CB   | 1:WR:184:ARG:CG   | 2.85                     | 0.40              |
| 1:WS:197:LEU:HA   | 1:WT:175:SER:CB   | 2.52                     | 0.40              |
| 5:L:4:ILE:HA      | 1:AI:372:ILE:HD12 | 2.03                     | 0.40              |
| 5:L:7:ILE:O       | 5:L:11:ILE:HG23   | 2.21                     | 0.40              |
| 5:N:7:ILE:HB      | 1:6:278:THR:HG21  | 2.02                     | 0.40              |
| 7:a:119:LEU:HD23  | 7:a:119:LEU:HA    | 1.98                     | 0.40              |
| 1:z:360:ARG:NH1   | 1:z:362:GLU:OE1   | 2.55                     | 0.40              |
| 1:AD:360:ARG:NH1  | 1:AD:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:AE:360:ARG:NH1  | 1:AE:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:AN:360:ARG:NH1  | 1:AN:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:WC:163:SER:OG   | 1:WC:166:VAL:O    | 2.38                     | 0.40              |
| 1:WF:120:LYS:HB3  | 1:WF:121:PHE:H    | 1.66                     | 0.40              |
| 1:WG:124:SER:O    | 1:WG:127:SER:N    | 2.55                     | 0.40              |
| 1:WG:187:ASP:HB3  | 1:WG:190:GLN:H    | 1.87                     | 0.40              |
| 1:WJ:144:ILE:O    | 1:WJ:147:LEU:HB2  | 2.21                     | 0.40              |
| 1:WL:191:ILE:HG23 | 1:WL:212:LEU:HD23 | 2.03                     | 0.40              |
| 1:WQ:214:ASP:OD1  | 1:WQ:218:HIS:N    | 2.49                     | 0.40              |
| 1:WR:201:ALA:C    | 1:WS:158:ALA:HB2  | 2.47                     | 0.40              |
| 3:E:6:SER:OG      | 3:E:7:GLU:N       | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:146:LEU:HD23 | 3:E:146:LEU:HA   | 1.80                     | 0.40              |
| 5:P:77:LYS:HE2   | 7:V:7:PHE:HB3    | 2.04                     | 0.40              |
| 6:U:72:HIS:HA    | 1:2:295:SER:HB3  | 2.02                     | 0.40              |
| 7:Y:119:LEU:HD12 | 7:Y:119:LEU:HA   | 1.84                     | 0.40              |
| 1:9:404:LEU:HD22 | 1:9:409:MET:HE3  | 2.02                     | 0.40              |
| 1:AD:235:LEU:HB3 | 1:AE:244:ARG:NH2 | 2.36                     | 0.40              |
| 1:AN:235:LEU:HB3 | 1:AO:244:ARG:NH2 | 2.36                     | 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   | 0     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 1     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 2     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 3     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 4     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 5     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 6     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 7     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 8     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | 9     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AA    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AB    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AC    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AD    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AE    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AF    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AG    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AH    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AI    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AJ    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AK    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AL    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AM    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AN    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AO    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AP    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | AQ    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | UI    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | UJ    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | UK    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | UL    | 151/560 (27%) | 142 (94%) | 7 (5%)  | 2 (1%)   | 9           | 38  |
| 1   | UM    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | UN    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | UO    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | UP    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 38  |
| 1   | WA    | 111/560 (20%) | 99 (89%)  | 9 (8%)  | 3 (3%)   | 4           | 27  |
| 1   | WB    | 109/560 (20%) | 94 (86%)  | 10 (9%) | 5 (5%)   | 2           | 18  |
| 1   | WC    | 106/560 (19%) | 96 (91%)  | 9 (8%)  | 1 (1%)   | 14          | 45  |
| 1   | WD    | 108/560 (19%) | 99 (92%)  | 4 (4%)  | 5 (5%)   | 2           | 18  |
| 1   | WE    | 110/560 (20%) | 98 (89%)  | 8 (7%)  | 4 (4%)   | 2           | 22  |
| 1   | WF    | 109/560 (20%) | 98 (90%)  | 8 (7%)  | 3 (3%)   | 4           | 26  |
| 1   | WG    | 110/560 (20%) | 98 (89%)  | 10 (9%) | 2 (2%)   | 6           | 33  |
| 1   | WH    | 93/560 (17%)  | 86 (92%)  | 5 (5%)  | 2 (2%)   | 5           | 30  |
| 1   | WI    | 93/560 (17%)  | 82 (88%)  | 5 (5%)  | 6 (6%)   | 1           | 14  |
| 1   | WJ    | 97/560 (17%)  | 89 (92%)  | 7 (7%)  | 1 (1%)   | 12          | 43  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | WK    | 96/560 (17%)  | 84 (88%)  | 9 (9%)  | 3 (3%)   | 3           | 25  |
| 1   | WL    | 81/560 (14%)  | 75 (93%)  | 4 (5%)  | 2 (2%)   | 4           | 28  |
| 1   | WM    | 78/560 (14%)  | 72 (92%)  | 4 (5%)  | 2 (3%)   | 4           | 27  |
| 1   | WN    | 80/560 (14%)  | 75 (94%)  | 2 (2%)  | 3 (4%)   | 2           | 21  |
| 1   | WO    | 94/560 (17%)  | 85 (90%)  | 7 (7%)  | 2 (2%)   | 5           | 31  |
| 1   | WP    | 98/560 (18%)  | 87 (89%)  | 6 (6%)  | 5 (5%)   | 1           | 17  |
| 1   | WQ    | 109/560 (20%) | 100 (92%) | 5 (5%)  | 4 (4%)   | 2           | 21  |
| 1   | WR    | 109/560 (20%) | 94 (86%)  | 8 (7%)  | 7 (6%)   | 1           | 14  |
| 1   | WS    | 109/560 (20%) | 96 (88%)  | 7 (6%)  | 6 (6%)   | 1           | 16  |
| 1   | WT    | 109/560 (20%) | 97 (89%)  | 5 (5%)  | 7 (6%)   | 1           | 14  |
| 1   | WU    | 110/560 (20%) | 101 (92%) | 8 (7%)  | 1 (1%)   | 14          | 45  |
| 1   | WV    | 108/560 (19%) | 97 (90%)  | 9 (8%)  | 2 (2%)   | 6           | 32  |
| 1   | WW    | 109/560 (20%) | 95 (87%)  | 9 (8%)  | 5 (5%)   | 2           | 18  |
| 1   | b     | 11/560 (2%)   | 10 (91%)  | 1 (9%)  | 0        | 100         | 100 |
| 1   | c     | 14/560 (2%)   | 12 (86%)  | 2 (14%) | 0        | 100         | 100 |
| 1   | d     | 18/560 (3%)   | 18 (100%) | 0       | 0        | 100         | 100 |
| 1   | e     | 14/560 (2%)   | 14 (100%) | 0       | 0        | 100         | 100 |
| 1   | f     | 19/560 (3%)   | 19 (100%) | 0       | 0        | 100         | 100 |
| 1   | g     | 14/560 (2%)   | 12 (86%)  | 2 (14%) | 0        | 100         | 100 |
| 1   | h     | 19/560 (3%)   | 19 (100%) | 0       | 0        | 100         | 100 |
| 1   | i     | 14/560 (2%)   | 14 (100%) | 0       | 0        | 100         | 100 |
| 1   | j     | 18/560 (3%)   | 17 (94%)  | 1 (6%)  | 0        | 100         | 100 |
| 1   | k     | 14/560 (2%)   | 14 (100%) | 0       | 0        | 100         | 100 |
| 1   | l     | 19/560 (3%)   | 19 (100%) | 0       | 0        | 100         | 100 |
| 1   | t     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | u     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | v     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | w     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | x     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | y     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | z     | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 2   | A     | 87/89 (98%)       | 85 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 2   | B     | 87/89 (98%)       | 86 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | C     | 87/89 (98%)       | 86 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | D     | 87/89 (98%)       | 85 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 3   | E     | 251/264 (95%)     | 231 (92%)   | 14 (6%)  | 6 (2%)   | 4           | 29  |
| 4   | F     | 205/245 (84%)     | 195 (95%)   | 10 (5%)  | 0        | 100         | 100 |
| 4   | G     | 207/245 (84%)     | 199 (96%)   | 6 (3%)   | 2 (1%)   | 12          | 43  |
| 4   | H     | 206/245 (84%)     | 201 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 4   | I     | 206/245 (84%)     | 199 (97%)   | 6 (3%)   | 1 (0%)   | 24          | 57  |
| 4   | J     | 207/245 (84%)     | 201 (97%)   | 4 (2%)   | 2 (1%)   | 12          | 43  |
| 5   | K     | 55/104 (53%)      | 53 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 5   | L     | 87/104 (84%)      | 87 (100%)   | 0        | 0        | 100         | 100 |
| 5   | M     | 89/104 (86%)      | 87 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 5   | N     | 89/104 (86%)      | 89 (100%)   | 0        | 0        | 100         | 100 |
| 5   | O     | 89/104 (86%)      | 89 (100%)   | 0        | 0        | 100         | 100 |
| 5   | P     | 88/104 (85%)      | 88 (100%)   | 0        | 0        | 100         | 100 |
| 6   | Q     | 132/138 (96%)     | 128 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 6   | R     | 115/138 (83%)     | 114 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 6   | S     | 119/138 (86%)     | 116 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 6   | T     | 121/138 (88%)     | 118 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 6   | U     | 117/138 (85%)     | 115 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 7   | V     | 131/134 (98%)     | 123 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 7   | W     | 130/134 (97%)     | 124 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 7   | X     | 131/134 (98%)     | 126 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 7   | Y     | 131/134 (98%)     | 127 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 7   | Z     | 131/134 (98%)     | 125 (95%)   | 5 (4%)   | 1 (1%)   | 16          | 48  |
| 7   | a     | 131/134 (98%)     | 125 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| All | All   | 12674/46523 (27%) | 12203 (96%) | 362 (3%) | 109 (1%) | 16          | 45  |

