



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:57 PM UTC

PDB ID : 8WLT / pdb\_00008wlt  
EMDB ID : EMD-37630  
Title : Cryo-EM structure of the membrane-anchored part of the flagellar motor-hook complex in the CCW state  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-10-01  
Resolution : 4.10 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

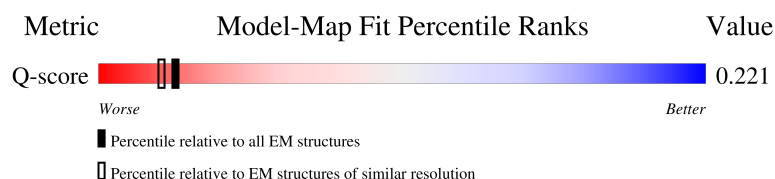
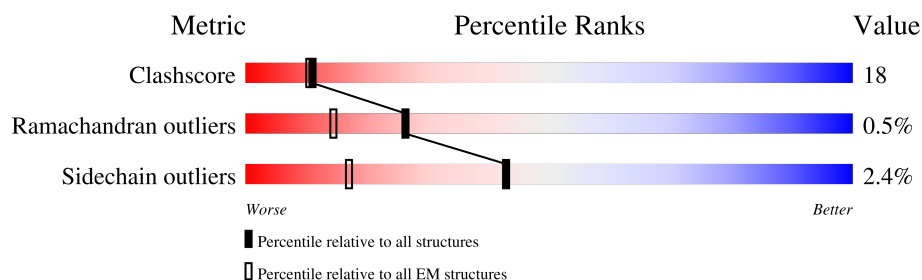
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | 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                       | 6458 ( 3.60 - 4.60 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 232    | <div> <div>31%</div> <div>66%</div> <div>23%</div> <div>9%</div> </div> |
| 1   | B     | 232    | <div> <div>31%</div> <div>66%</div> <div>23%</div> <div>9%</div> </div> |
| 1   | C     | 232    | <div> <div>29%</div> <div>66%</div> <div>24%</div> <div>9%</div> </div> |
| 1   | D     | 232    | <div> <div>26%</div> <div>67%</div> <div>23%</div> <div>9%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 232    |                  |
| 1   | F     | 232    |                  |
| 1   | G     | 232    |                  |
| 1   | H     | 232    |                  |
| 1   | I     | 232    |                  |
| 1   | J     | 232    |                  |
| 1   | K     | 232    |                  |
| 1   | L     | 232    |                  |
| 1   | M     | 232    |                  |
| 1   | N     | 232    |                  |
| 1   | O     | 232    |                  |
| 1   | P     | 232    |                  |
| 1   | Q     | 232    |                  |
| 1   | R     | 232    |                  |
| 1   | S     | 232    |                  |
| 1   | T     | 232    |                  |
| 1   | U     | 232    |                  |
| 1   | V     | 232    |                  |
| 1   | W     | 232    |                  |
| 1   | X     | 232    |                  |
| 1   | Y     | 232    |                  |
| 1   | Z     | 232    |                  |
| 2   | a     | 365    |                  |
| 2   | b     | 365    |                  |
| 2   | c     | 365    |                  |

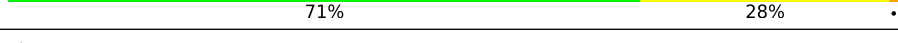
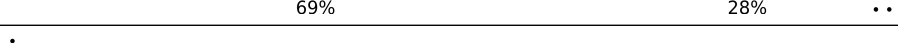
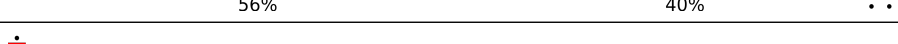
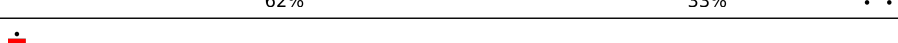
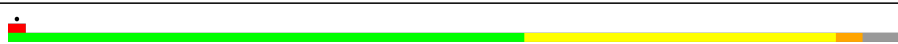
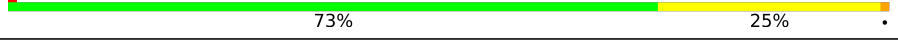
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | d     | 365    |                  |
| 2   | e     | 365    |                  |
| 2   | f     | 365    |                  |
| 2   | g     | 365    |                  |
| 2   | h     | 365    |                  |
| 2   | i     | 365    |                  |
| 2   | j     | 365    |                  |
| 2   | k     | 365    |                  |
| 2   | l     | 365    |                  |
| 2   | m     | 365    |                  |
| 2   | n     | 365    |                  |
| 2   | o     | 365    |                  |
| 2   | p     | 365    |                  |
| 2   | q     | 365    |                  |
| 2   | r     | 365    |                  |
| 2   | s     | 365    |                  |
| 2   | t     | 365    |                  |
| 2   | u     | 365    |                  |
| 2   | v     | 365    |                  |
| 2   | w     | 365    |                  |
| 2   | x     | 365    |                  |
| 2   | y     | 365    |                  |
| 2   | z     | 365    |                  |
| 3   | 0     | 260    |                  |
| 3   | 1     | 260    |                  |