All (109) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WO    | 168 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WR    | 123 | ILE  |
| 1   | WR    | 165 | PHE  |
| 1   | WR    | 166 | VAL  |
| 1   | WS    | 187 | ASP  |
| 3   | E     | 188 | LEU  |
| 3   | E     | 190 | VAL  |
| 4   | J     | 83  | ALA  |
| 1   | WB    | 148 | GLY  |
| 1   | WB    | 163 | SER  |
| 1   | WD    | 146 | THR  |
| 1   | WD    | 148 | GLY  |
| 1   | WF    | 118 | GLN  |
| 1   | WI    | 146 | THR  |
| 1   | WI    | 160 | PRO  |
| 1   | WI    | 170 | LYS  |
| 1   | WK    | 166 | VAL  |
| 1   | WM    | 148 | GLY  |
| 1   | WN    | 146 | THR  |
| 1   | WN    | 148 | GLY  |
| 1   | WP    | 146 | THR  |
| 1   | WQ    | 146 | THR  |
| 1   | WQ    | 148 | GLY  |
| 1   | WQ    | 169 | GLN  |
| 1   | WS    | 146 | THR  |
| 1   | WT    | 146 | THR  |
| 1   | WT    | 162 | PRO  |
| 1   | WW    | 146 | THR  |
| 1   | WW    | 148 | GLY  |
| 3   | E     | 167 | ASN  |
| 3   | E     | 213 | ILE  |
| 4   | G     | 83  | ALA  |
| 4   | I     | 160 | GLN  |
| 1   | UI    | 162 | PRO  |
| 1   | UJ    | 162 | PRO  |
| 1   | UK    | 162 | PRO  |
| 1   | UL    | 162 | PRO  |
| 1   | UM    | 162 | PRO  |
| 1   | UN    | 162 | PRO  |
| 1   | UO    | 162 | PRO  |
| 1   | UP    | 162 | PRO  |
| 1   | WB    | 146 | THR  |
| 1   | WB    | 164 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WD    | 118 | GLN  |
| 1   | WE    | 160 | PRO  |
| 1   | WE    | 162 | PRO  |
| 1   | WI    | 148 | GLY  |
| 1   | WP    | 148 | GLY  |
| 1   | WS    | 118 | GLN  |
| 1   | WS    | 169 | GLN  |
| 1   | WT    | 165 | PHE  |
| 1   | WW    | 118 | GLN  |
| 1   | WW    | 168 | GLU  |
| 3   | E     | 189 | PRO  |
| 1   | UI    | 163 | SER  |
| 1   | UJ    | 163 | SER  |
| 1   | UK    | 163 | SER  |
| 1   | UL    | 163 | SER  |
| 1   | UM    | 163 | SER  |
| 1   | UN    | 163 | SER  |
| 1   | UO    | 163 | SER  |
| 1   | UP    | 163 | SER  |
| 1   | WA    | 182 | PRO  |
| 1   | WB    | 182 | PRO  |
| 1   | WD    | 165 | PHE  |
| 1   | WD    | 182 | PRO  |
| 1   | WE    | 182 | PRO  |
| 1   | WF    | 182 | PRO  |
| 1   | WG    | 182 | PRO  |
| 1   | WH    | 165 | PHE  |
| 1   | WH    | 182 | PRO  |
| 1   | WI    | 169 | GLN  |
| 1   | WI    | 182 | PRO  |
| 1   | WJ    | 182 | PRO  |
| 1   | WK    | 182 | PRO  |
| 1   | WL    | 182 | PRO  |
| 1   | WM    | 182 | PRO  |
| 1   | WN    | 182 | PRO  |
| 1   | WO    | 182 | PRO  |
| 1   | WP    | 182 | PRO  |
| 1   | WQ    | 182 | PRO  |
| 1   | WR    | 112 | GLY  |
| 1   | WR    | 182 | PRO  |
| 1   | WS    | 182 | PRO  |
| 1   | WT    | 182 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WU    | 182 | PRO  |
| 1   | WV    | 148 | GLY  |
| 1   | WV    | 182 | PRO  |
| 1   | WW    | 182 | PRO  |
| 1   | WK    | 168 | GLU  |
| 1   | WR    | 121 | PHE  |
| 1   | WT    | 163 | SER  |
| 4   | G     | 162 | PRO  |
| 1   | WC    | 182 | PRO  |
| 1   | WE    | 221 | THR  |
| 1   | WG    | 163 | SER  |
| 3   | E     | 187 | ALA  |
| 7   | Z     | 58  | ALA  |
| 1   | WA    | 160 | PRO  |
| 1   | WF    | 162 | PRO  |
| 1   | WL    | 148 | GLY  |
| 1   | WS    | 148 | GLY  |
| 1   | WT    | 148 | GLY  |
| 1   | WA    | 148 | GLY  |
| 1   | WP    | 123 | ILE  |
| 1   | WR    | 148 | GLY  |
| 1   | WP    | 160 | PRO  |
| 1   | WT    | 161 | LYS  |
| 4   | J     | 229 | VAL  |

### 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   | 0     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 1     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 2     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 3     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 4     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | 5     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 6     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 7     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 8     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | 9     | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AA    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AB    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AC    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AD    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AE    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AF    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AG    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AH    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AI    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AJ    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AK    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AL    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AM    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AN    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AO    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AP    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | AQ    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 77 |
| 1   | UI    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 48 |
| 1   | UJ    | 128/467 (27%) | 121 (94%) | 7 (6%)   | 19          | 45 |
| 1   | UK    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 48 |
| 1   | UL    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 48 |
| 1   | UM    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 48 |
| 1   | UN    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 48 |
| 1   | UO    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 48 |
| 1   | UP    | 128/467 (27%) | 121 (94%) | 7 (6%)   | 19          | 45 |
| 1   | WA    | 95/467 (20%)  | 91 (96%)  | 4 (4%)   | 26          | 50 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | WB    | 93/467 (20%) | 86 (92%)  | 7 (8%)   | 12          | 38  |
| 1   | WC    | 91/467 (20%) | 83 (91%)  | 8 (9%)   | 9           | 33  |
| 1   | WD    | 92/467 (20%) | 88 (96%)  | 4 (4%)   | 26          | 50  |
| 1   | WE    | 94/467 (20%) | 87 (93%)  | 7 (7%)   | 13          | 38  |
| 1   | WF    | 93/467 (20%) | 84 (90%)  | 9 (10%)  | 8           | 29  |
| 1   | WG    | 94/467 (20%) | 85 (90%)  | 9 (10%)  | 8           | 29  |
| 1   | WH    | 79/467 (17%) | 75 (95%)  | 4 (5%)   | 21          | 46  |
| 1   | WI    | 79/467 (17%) | 75 (95%)  | 4 (5%)   | 21          | 46  |
| 1   | WJ    | 83/467 (18%) | 80 (96%)  | 3 (4%)   | 31          | 54  |
| 1   | WK    | 82/467 (18%) | 76 (93%)  | 6 (7%)   | 13          | 39  |
| 1   | WL    | 69/467 (15%) | 67 (97%)  | 2 (3%)   | 37          | 58  |
| 1   | WM    | 66/467 (14%) | 64 (97%)  | 2 (3%)   | 36          | 57  |
| 1   | WN    | 68/467 (15%) | 66 (97%)  | 2 (3%)   | 37          | 58  |
| 1   | WO    | 80/467 (17%) | 76 (95%)  | 4 (5%)   | 22          | 47  |
| 1   | WP    | 83/467 (18%) | 80 (96%)  | 3 (4%)   | 31          | 54  |
| 1   | WQ    | 93/467 (20%) | 90 (97%)  | 3 (3%)   | 34          | 56  |
| 1   | WR    | 93/467 (20%) | 85 (91%)  | 8 (9%)   | 10          | 33  |
| 1   | WS    | 93/467 (20%) | 89 (96%)  | 4 (4%)   | 26          | 50  |
| 1   | WT    | 93/467 (20%) | 86 (92%)  | 7 (8%)   | 12          | 38  |
| 1   | WU    | 94/467 (20%) | 88 (94%)  | 6 (6%)   | 16          | 42  |
| 1   | WV    | 92/467 (20%) | 81 (88%)  | 11 (12%) | 5           | 21  |
| 1   | WW    | 93/467 (20%) | 85 (91%)  | 8 (9%)   | 10          | 33  |
| 1   | b     | 8/467 (2%)   | 8 (100%)  | 0        | 100         | 100 |
| 1   | c     | 11/467 (2%)  | 11 (100%) | 0        | 100         | 100 |
| 1   | d     | 14/467 (3%)  | 12 (86%)  | 2 (14%)  | 3           | 17  |
| 1   | e     | 11/467 (2%)  | 11 (100%) | 0        | 100         | 100 |
| 1   | f     | 15/467 (3%)  | 15 (100%) | 0        | 100         | 100 |
| 1   | g     | 11/467 (2%)  | 11 (100%) | 0        | 100         | 100 |
| 1   | h     | 15/467 (3%)  | 15 (100%) | 0        | 100         | 100 |
| 1   | i     | 11/467 (2%)  | 11 (100%) | 0        | 100         | 100 |
| 1   | j     | 14/467 (3%)  | 13 (93%)  | 1 (7%)   | 13          | 39  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | k     | 11/467 (2%)   | 11 (100%)  | 0        | 100         | 100 |
| 1   | l     | 15/467 (3%)   | 15 (100%)  | 0        | 100         | 100 |
| 1   | t     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 1   | u     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 1   | v     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 1   | w     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 1   | x     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 1   | y     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 1   | z     | 141/467 (30%) | 140 (99%)  | 1 (1%)   | 76          | 77  |
| 2   | A     | 74/74 (100%)  | 72 (97%)   | 2 (3%)   | 39          | 59  |
| 2   | B     | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 2   | C     | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 2   | D     | 74/74 (100%)  | 72 (97%)   | 2 (3%)   | 39          | 59  |
| 3   | E     | 210/221 (95%) | 208 (99%)  | 2 (1%)   | 68          | 74  |
| 4   | F     | 177/204 (87%) | 175 (99%)  | 2 (1%)   | 65          | 73  |
| 4   | G     | 179/204 (88%) | 174 (97%)  | 5 (3%)   | 38          | 58  |
| 4   | H     | 178/204 (87%) | 176 (99%)  | 2 (1%)   | 65          | 73  |
| 4   | I     | 178/204 (87%) | 175 (98%)  | 3 (2%)   | 53          | 67  |
| 4   | J     | 179/204 (88%) | 178 (99%)  | 1 (1%)   | 78          | 79  |
| 5   | K     | 45/79 (57%)   | 43 (96%)   | 2 (4%)   | 25          | 49  |
| 5   | L     | 68/79 (86%)   | 66 (97%)   | 2 (3%)   | 37          | 58  |
| 5   | M     | 70/79 (89%)   | 65 (93%)   | 5 (7%)   | 13          | 39  |
| 5   | N     | 70/79 (89%)   | 67 (96%)   | 3 (4%)   | 26          | 50  |
| 5   | O     | 70/79 (89%)   | 68 (97%)   | 2 (3%)   | 37          | 58  |
| 5   | P     | 69/79 (87%)   | 65 (94%)   | 4 (6%)   | 18          | 44  |
| 6   | Q     | 110/113 (97%) | 109 (99%)  | 1 (1%)   | 70          | 74  |
| 6   | R     | 101/113 (89%) | 100 (99%)  | 1 (1%)   | 68          | 74  |
| 6   | S     | 103/113 (91%) | 99 (96%)   | 4 (4%)   | 28          | 52  |
| 6   | T     | 104/113 (92%) | 103 (99%)  | 1 (1%)   | 68          | 74  |
| 6   | U     | 102/113 (90%) | 100 (98%)  | 2 (2%)   | 48          | 65  |
| 7   | V     | 104/105 (99%) | 104 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 7   | W     | 104/105 (99%)     | 104 (100%)  | 0        | 100         | 100 |
| 7   | X     | 104/105 (99%)     | 104 (100%)  | 0        | 100         | 100 |
| 7   | Y     | 104/105 (99%)     | 103 (99%)   | 1 (1%)   | 68          | 74  |
| 7   | Z     | 104/105 (99%)     | 102 (98%)   | 2 (2%)   | 50          | 66  |
| 7   | a     | 104/105 (99%)     | 104 (100%)  | 0        | 100         | 100 |
| All | All   | 10879/38698 (28%) | 10618 (98%) | 261 (2%) | 43          | 62  |