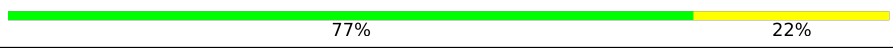
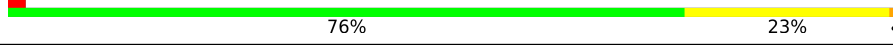
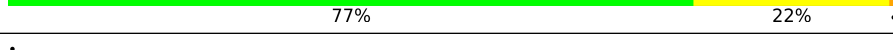
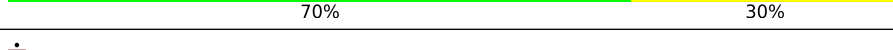
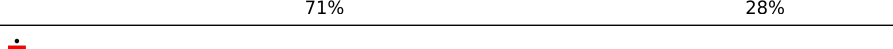
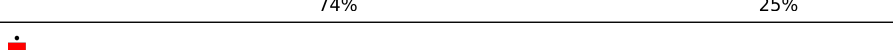
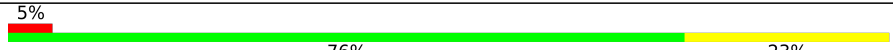
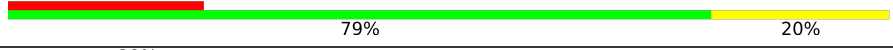
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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 3   | 2     | 260    |  67% 31%       |
| 3   | 3     | 260    |  65% 35%       |
| 3   | 4     | 260    |  65% 34%       |
| 3   | 5     | 260    |  63% 35%       |
| 3   | 6     | 260    |  67% 32%       |
| 3   | 7     | 260    |  66% 32%       |
| 3   | 8     | 260    |  66% 30%       |
| 3   | 9     | 260    |  71% 28%       |
| 3   | AF    | 260    |  69% 28%       |
| 3   | AG    | 260    |  56% 40%       |
| 3   | AH    | 260    |  62% 33%       |
| 3   | AI    | 260    |  60% 37%     |
| 3   | AJ    | 260    |  62% 33%     |
| 3   | AK    | 260    |  62% 30% 7%  |
| 3   | AL    | 260    |  57% 36% 5%  |
| 3   | AM    | 260    |  58% 35% 5%  |
| 3   | AN    | 260    |  66% 28% 5%  |
| 3   | ZA    | 260    |  65% 34%     |
| 3   | ZB    | 260    |  67% 31%     |
| 3   | ZC    | 260    |  68% 31%     |
| 3   | ZD    | 260    |  63% 35%     |
| 3   | ZE    | 260    |  68% 30%     |
| 4   | ZF    | 403    |  29% 78% 21% |
| 4   | ZG    | 403    |  73% 25%     |
| 4   | ZH    | 403    |  76% 23%     |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | ZI    | 403    |    |
| 4   | ZJ    | 403    |    |
| 4   | ZK    | 403    |    |
| 4   | ZL    | 403    |    |
| 4   | ZM    | 403    |    |
| 4   | ZN    | 403    |    |
| 4   | ZO    | 403    |    |
| 4   | ZP    | 403    |    |
| 4   | ZQ    | 403    |    |
| 4   | ZR    | 403    |    |
| 4   | ZS    | 403    |    |
| 4   | ZT    | 403    |  |
| 4   | ZU    | 403    |  |
| 4   | ZV    | 403    |  |
| 4   | ZW    | 403    |  |
| 4   | ZX    | 403    |  |
| 4   | ZY    | 403    |  |
| 4   | ZZ    | 403    |  |
| 4   | Za    | 403    |  |
| 4   | Zb    | 403    |  |
| 4   | Zc    | 403    |  |
| 4   | Zd    | 403    |  |
| 4   | Ze    | 403    |  |
| 4   | Zf    | 403    |  |
| 4   | Zg    | 403    |  |

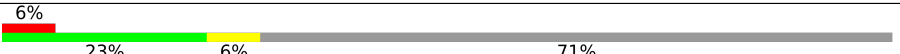
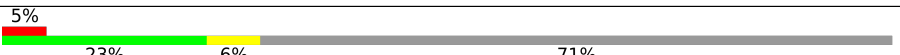
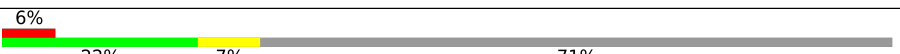
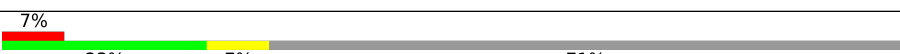
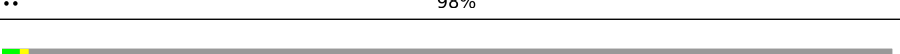
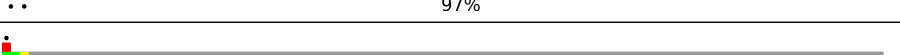
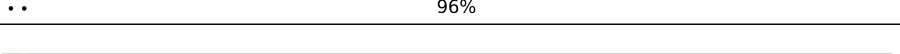
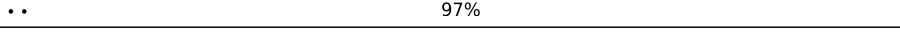
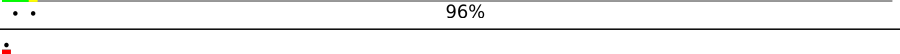
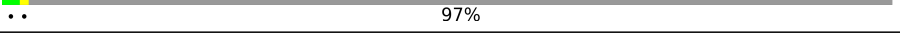
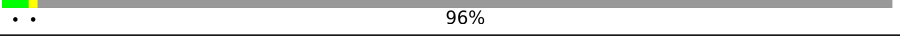
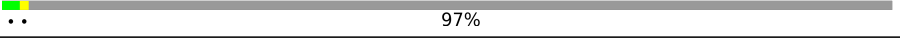
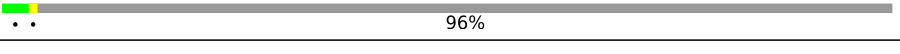
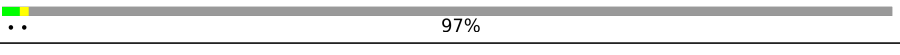
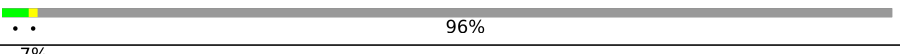
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | Zh    | 403    |                  |
| 5   | AA    | 251    |                  |
| 5   | AB    | 251    |                  |
| 5   | AC    | 251    |                  |
| 5   | AD    | 251    |                  |
| 5   | AE    | 251    |                  |
| 6   | AO    | 560    |                  |
| 6   | AP    | 560    |                  |
| 6   | AQ    | 560    |                  |
| 6   | AR    | 560    |                  |
| 6   | AS    | 560    |                  |
| 6   | AT    | 560    |                  |
| 6   | AU    | 560    |                  |
| 6   | AV    | 560    |                  |
| 6   | AW    | 560    |                  |
| 6   | AX    | 560    |                  |
| 6   | AY    | 560    |                  |
| 6   | AZ    | 560    |                  |
| 6   | Aa    | 560    |                  |
| 6   | Ac    | 560    |                  |
| 6   | Ad    | 560    |                  |
| 6   | Ae    | 560    |                  |
| 6   | Af    | 560    |                  |
| 6   | Ag    | 560    |                  |
| 6   | Ah    | 560    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                      |
|-----|-------|--------|-------------------------------------------------------------------------------------------------------|
| 6   | Ai    | 560    | <br>5% 23% 7% 71%   |
| 6   | Aj    | 560    | <br>5% 22% 7% 71%   |
| 6   | Ak    | 560    | <br>6% 22% 7% 71%   |
| 6   | Al    | 560    | <br>6% 23% 6% 71%   |
| 6   | Am    | 560    | <br>5% 23% 6% 71%   |
| 6   | An    | 560    | <br>6% 22% 7% 71%   |
| 6   | Ao    | 560    | <br>7% 23% 7% 71%   |
| 6   | Ap    | 560    | <br>6% 23% 6% 71%   |
| 6   | BG    | 560    | <br>98%             |
| 6   | BH    | 560    | <br>97%             |
| 6   | BI    | 560    | <br>96%             |
| 6   | BJ    | 560    | <br>97%             |
| 6   | BK    | 560    | <br>96%            |
| 6   | BL    | 560    | <br>97%           |
| 6   | BM    | 560    | <br>96%           |
| 6   | BN    | 560    | <br>97%           |
| 6   | BO    | 560    | <br>96%           |
| 6   | BP    | 560    | <br>97%           |
| 6   | BQ    | 560    | <br>96%           |
| 6   | BR    | 560    | <br>7% 22% 7% 71% |
| 6   | BS    | 560    | <br>6% 22% 7% 71% |
| 6   | BT    | 560    | <br>6% 23% 6% 71% |
| 6   | BU    | 560    | <br>6% 22% 7% 71% |
| 6   | BV    | 560    | <br>5% 23% 7% 71% |
| 6   | BW    | 560    | <br>23% 7% 71%    |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | BX    | 560    |                  |
| 6   | UI    | 560    |                  |
| 6   | UJ    | 560    |                  |
| 6   | UK    | 560    |                  |
| 6   | UL    | 560    |                  |
| 6   | UM    | 560    |                  |
| 6   | UN    | 560    |                  |
| 6   | UO    | 560    |                  |
| 6   | UP    | 560    |                  |
| 6   | WA    | 560    |                  |
| 6   | WB    | 560    |                  |
| 6   | WC    | 560    |                  |
| 6   | WD    | 560    |                  |
| 6   | WE    | 560    |                  |
| 6   | WF    | 560    |                  |
| 6   | WG    | 560    |                  |
| 6   | WH    | 560    |                  |
| 6   | WI    | 560    |                  |
| 6   | WJ    | 560    |                  |
| 6   | WK    | 560    |                  |
| 6   | WL    | 560    |                  |
| 6   | WM    | 560    |                  |
| 6   | WN    | 560    |                  |
| 6   | WO    | 560    |                  |
| 6   | WP    | 560    |                  |