All (261) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | UI    | 98  | LEU  |
| 1   | UI    | 127 | SER  |
| 1   | UI    | 154 | ARG  |
| 1   | UI    | 159 | MET  |
| 1   | UI    | 165 | PHE  |
| 1   | UI    | 219 | LEU  |
| 1   | UJ    | 98  | LEU  |
| 1   | UJ    | 103 | GLN  |
| 1   | UJ    | 127 | SER  |
| 1   | UJ    | 154 | ARG  |
| 1   | UJ    | 159 | MET  |
| 1   | UJ    | 165 | PHE  |
| 1   | UJ    | 268 | LEU  |
| 1   | UK    | 98  | LEU  |
| 1   | UK    | 127 | SER  |
| 1   | UK    | 154 | ARG  |
| 1   | UK    | 159 | MET  |
| 1   | UK    | 165 | PHE  |
| 1   | UK    | 219 | LEU  |
| 1   | UL    | 98  | LEU  |
| 1   | UL    | 127 | SER  |
| 1   | UL    | 154 | ARG  |
| 1   | UL    | 159 | MET  |
| 1   | UL    | 167 | ARG  |
| 1   | UL    | 219 | LEU  |
| 1   | UM    | 98  | LEU  |
| 1   | UM    | 127 | SER  |
| 1   | UM    | 154 | ARG  |
| 1   | UM    | 159 | MET  |
| 1   | UM    | 165 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | UM    | 219 | LEU  |
| 1   | UN    | 98  | LEU  |
| 1   | UN    | 127 | SER  |
| 1   | UN    | 154 | ARG  |
| 1   | UN    | 159 | MET  |
| 1   | UN    | 165 | PHE  |
| 1   | UN    | 219 | LEU  |
| 1   | UO    | 98  | LEU  |
| 1   | UO    | 127 | SER  |
| 1   | UO    | 154 | ARG  |
| 1   | UO    | 159 | MET  |
| 1   | UO    | 165 | PHE  |
| 1   | UO    | 219 | LEU  |
| 1   | UP    | 98  | LEU  |
| 1   | UP    | 127 | SER  |
| 1   | UP    | 154 | ARG  |
| 1   | UP    | 159 | MET  |
| 1   | UP    | 165 | PHE  |
| 1   | UP    | 167 | ARG  |
| 1   | UP    | 219 | LEU  |
| 1   | WA    | 114 | GLU  |
| 1   | WA    | 123 | ILE  |
| 1   | WA    | 167 | ARG  |
| 1   | WA    | 170 | LYS  |
| 1   | WB    | 119 | GLU  |
| 1   | WB    | 120 | LYS  |
| 1   | WB    | 137 | GLU  |
| 1   | WB    | 159 | MET  |
| 1   | WB    | 164 | LEU  |
| 1   | WB    | 166 | VAL  |
| 1   | WB    | 169 | GLN  |
| 1   | WC    | 115 | LEU  |
| 1   | WC    | 120 | LYS  |
| 1   | WC    | 128 | GLU  |
| 1   | WC    | 134 | ARG  |
| 1   | WC    | 164 | LEU  |
| 1   | WC    | 166 | VAL  |
| 1   | WC    | 168 | GLU  |
| 1   | WC    | 170 | LYS  |
| 1   | WD    | 114 | GLU  |
| 1   | WD    | 115 | LEU  |
| 1   | WD    | 159 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WD    | 167 | ARG  |
| 1   | WE    | 114 | GLU  |
| 1   | WE    | 123 | ILE  |
| 1   | WE    | 128 | GLU  |
| 1   | WE    | 134 | ARG  |
| 1   | WE    | 160 | PRO  |
| 1   | WE    | 161 | LYS  |
| 1   | WE    | 164 | LEU  |
| 1   | WF    | 111 | VAL  |
| 1   | WF    | 113 | PHE  |
| 1   | WF    | 123 | ILE  |
| 1   | WF    | 134 | ARG  |
| 1   | WF    | 142 | ARG  |
| 1   | WF    | 159 | MET  |
| 1   | WF    | 161 | LYS  |
| 1   | WF    | 162 | PRO  |
| 1   | WF    | 166 | VAL  |
| 1   | WG    | 111 | VAL  |
| 1   | WG    | 114 | GLU  |
| 1   | WG    | 115 | LEU  |
| 1   | WG    | 120 | LYS  |
| 1   | WG    | 129 | GLN  |
| 1   | WG    | 134 | ARG  |
| 1   | WG    | 164 | LEU  |
| 1   | WG    | 170 | LYS  |
| 1   | WG    | 190 | GLN  |
| 1   | WH    | 134 | ARG  |
| 1   | WH    | 159 | MET  |
| 1   | WH    | 168 | GLU  |
| 1   | WH    | 221 | THR  |
| 1   | WI    | 165 | PHE  |
| 1   | WI    | 168 | GLU  |
| 1   | WI    | 169 | GLN  |
| 1   | WI    | 170 | LYS  |
| 1   | WJ    | 123 | ILE  |
| 1   | WJ    | 167 | ARG  |
| 1   | WJ    | 169 | GLN  |
| 1   | WK    | 129 | GLN  |
| 1   | WK    | 164 | LEU  |
| 1   | WK    | 165 | PHE  |
| 1   | WK    | 167 | ARG  |
| 1   | WK    | 170 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WK    | 187 | ASP  |
| 1   | WL    | 159 | MET  |
| 1   | WL    | 221 | THR  |
| 1   | WM    | 159 | MET  |
| 1   | WM    | 221 | THR  |
| 1   | WN    | 159 | MET  |
| 1   | WN    | 221 | THR  |
| 1   | WO    | 159 | MET  |
| 1   | WO    | 169 | GLN  |
| 1   | WO    | 170 | LYS  |
| 1   | WO    | 221 | THR  |
| 1   | WP    | 154 | ARG  |
| 1   | WP    | 161 | LYS  |
| 1   | WP    | 165 | PHE  |
| 1   | WQ    | 114 | GLU  |
| 1   | WQ    | 134 | ARG  |
| 1   | WQ    | 159 | MET  |
| 1   | WR    | 114 | GLU  |
| 1   | WR    | 117 | ASP  |
| 1   | WR    | 128 | GLU  |
| 1   | WR    | 129 | GLN  |
| 1   | WR    | 164 | LEU  |
| 1   | WR    | 166 | VAL  |
| 1   | WR    | 169 | GLN  |
| 1   | WR    | 170 | LYS  |
| 1   | WS    | 114 | GLU  |
| 1   | WS    | 134 | ARG  |
| 1   | WS    | 159 | MET  |
| 1   | WS    | 221 | THR  |
| 1   | WT    | 119 | GLU  |
| 1   | WT    | 123 | ILE  |
| 1   | WT    | 134 | ARG  |
| 1   | WT    | 159 | MET  |
| 1   | WT    | 161 | LYS  |
| 1   | WT    | 165 | PHE  |
| 1   | WT    | 167 | ARG  |
| 1   | WU    | 114 | GLU  |
| 1   | WU    | 123 | ILE  |
| 1   | WU    | 134 | ARG  |
| 1   | WU    | 159 | MET  |
| 1   | WU    | 161 | LYS  |
| 1   | WU    | 164 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | WV    | 114 | GLU  |
| 1   | WV    | 115 | LEU  |
| 1   | WV    | 120 | LYS  |
| 1   | WV    | 128 | GLU  |
| 1   | WV    | 129 | GLN  |
| 1   | WV    | 134 | ARG  |
| 1   | WV    | 164 | LEU  |
| 1   | WV    | 166 | VAL  |
| 1   | WV    | 169 | GLN  |
| 1   | WV    | 170 | LYS  |
| 1   | WV    | 187 | ASP  |
| 1   | WW    | 114 | GLU  |
| 1   | WW    | 115 | LEU  |
| 1   | WW    | 134 | ARG  |
| 1   | WW    | 159 | MET  |
| 1   | WW    | 167 | ARG  |
| 1   | WW    | 168 | GLU  |
| 1   | WW    | 169 | GLN  |
| 1   | WW    | 221 | THR  |
| 2   | A     | 7   | MET  |
| 2   | A     | 15  | LYS  |
| 2   | D     | 9   | MET  |
| 2   | D     | 14  | MET  |
| 3   | E     | 185 | MET  |
| 3   | E     | 214 | PHE  |
| 4   | F     | 123 | MET  |
| 4   | F     | 160 | GLN  |
| 4   | G     | 48  | ILE  |
| 4   | G     | 140 | ARG  |
| 4   | G     | 160 | GLN  |
| 4   | G     | 162 | PRO  |
| 4   | G     | 209 | MET  |
| 4   | H     | 143 | ARG  |
| 4   | H     | 152 | ARG  |
| 4   | I     | 187 | PHE  |
| 4   | I     | 205 | MET  |
| 4   | I     | 241 | GLN  |
| 4   | J     | 230 | ASP  |
| 5   | K     | 15  | GLN  |
| 5   | K     | 19  | MET  |
| 5   | L     | 15  | GLN  |
| 5   | L     | 19  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 7   | ILE  |
| 5   | M     | 11  | ILE  |
| 5   | M     | 14  | LEU  |
| 5   | M     | 15  | GLN  |
| 5   | M     | 19  | MET  |
| 5   | N     | 15  | GLN  |
| 5   | N     | 19  | MET  |
| 5   | N     | 97  | GLN  |
| 5   | O     | 15  | GLN  |
| 5   | O     | 19  | MET  |
| 5   | P     | 15  | GLN  |
| 5   | P     | 19  | MET  |
| 5   | P     | 57  | GLU  |
| 5   | P     | 91  | LYS  |
| 6   | Q     | 101 | ASP  |
| 6   | R     | 55  | ARG  |
| 6   | S     | 65  | LEU  |
| 6   | S     | 69  | SER  |
| 6   | S     | 71  | HIS  |
| 6   | S     | 72  | HIS  |
| 6   | T     | 76  | GLN  |
| 6   | U     | 65  | LEU  |
| 6   | U     | 104 | ARG  |
| 7   | Y     | 101 | GLU  |
| 7   | Z     | 6   | ILE  |
| 7   | Z     | 127 | LEU  |
| 1   | d     | 318 | ASN  |
| 1   | d     | 319 | GLN  |
| 1   | j     | 319 | GLN  |
| 1   | t     | 295 | SER  |
| 1   | u     | 295 | SER  |
| 1   | v     | 295 | SER  |
| 1   | w     | 295 | SER  |
| 1   | x     | 295 | SER  |
| 1   | y     | 295 | SER  |
| 1   | z     | 295 | SER  |
| 1   | 1     | 295 | SER  |
| 1   | 2     | 295 | SER  |
| 1   | 3     | 295 | SER  |
| 1   | 4     | 295 | SER  |
| 1   | 5     | 295 | SER  |
| 1   | 6     | 295 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7     | 295 | SER  |
| 1   | 8     | 295 | SER  |
| 1   | 9     | 295 | SER  |
| 1   | 0     | 295 | SER  |
| 1   | AA    | 295 | SER  |
| 1   | AB    | 295 | SER  |
| 1   | AC    | 295 | SER  |
| 1   | AD    | 295 | SER  |
| 1   | AE    | 295 | SER  |
| 1   | AF    | 295 | SER  |
| 1   | AG    | 295 | SER  |
| 1   | AH    | 295 | SER  |
| 1   | AI    | 295 | SER  |
| 1   | AJ    | 295 | SER  |
| 1   | AK    | 295 | SER  |
| 1   | AL    | 295 | SER  |
| 1   | AM    | 295 | SER  |
| 1   | AN    | 295 | SER  |
| 1   | AO    | 295 | SER  |
| 1   | AP    | 295 | SER  |
| 1   | AQ    | 295 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (331) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | UI    | 69  | GLN  |
| 1   | UI    | 94  | HIS  |
| 1   | UI    | 196 | HIS  |
| 1   | UJ    | 94  | HIS  |
| 1   | UJ    | 245 | HIS  |
| 1   | UK    | 94  | HIS  |
| 1   | UK    | 196 | HIS  |
| 1   | UL    | 69  | GLN  |
| 1   | UL    | 94  | HIS  |
| 1   | UL    | 196 | HIS  |
| 1   | UM    | 94  | HIS  |
| 1   | UM    | 196 | HIS  |
| 1   | UN    | 69  | GLN  |
| 1   | UN    | 94  | HIS  |
| 1   | UN    | 196 | HIS  |
| 1   | UO    | 69  | GLN  |
| 1   | UO    | 94  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | UO    | 196 | HIS  |
| 1   | UP    | 94  | HIS  |
| 1   | UP    | 196 | HIS  |
| 1   | WA    | 156 | HIS  |
| 1   | WB    | 131 | ASN  |
| 1   | WB    | 169 | GLN  |
| 1   | WC    | 129 | GLN  |
| 1   | WC    | 190 | GLN  |
| 1   | WD    | 190 | GLN  |
| 1   | WE    | 156 | HIS  |
| 1   | WE    | 209 | ASN  |
| 1   | WF    | 118 | GLN  |
| 1   | WG    | 118 | GLN  |
| 1   | WH    | 156 | HIS  |
| 1   | WI    | 129 | GLN  |
| 1   | WI    | 156 | HIS  |
| 1   | WJ    | 169 | GLN  |
| 1   | WJ    | 209 | ASN  |
| 1   | WO    | 209 | ASN  |
| 1   | WP    | 169 | GLN  |
| 1   | WP    | 209 | ASN  |
| 1   | WR    | 129 | GLN  |
| 1   | WR    | 156 | HIS  |
| 1   | WT    | 156 | HIS  |
| 1   | WT    | 209 | ASN  |
| 1   | WV    | 118 | GLN  |
| 1   | WV    | 169 | GLN  |
| 2   | D     | 39  | GLN  |
| 3   | E     | 162 | ASN  |
| 3   | E     | 182 | ASN  |
| 4   | F     | 119 | GLN  |
| 4   | F     | 141 | GLN  |
| 4   | F     | 160 | GLN  |
| 4   | G     | 86  | ASN  |
| 4   | G     | 87  | GLN  |
| 4   | G     | 241 | GLN  |
| 4   | H     | 160 | GLN  |
| 4   | H     | 184 | GLN  |
| 4   | I     | 160 | GLN  |
| 4   | I     | 184 | GLN  |
| 4   | I     | 233 | GLN  |
| 4   | I     | 241 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 87  | GLN  |
| 4   | J     | 114 | GLN  |
| 4   | J     | 155 | ASN  |
| 5   | K     | 103 | GLN  |
| 5   | M     | 13  | GLN  |
| 5   | M     | 15  | GLN  |
| 5   | M     | 83  | GLN  |
| 5   | M     | 103 | GLN  |
| 5   | N     | 87  | GLN  |
| 5   | O     | 39  | HIS  |
| 5   | O     | 55  | GLN  |
| 5   | O     | 83  | GLN  |
| 5   | O     | 87  | GLN  |
| 5   | O     | 97  | GLN  |
| 5   | P     | 55  | GLN  |
| 5   | P     | 76  | GLN  |
| 5   | P     | 87  | GLN  |
| 6   | Q     | 17  | ASN  |
| 6   | Q     | 71  | HIS  |
| 6   | R     | 21  | GLN  |
| 6   | R     | 29  | ASN  |
| 6   | R     | 92  | GLN  |
| 6   | R     | 98  | ASN  |
| 6   | R     | 117 | GLN  |
| 6   | S     | 32  | ASN  |
| 6   | S     | 76  | GLN  |
| 6   | S     | 92  | GLN  |
| 6   | S     | 135 | GLN  |
| 6   | T     | 21  | GLN  |
| 6   | T     | 32  | ASN  |
| 6   | T     | 72  | HIS  |
| 6   | T     | 76  | GLN  |
| 6   | T     | 98  | ASN  |
| 6   | T     | 117 | GLN  |
| 6   | U     | 13  | GLN  |
| 6   | U     | 72  | HIS  |
| 6   | U     | 76  | GLN  |
| 6   | U     | 92  | GLN  |
| 6   | U     | 112 | ASN  |
| 7   | V     | 30  | ASN  |
| 7   | V     | 115 | ASN  |
| 7   | W     | 22  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | X     | 40  | GLN  |
| 7   | X     | 50  | GLN  |
| 7   | X     | 57  | GLN  |
| 7   | X     | 134 | GLN  |
| 7   | Y     | 82  | ASN  |
| 7   | Z     | 17  | GLN  |
| 7   | Z     | 115 | ASN  |
| 7   | a     | 5   | ASN  |
| 7   | a     | 57  | GLN  |
| 7   | a     | 115 | ASN  |
| 1   | b     | 319 | GLN  |
| 1   | e     | 324 | ASN  |
| 1   | f     | 324 | ASN  |
| 1   | i     | 318 | ASN  |
| 1   | j     | 318 | ASN  |
| 1   | k     | 318 | ASN  |
| 1   | l     | 318 | ASN  |
| 1   | t     | 234 | GLN  |
| 1   | t     | 303 | GLN  |
| 1   | t     | 378 | ASN  |
| 1   | t     | 434 | ASN  |
| 1   | u     | 234 | GLN  |
| 1   | u     | 281 | HIS  |
| 1   | u     | 303 | GLN  |
| 1   | u     | 374 | HIS  |
| 1   | u     | 378 | ASN  |
| 1   | u     | 434 | ASN  |
| 1   | v     | 234 | GLN  |
| 1   | v     | 303 | GLN  |
| 1   | v     | 374 | HIS  |
| 1   | v     | 378 | ASN  |
| 1   | v     | 434 | ASN  |
| 1   | w     | 234 | GLN  |
| 1   | w     | 303 | GLN  |
| 1   | w     | 374 | HIS  |
| 1   | w     | 378 | ASN  |
| 1   | w     | 434 | ASN  |
| 1   | x     | 234 | GLN  |
| 1   | x     | 303 | GLN  |
| 1   | x     | 374 | HIS  |
| 1   | x     | 378 | ASN  |
| 1   | x     | 434 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | y     | 234 | GLN  |
| 1   | y     | 374 | HIS  |
| 1   | y     | 378 | ASN  |
| 1   | y     | 434 | ASN  |
| 1   | z     | 231 | ASN  |
| 1   | z     | 234 | GLN  |
| 1   | z     | 303 | GLN  |
| 1   | z     | 374 | HIS  |
| 1   | z     | 378 | ASN  |
| 1   | z     | 434 | ASN  |
| 1   | 1     | 231 | ASN  |
| 1   | 1     | 234 | GLN  |
| 1   | 1     | 297 | GLN  |
| 1   | 1     | 299 | ASN  |
| 1   | 1     | 303 | GLN  |
| 1   | 1     | 374 | HIS  |
| 1   | 1     | 378 | ASN  |
| 1   | 1     | 434 | ASN  |
| 1   | 2     | 231 | ASN  |
| 1   | 2     | 234 | GLN  |
| 1   | 2     | 303 | GLN  |
| 1   | 2     | 374 | HIS  |
| 1   | 2     | 378 | ASN  |
| 1   | 2     | 434 | ASN  |
| 1   | 3     | 231 | ASN  |
| 1   | 3     | 234 | GLN  |
| 1   | 3     | 281 | HIS  |
| 1   | 3     | 303 | GLN  |
| 1   | 3     | 374 | HIS  |
| 1   | 3     | 378 | ASN  |
| 1   | 3     | 434 | ASN  |
| 1   | 4     | 231 | ASN  |
| 1   | 4     | 234 | GLN  |
| 1   | 4     | 303 | GLN  |
| 1   | 4     | 374 | HIS  |
| 1   | 4     | 378 | ASN  |
| 1   | 4     | 434 | ASN  |
| 1   | 5     | 231 | ASN  |
| 1   | 5     | 234 | GLN  |
| 1   | 5     | 263 | HIS  |
| 1   | 5     | 281 | HIS  |
| 1   | 5     | 299 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 303 | GLN  |
| 1   | 5     | 374 | HIS  |
| 1   | 5     | 378 | ASN  |
| 1   | 5     | 434 | ASN  |
| 1   | 6     | 231 | ASN  |
| 1   | 6     | 234 | GLN  |
| 1   | 6     | 281 | HIS  |
| 1   | 6     | 297 | GLN  |
| 1   | 6     | 303 | GLN  |
| 1   | 6     | 374 | HIS  |
| 1   | 6     | 378 | ASN  |
| 1   | 6     | 434 | ASN  |
| 1   | 7     | 231 | ASN  |
| 1   | 7     | 234 | GLN  |
| 1   | 7     | 281 | HIS  |
| 1   | 7     | 299 | ASN  |
| 1   | 7     | 303 | GLN  |
| 1   | 7     | 374 | HIS  |
| 1   | 7     | 378 | ASN  |
| 1   | 7     | 434 | ASN  |
| 1   | 8     | 231 | ASN  |
| 1   | 8     | 234 | GLN  |
| 1   | 8     | 303 | GLN  |
| 1   | 8     | 374 | HIS  |
| 1   | 8     | 378 | ASN  |
| 1   | 8     | 434 | ASN  |
| 1   | 9     | 231 | ASN  |
| 1   | 9     | 234 | GLN  |
| 1   | 9     | 303 | GLN  |
| 1   | 9     | 374 | HIS  |
| 1   | 9     | 378 | ASN  |
| 1   | 9     | 434 | ASN  |
| 1   | 0     | 231 | ASN  |
| 1   | 0     | 234 | GLN  |
| 1   | 0     | 281 | HIS  |
| 1   | 0     | 303 | GLN  |
| 1   | 0     | 374 | HIS  |
| 1   | 0     | 378 | ASN  |
| 1   | 0     | 434 | ASN  |
| 1   | AA    | 231 | ASN  |
| 1   | AA    | 234 | GLN  |
| 1   | AA    | 303 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 374 | HIS  |
| 1   | AA    | 378 | ASN  |
| 1   | AA    | 434 | ASN  |
| 1   | AB    | 231 | ASN  |
| 1   | AB    | 234 | GLN  |
| 1   | AB    | 265 | GLN  |
| 1   | AB    | 303 | GLN  |
| 1   | AB    | 374 | HIS  |
| 1   | AB    | 378 | ASN  |
| 1   | AB    | 434 | ASN  |
| 1   | AC    | 231 | ASN  |
| 1   | AC    | 234 | GLN  |
| 1   | AC    | 281 | HIS  |
| 1   | AC    | 303 | GLN  |
| 1   | AC    | 374 | HIS  |
| 1   | AC    | 378 | ASN  |
| 1   | AC    | 434 | ASN  |
| 1   | AD    | 231 | ASN  |
| 1   | AD    | 234 | GLN  |
| 1   | AD    | 297 | GLN  |
| 1   | AD    | 303 | GLN  |
| 1   | AD    | 365 | ASN  |
| 1   | AD    | 374 | HIS  |
| 1   | AD    | 378 | ASN  |
| 1   | AD    | 434 | ASN  |
| 1   | AE    | 231 | ASN  |
| 1   | AE    | 234 | GLN  |
| 1   | AE    | 297 | GLN  |
| 1   | AE    | 303 | GLN  |
| 1   | AE    | 374 | HIS  |
| 1   | AE    | 378 | ASN  |
| 1   | AE    | 434 | ASN  |
| 1   | AF    | 231 | ASN  |
| 1   | AF    | 234 | GLN  |
| 1   | AF    | 246 | GLN  |
| 1   | AF    | 281 | HIS  |
| 1   | AF    | 303 | GLN  |
| 1   | AF    | 374 | HIS  |
| 1   | AF    | 378 | ASN  |
| 1   | AF    | 434 | ASN  |
| 1   | AG    | 231 | ASN  |
| 1   | AG    | 234 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AG    | 303 | GLN  |
| 1   | AG    | 378 | ASN  |
| 1   | AG    | 434 | ASN  |
| 1   | AH    | 231 | ASN  |
| 1   | AH    | 234 | GLN  |
| 1   | AH    | 281 | HIS  |
| 1   | AH    | 303 | GLN  |
| 1   | AH    | 378 | ASN  |
| 1   | AH    | 434 | ASN  |
| 1   | AI    | 231 | ASN  |
| 1   | AI    | 234 | GLN  |
| 1   | AI    | 303 | GLN  |
| 1   | AI    | 374 | HIS  |
| 1   | AI    | 378 | ASN  |
| 1   | AI    | 434 | ASN  |
| 1   | AJ    | 231 | ASN  |
| 1   | AJ    | 234 | GLN  |
| 1   | AJ    | 281 | HIS  |
| 1   | AJ    | 303 | GLN  |
| 1   | AJ    | 374 | HIS  |
| 1   | AJ    | 378 | ASN  |
| 1   | AJ    | 434 | ASN  |
| 1   | AK    | 231 | ASN  |
| 1   | AK    | 234 | GLN  |
| 1   | AK    | 281 | HIS  |
| 1   | AK    | 303 | GLN  |
| 1   | AK    | 374 | HIS  |
| 1   | AK    | 378 | ASN  |
| 1   | AK    | 434 | ASN  |
| 1   | AL    | 234 | GLN  |
| 1   | AL    | 281 | HIS  |
| 1   | AL    | 303 | GLN  |
| 1   | AL    | 374 | HIS  |
| 1   | AL    | 378 | ASN  |
| 1   | AL    | 434 | ASN  |
| 1   | AM    | 234 | GLN  |
| 1   | AM    | 303 | GLN  |
| 1   | AM    | 374 | HIS  |
| 1   | AM    | 378 | ASN  |
| 1   | AM    | 434 | ASN  |
| 1   | AN    | 234 | GLN  |
| 1   | AN    | 374 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AN    | 378 | ASN  |
| 1   | AN    | 434 | ASN  |
| 1   | AO    | 234 | GLN  |
| 1   | AO    | 297 | GLN  |
| 1   | AO    | 303 | GLN  |
| 1   | AO    | 374 | HIS  |
| 1   | AO    | 378 | ASN  |
| 1   | AO    | 434 | ASN  |
| 1   | AP    | 234 | GLN  |
| 1   | AP    | 297 | GLN  |
| 1   | AP    | 303 | GLN  |
| 1   | AP    | 359 | GLN  |
| 1   | AP    | 374 | HIS  |
| 1   | AP    | 378 | ASN  |
| 1   | AP    | 434 | ASN  |
| 1   | AQ    | 234 | GLN  |
| 1   | AQ    | 303 | GLN  |
| 1   | AQ    | 374 | HIS  |
| 1   | AQ    | 378 | ASN  |
| 1   | AQ    | 434 | 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