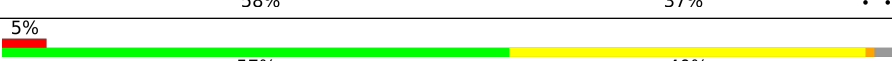
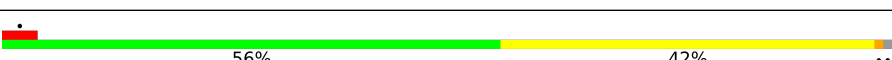
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | WQ    | 560    |                  |
| 6   | WR    | 560    |                  |
| 6   | WS    | 560    |                  |
| 6   | WT    | 560    |                  |
| 6   | WU    | 560    |                  |
| 6   | WV    | 560    |                  |
| 6   | WW    | 560    |                  |
| 7   | Ab    | 89     |                  |
| 7   | Aq    | 89     |                  |
| 7   | Ar    | 89     |                  |
| 7   | As    | 89     |                  |
| 8   | At    | 264    |                  |
| 9   | Au    | 245    |                  |
| 9   | Av    | 245    |                  |
| 9   | Aw    | 245    |                  |
| 9   | Ax    | 245    |                  |
| 9   | Ay    | 245    |                  |
| 10  | A1    | 104    |                  |
| 10  | A2    | 104    |                  |
| 10  | A3    | 104    |                  |
| 10  | A4    | 104    |                  |
| 10  | A5    | 104    |                  |
| 10  | Az    | 104    |                  |
| 11  | A0    | 138    |                  |
| 11  | A6    | 138    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 11  | A7    | 138    |  |
| 11  | A8    | 138    |  |
| 11  | A9    | 138    |  |
| 12  | BA    | 134    |  |
| 12  | BB    | 134    |  |
| 12  | BC    | 134    |  |
| 12  | BD    | 134    |  |
| 12  | BE    | 134    |  |
| 12  | BF    | 134    |  |

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 338664 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 L-ring protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | B     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | C     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | D     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | E     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | F     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | G     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | H     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | I     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | J     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | K     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | L     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | M     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | N     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | O     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | P     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | Q     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | R     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | S     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | T     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | U     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | V     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | W     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | X     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | Y     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |
| 1   | Z     | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 985 | 282 | 309 | 4 |         |       |

- Molecule 2 is a protein called Flagellar P-ring protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | a     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | b     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | c     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | d     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | e     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | f     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | g     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | h     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | i     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | j     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | k     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | l     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | m     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | n     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | o     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | p     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | q     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | r     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | s     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | t     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | u     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | v     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | w     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | x     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | y     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |
| 2   | z     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1364 | 405 | 446 | 13 |         |       |

- Molecule 3 is a protein called Flagellar basal-body rod protein FlgG.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 0     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1866  | 1154 | 327 | 379 | 6 |         |       |
| 3   | 1     | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1894  | 1172 | 331 | 385 | 6 |         |       |
| 3   | 2     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 3   | 3     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | 4     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | 5     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | 6     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | 7     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | 8     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | 9     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | ZA    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | ZB    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | ZC    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | ZD    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | ZE    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 3   | AF    | 254      | Total<br>1903 | C<br>1175 | N<br>334 | O<br>389 | S<br>5 | 0       | 0     |
| 3   | AG    | 255      | Total<br>1911 | C<br>1181 | N<br>335 | O<br>390 | S<br>5 | 0       | 0     |
| 3   | AH    | 256      | Total<br>1919 | C<br>1186 | N<br>336 | O<br>391 | S<br>6 | 0       | 0     |
| 3   | AI    | 254      | Total<br>1903 | C<br>1175 | N<br>334 | O<br>389 | S<br>5 | 0       | 0     |
| 3   | AJ    | 255      | Total<br>1911 | C<br>1181 | N<br>335 | O<br>390 | S<br>5 | 0       | 0     |
| 3   | AK    | 243      | Total<br>1823 | C<br>1127 | N<br>318 | O<br>373 | S<br>5 | 0       | 0     |
| 3   | AL    | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |
| 3   | AM    | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |
| 3   | AN    | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |

- Molecule 4 is a protein called Flagellar hook protein FlgE.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | ZF    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZG    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZH    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZI    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZJ    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZK    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZL    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZM    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZN    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZO    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZP    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZQ    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZR    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZS    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZT    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZU    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZV    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZW    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZX    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZY    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | ZZ    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | Za    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Zb    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Zc    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Zd    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Ze    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Zf    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Zg    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 4   | Zh    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |

- Molecule 5 is a protein called Flagellar basal-body rod protein FlgF.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | AA    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1804  | 1106 | 324 | 367 | 7 |         |       |
| 5   | AB    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |
| 5   | AC    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1820  | 1116 | 326 | 369 | 9 |         |       |
| 5   | AD    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1820  | 1116 | 326 | 369 | 9 |         |       |
| 5   | AE    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |