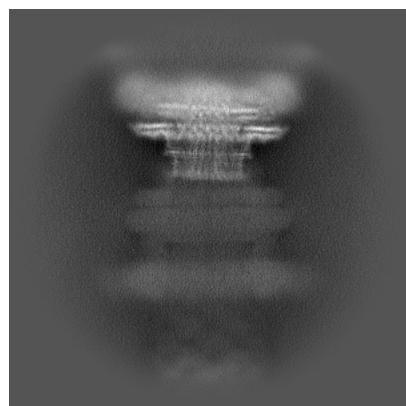
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37605. These allow visual inspection of the internal detail of the map and identification of artifacts.

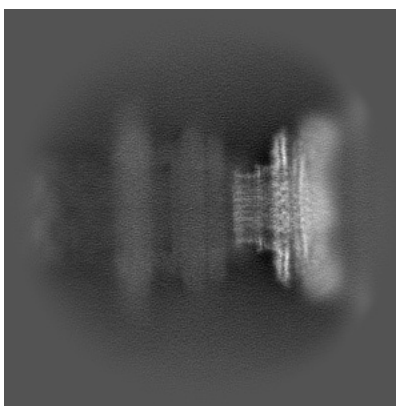
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

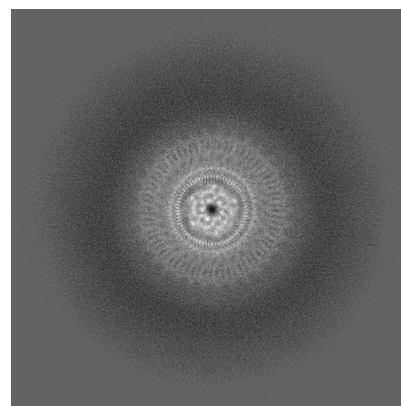
#### 6.1.1 Primary map



X

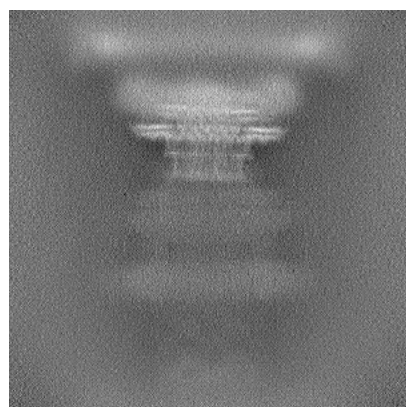


Y

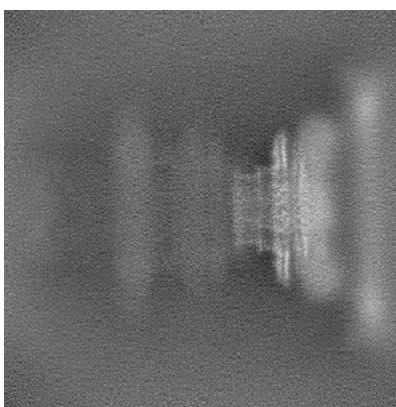


Z

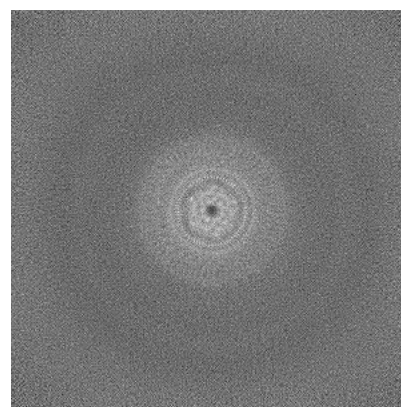
#### 6.1.2 Raw map



X



Y

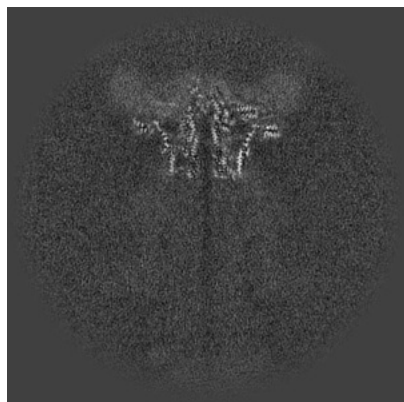


Z

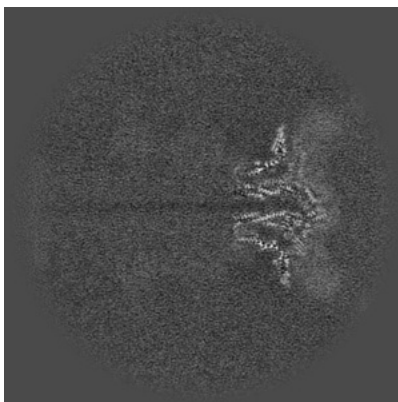
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

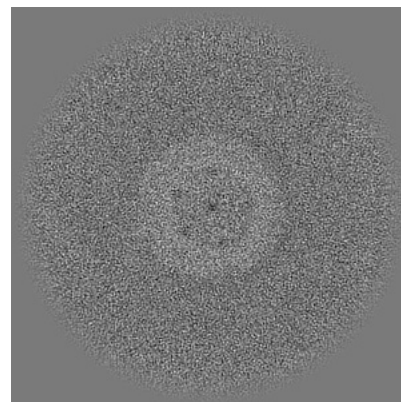
### 6.2.1 Primary map



X Index: 256

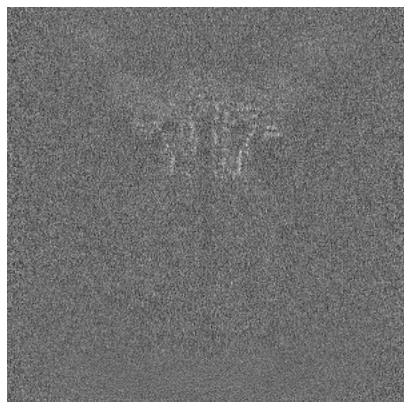


Y Index: 256

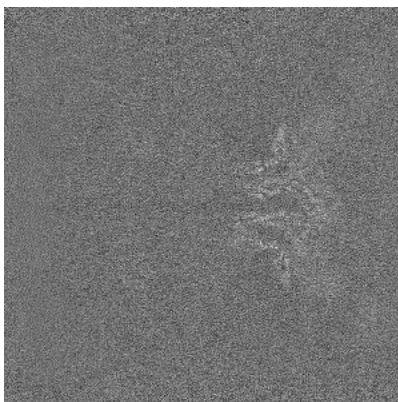


Z Index: 256

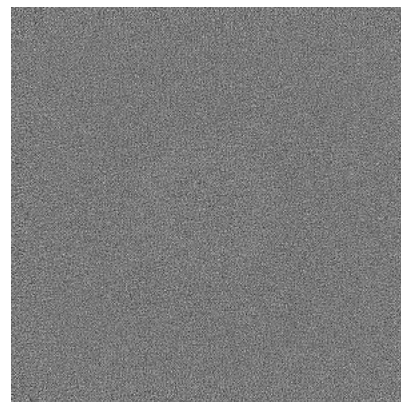
### 6.2.2 Raw map



X Index: 256



Y Index: 256

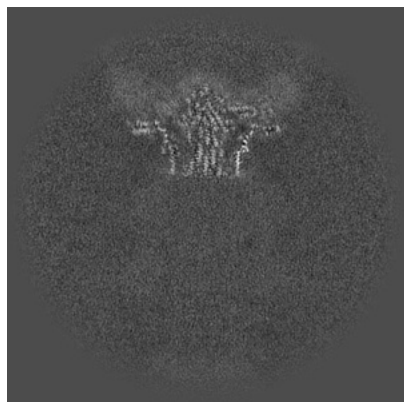


Z Index: 256

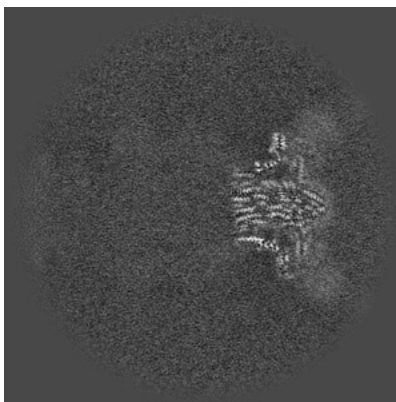
The images above show central slices of the map in three orthogonal directions.

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

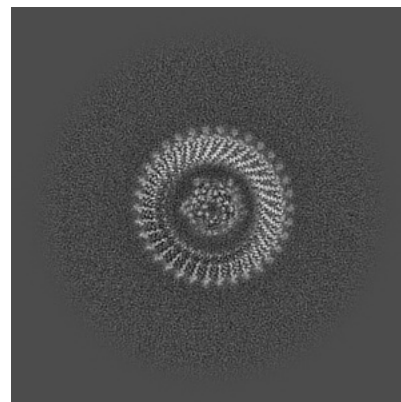
### 6.3.1 Primary map



X Index: 244

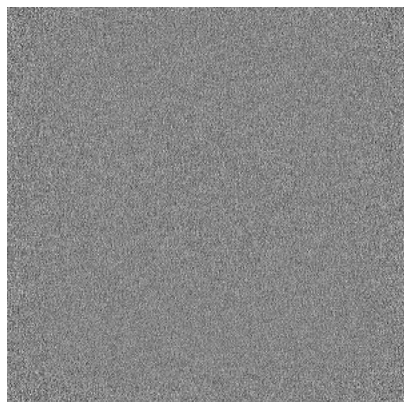


Y Index: 265

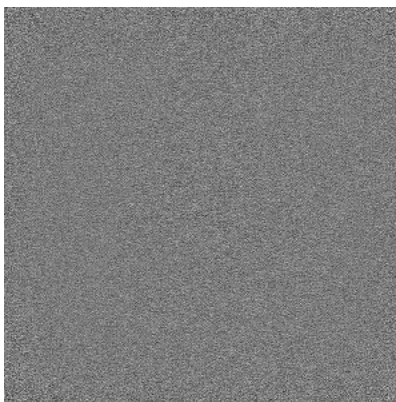


Z Index: 358

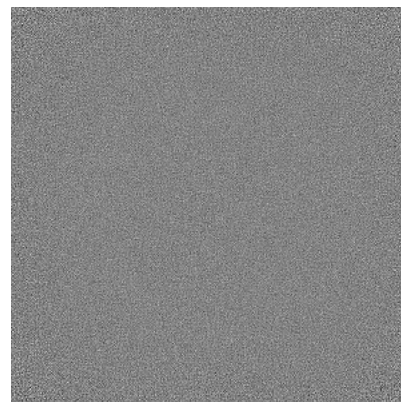
### 6.3.2 Raw map



X Index: 0



Y Index: 0

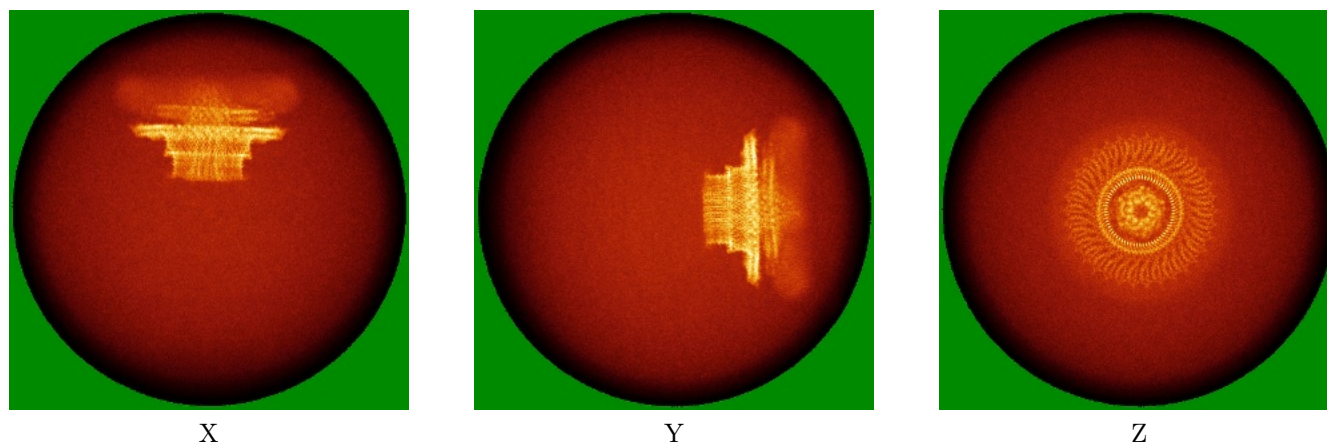


Z Index: 0

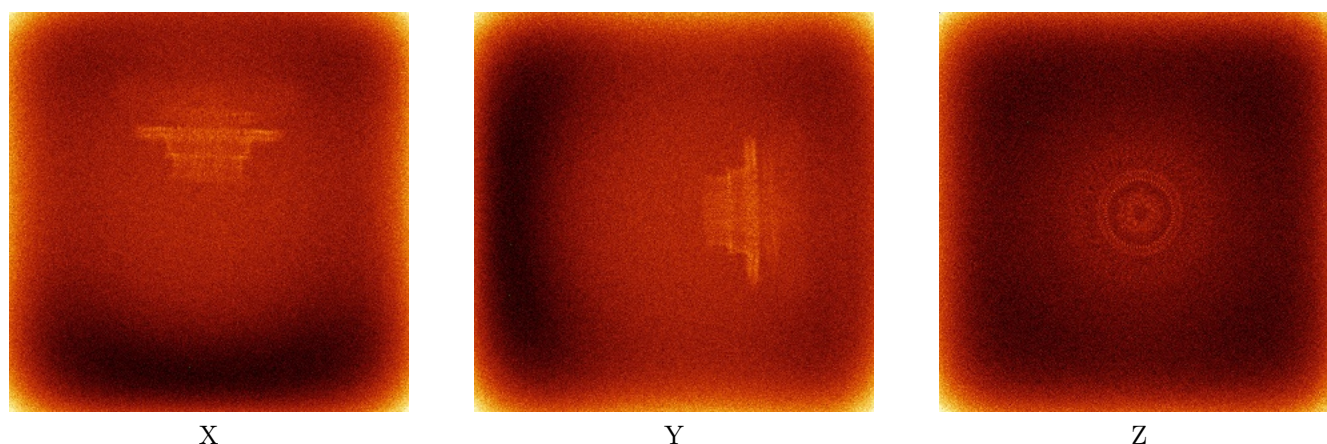
The images above show the largest variance slices of the map in three orthogonal directions.

## 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](#)

This section was not generated.

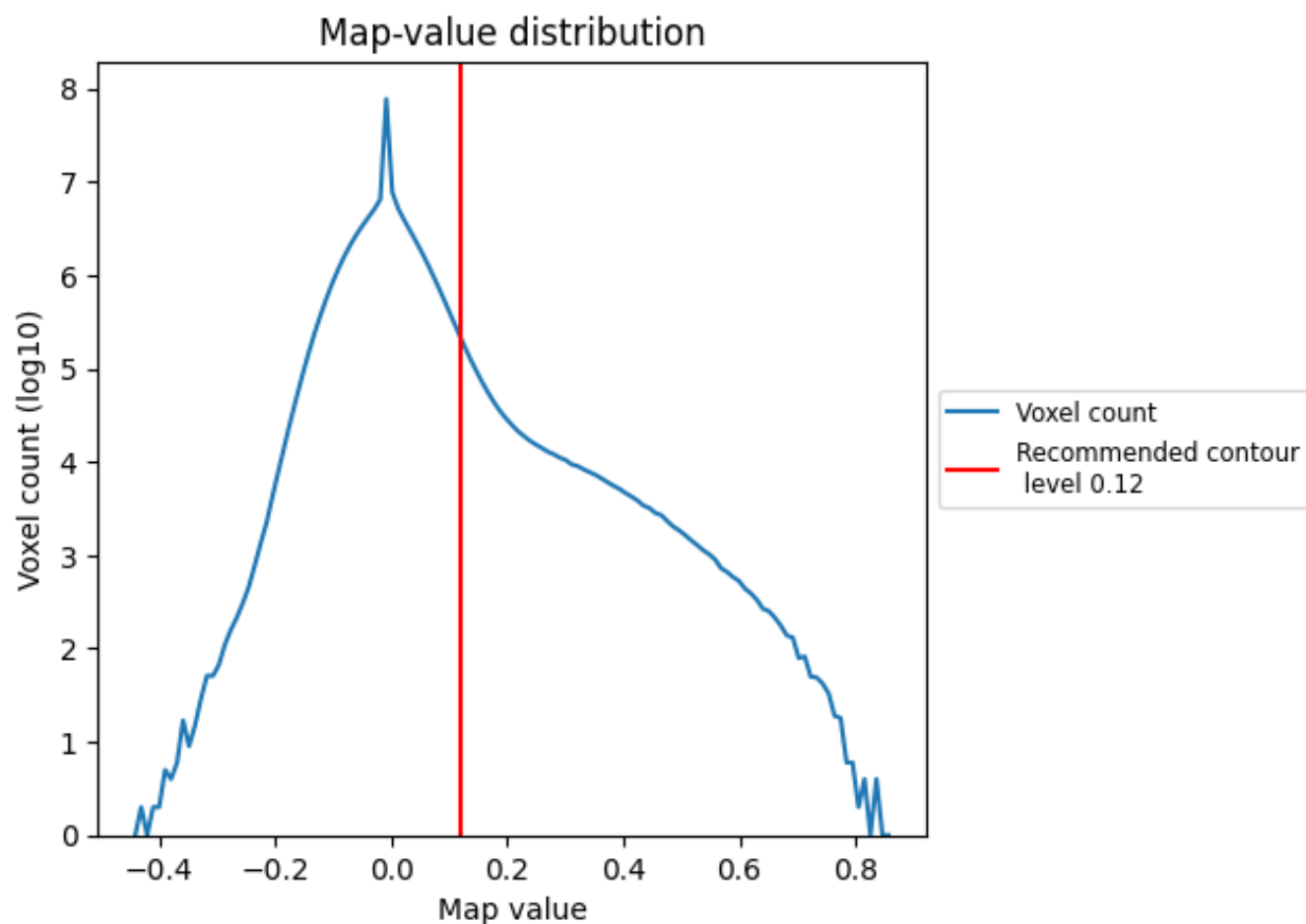
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

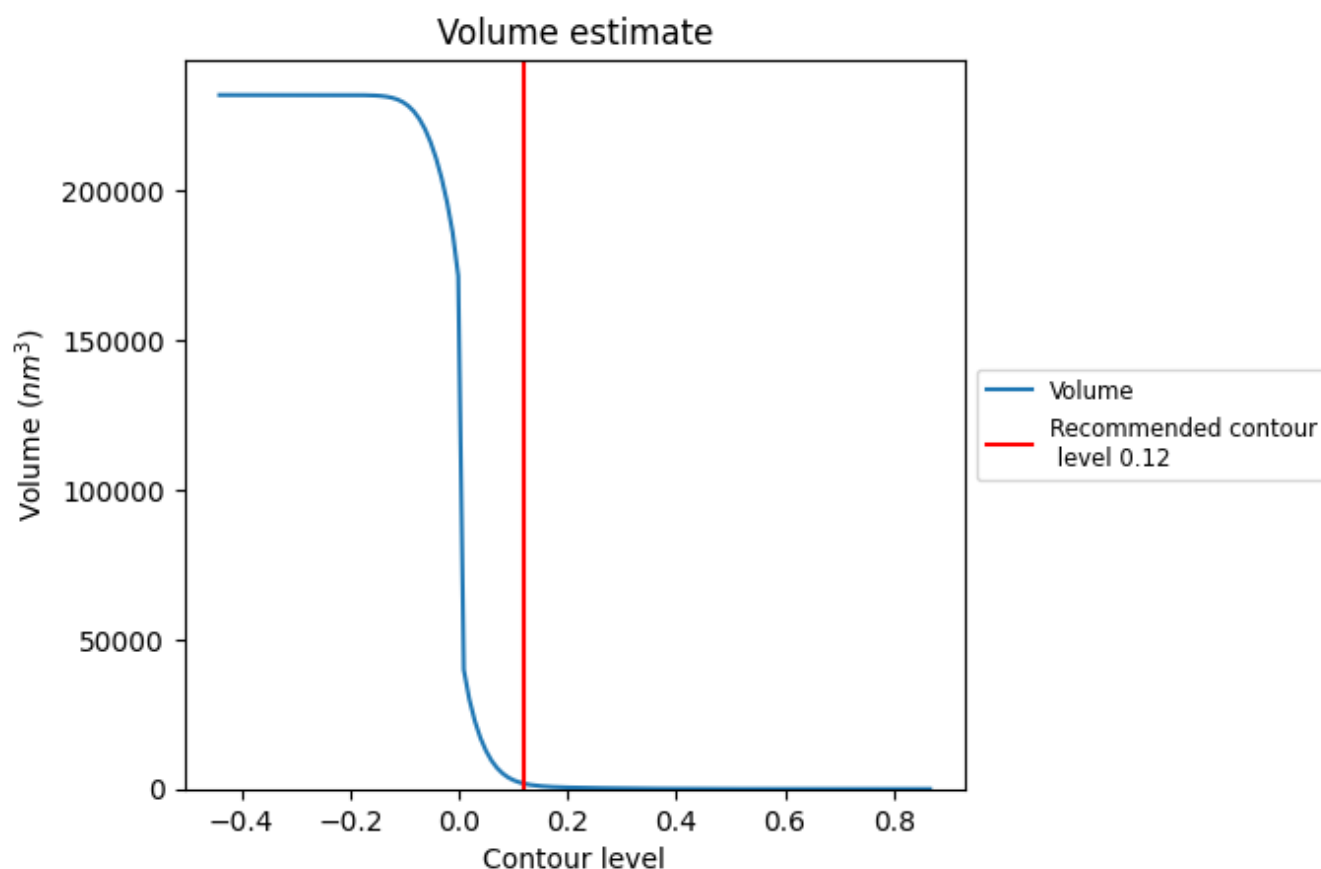
This section contains the results of statistical analysis of the map.

### 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.

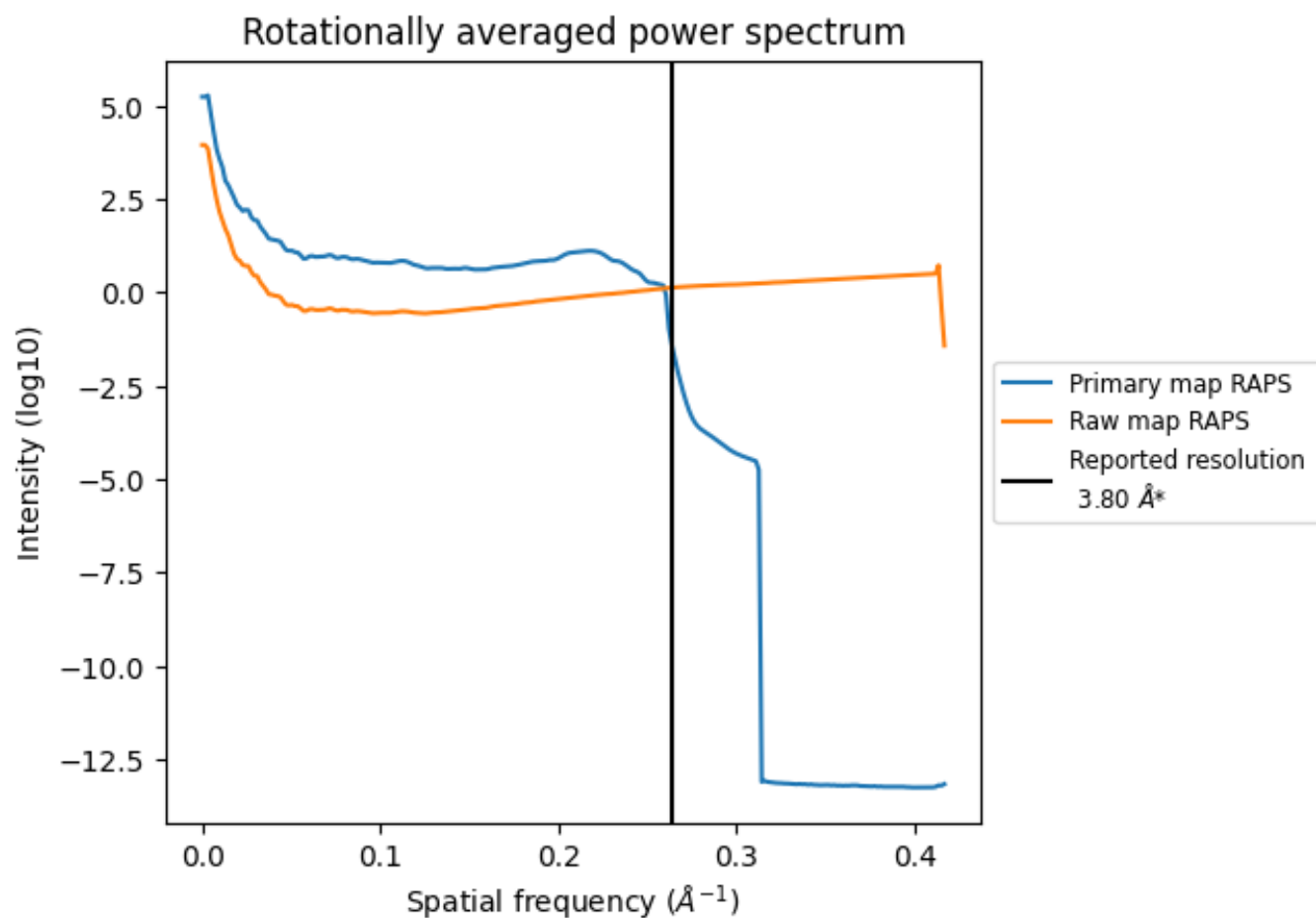
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1782 nm<sup>3</sup>; this corresponds to an approximate mass of 1610 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 ⓘ

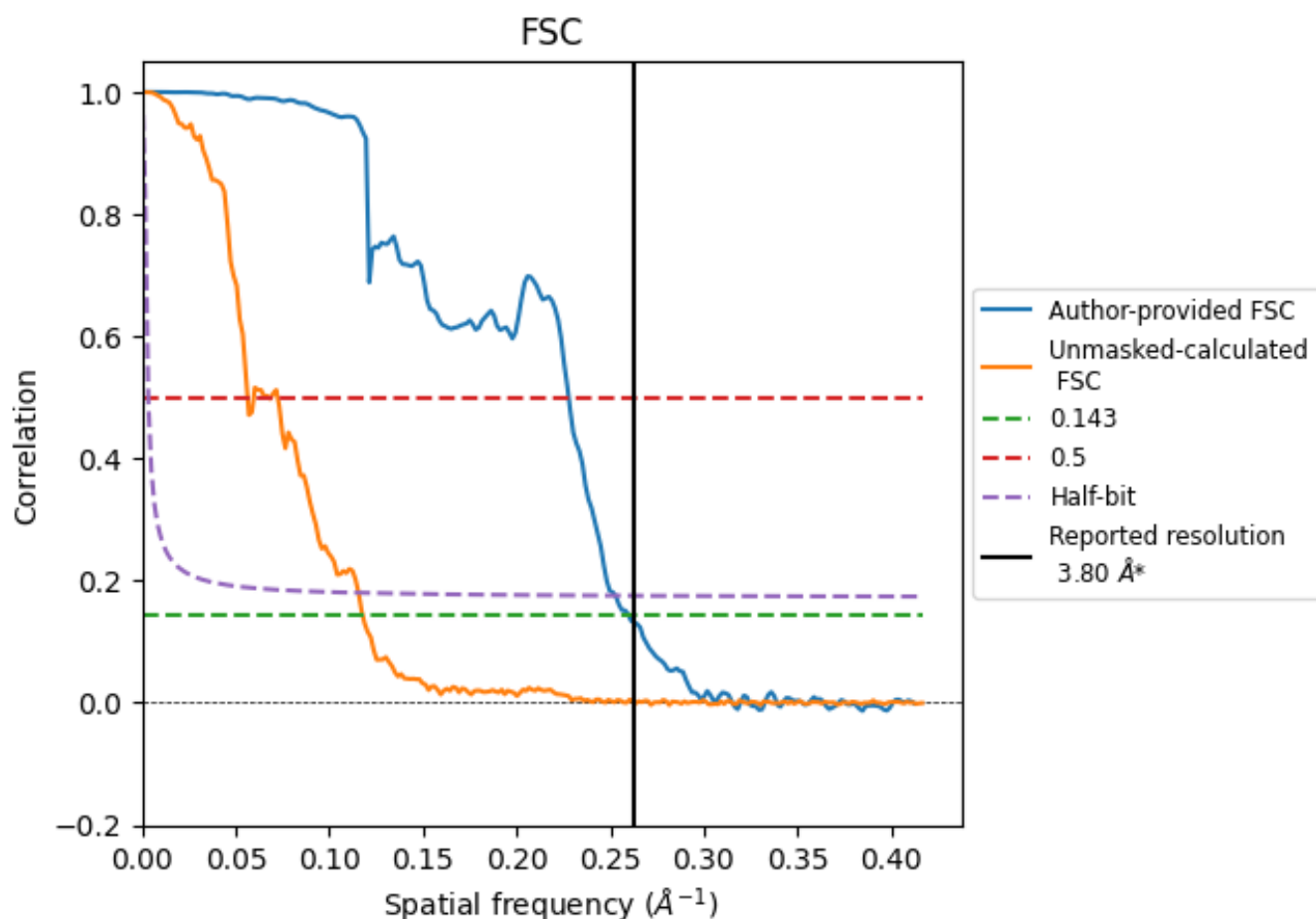


\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$

## 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  $0.263 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.80                               | -     | -        |
| Author-provided FSC curve | 3.85                               | 4.39  | 3.96     |
| Unmasked-calculated*      | 8.49                               | 17.76 | 8.65     |

\*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 8.49 differs from the reported value 3.8 by more than 10 %

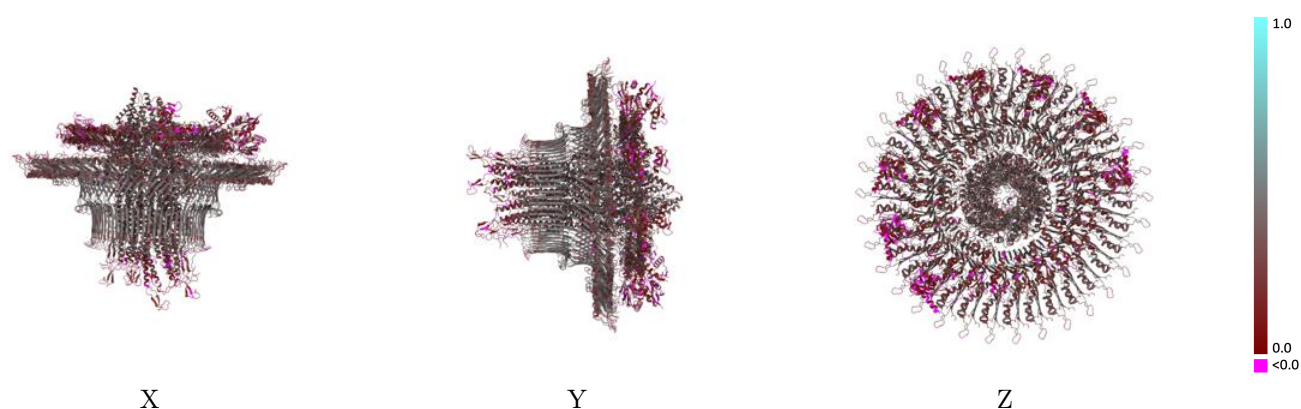
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37605 and PDB model 8WKQ. Per-residue inclusion information can be found in section 3 on page 13.

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

This section was not generated.

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

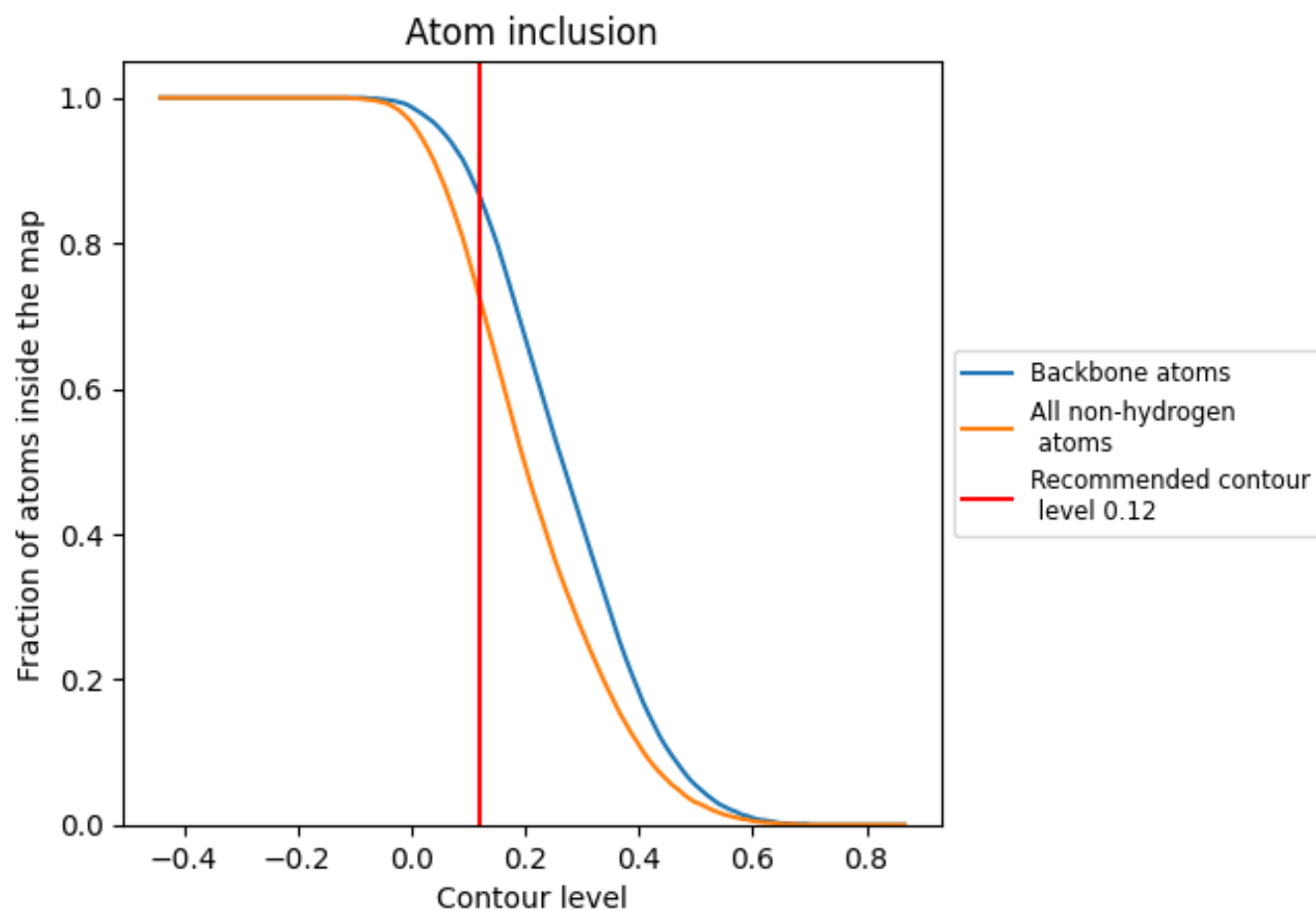


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% 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   |  0.7250   |  0.3190   |
| 0     |  0.8170   |  0.3700   |
| 1     |  0.8140   |  0.3590   |
| 2     |  0.8250   |  0.3680   |
| 3     |  0.8290   |  0.3720   |
| 4     |  0.8250   |  0.3740   |
| 5     |  0.8190   |  0.3730   |
| 6     |  0.8280   |  0.3770   |
| 7     |  0.8200   |  0.3750   |
| 8     |  0.8340   |  0.3860   |
| 9     |  0.8330   |  0.3850   |
| A     |  0.7670   |  0.3160   |
| AA    |  0.8140   |  0.3660   |
| AB    |  0.8210   |  0.3660   |
| AC    |  0.8210  |  0.3690  |
| AD    |  0.8240 |  0.3640 |
| AE    |  0.8180 |  0.3720 |
| AF    |  0.8290 |  0.3590 |
| AG    |  0.8120 |  0.3470 |
| AH    |  0.8200 |  0.3540 |
| AI    |  0.8010 |  0.3490 |
| AJ    |  0.8220 |  0.3610 |
| AK    |  0.8270 |  0.3650 |
| AL    |  0.8140 |  0.3620 |
| AM    |  0.8110 |  0.3650 |
| AN    |  0.8040 |  0.3640 |
| AO    |  0.8250 |  0.3750 |
| AP    |  0.8220 |  0.3740 |
| AQ    |  0.8160 |  0.3700 |
| B     |  0.8150 |  0.3480 |
| C     |  0.8200 |  0.3510 |
| D     |  0.8090 |  0.3460 |
| E     |  0.7840 |  0.3500 |
| F     |  0.7940 |  0.3610 |
| G     |  0.8120 |  0.3750 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| H     |  0.7990   |  0.3690   |
| I     |  0.7870   |  0.3680   |
| J     |  0.7640   |  0.3640   |
| K     |  0.7300   |  0.3590   |
| L     |  0.7890   |  0.3540   |
| M     |  0.7750   |  0.3500   |
| N     |  0.7680   |  0.3580   |
| O     |  0.7610   |  0.3430   |
| P     |  0.7660   |  0.3520   |
| Q     |  0.7750   |  0.3790   |
| R     |  0.7740   |  0.3690   |
| S     |  0.7420   |  0.3670   |
| T     |  0.7260   |  0.3610   |
| U     |  0.6610   |  0.3390   |
| UI    |  0.5160   |  0.2040   |
| UJ    |  0.4890   |  0.1640   |
| UK    |  0.4160   |  0.1540   |
| UL    |  0.3670  |  0.1180  |
| UM    |  0.2850 |  0.0510 |
| UN    |  0.3590 |  0.0800 |
| UO    |  0.4200 |  0.1310 |
| UP    |  0.4760 |  0.1390 |
| V     |  0.5020 |  0.3110 |
| W     |  0.4120 |  0.2850 |
| WA    |  0.7920 |  0.3380 |
| WB    |  0.7910 |  0.3290 |
| WC    |  0.8040 |  0.3460 |
| WD    |  0.7890 |  0.3400 |
| WE    |  0.7680 |  0.3210 |
| WF    |  0.7780 |  0.3230 |
| WG    |  0.7460 |  0.2860 |
| WH    |  0.7690 |  0.2810 |
| WI    |  0.7200 |  0.2360 |
| WJ    |  0.6920 |  0.2170 |
| WK    |  0.6500 |  0.1970 |
| WL    |  0.6770 |  0.1880 |
| WM    |  0.7090 |  0.2250 |
| WN    |  0.6880 |  0.1660 |
| WO    |  0.6630 |  0.1650 |
| WP    |  0.7480 |  0.2330 |
| WQ    |  0.7300 |  0.2510 |
| WR    |  0.7300 |  0.2820 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| WS    |  0.7870   |  0.2910   |
| WT    |  0.7950   |  0.3240   |
| WU    |  0.7600   |  0.2930   |
| WV    |  0.7590   |  0.2860   |
| WW    |  0.7790   |  0.3220   |
| X     |  0.3500   |  0.2540   |
| Y     |  0.2900   |  0.2230   |
| Z     |  0.2590   |  0.2420   |
| a     |  0.2050   |  0.2240   |
| b     |  0.6670   |  0.3370   |
| c     |  0.5050   |  0.3570   |
| d     |  0.5640   |  0.3320   |
| e     |  0.2430   |  0.2510   |
| f     |  0.4930   |  0.2610   |
| g     |  0.0870   |  0.1150   |
| h     |  0.4360   |  0.2610   |
| i     |  0.0680   |  0.1250   |
| j     |  0.4510   |  0.2720   |
| k     |  0.0780   |  0.1940   |
| l     |  0.3360   |  0.2730   |
| t     |  0.8270  |  0.3780  |
| u     |  0.8270 |  0.3630 |
| v     |  0.8240 |  0.3710 |
| w     |  0.8280 |  0.3750 |
| x     |  0.8300 |  0.3680 |
| y     |  0.8260 |  0.3730 |
| z     |  0.8250 |  0.3740 |