- Molecule 6 is a protein called Flagellar M-ring protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | AR    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AS    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AT    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AU    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | AV    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AW    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AX    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AY    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AZ    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Aa    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ac    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ad    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ae    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Af    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ag    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ah    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ai    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Aj    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ak    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Al    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Am    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | An    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ao    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | Ap    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AO    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | AP    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | AQ    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | UI    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UJ    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UK    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UL    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UM    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UN    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UO    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | UP    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 733 | 211 | 226 | 2 |         |       |
| 6   | WA    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 849   | 534 | 148 | 166 | 1 |         |       |
| 6   | WB    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 836   | 526 | 146 | 163 | 1 |         |       |
| 6   | WC    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 812   | 510 | 142 | 159 | 1 |         |       |
| 6   | WD    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 522 | 144 | 160 | 1 |         |       |
| 6   | WE    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 147 | 164 | 1 |         |       |
| 6   | WF    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 6   | WG    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 147 | 164 | 1 |         |       |
| 6   | WH    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 439 | 126 | 137 | 1 |         |       |
| 6   | WI    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 439 | 126 | 137 | 1 |         |       |
| 6   | WJ    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 462 | 131 | 143 | 1 |         |       |
| 6   | WK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 729   | 456 | 130 | 142 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | WL    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 622   | 389 | 110 | 122 | 1 |         |       |
| 6   | WM    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 596   | 372 | 107 | 116 | 1 |         |       |
| 6   | WN    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 611   | 380 | 109 | 121 | 1 |         |       |
| 6   | WO    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 448 | 127 | 138 | 1 |         |       |
| 6   | WP    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 464 | 132 | 144 | 1 |         |       |
| 6   | WQ    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 6   | WR    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 6   | WS    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 6   | WT    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 6   | WU    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 147 | 164 | 1 |         |       |
| 6   | WV    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 521 | 144 | 161 | 1 |         |       |
| 6   | WW    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 526 | 145 | 162 | 1 |         |       |
| 6   | BG    | 13       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 81    | 50  | 15  | 16  |   |         |       |
| 6   | BH    | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 6   | BI    | 20       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 133   | 83  | 23  | 27  |   |         |       |
| 6   | BJ    | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 6   | BK    | 21       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 140   | 88  | 24  | 28  |   |         |       |
| 6   | BL    | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 6   | BM    | 21       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 140   | 88  | 24  | 28  |   |         |       |
| 6   | BN    | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 6   | BO    | 20       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 133   | 83  | 23  | 27  |   |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | BP    | 16       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 103   | 64  | 19  | 20  |   |         |       |
| 6   | BQ    | 21       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 140   | 88  | 24  | 28  |   |         |       |
| 6   | BR    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | BS    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | BT    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | BU    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | BV    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | BW    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |
| 6   | BX    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 776 | 237 | 259 | 3 |         |       |

- Molecule 7 is a protein called Flagellar biosynthetic protein FliQ.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | Ab    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 7   | Aq    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 7   | Ar    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 7   | As    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |

- Molecule 8 is a protein called Flagellar biosynthetic protein FliR.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | At    | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1945  | 1305 | 307 | 318 | 15 |         |       |

- Molecule 9 is a protein called Flagellar biosynthetic protein FliP.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | Au    | 207      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1605  | 1072 | 249 | 272 | 12 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | Av    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1626  | 1086 | 252 | 276 | 12 |         |       |
| 9   | Aw    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1614  | 1077 | 251 | 274 | 12 |         |       |
| 9   | Ax    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1614  | 1077 | 251 | 274 | 12 |         |       |
| 9   | Ay    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |

- Molecule 10 is a protein called Flagellar hook-basal body complex protein FliE.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | Az    | 59       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 429   | 265 | 74  | 83  | 7 |         |       |
| 10  | A1    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 672   | 415 | 121 | 129 | 7 |         |       |
| 10  | A2    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 686   | 424 | 123 | 132 | 7 |         |       |
| 10  | A3    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 686   | 424 | 123 | 132 | 7 |         |       |
| 10  | A4    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 686   | 424 | 123 | 132 | 7 |         |       |
| 10  | A5    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 679   | 420 | 122 | 130 | 7 |         |       |

- Molecule 11 is a protein called Flagellar basal body rod protein FlgB.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | A6    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1030  | 633 | 189 | 203 | 5 |         |       |
| 11  | A7    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 583 | 172 | 182 | 5 |         |       |
| 11  | A8    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 598 | 177 | 187 | 5 |         |       |
| 11  | A9    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 982   | 606 | 182 | 189 | 5 |         |       |
| 11  | A0    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 588 | 172 | 185 | 5 |         |       |

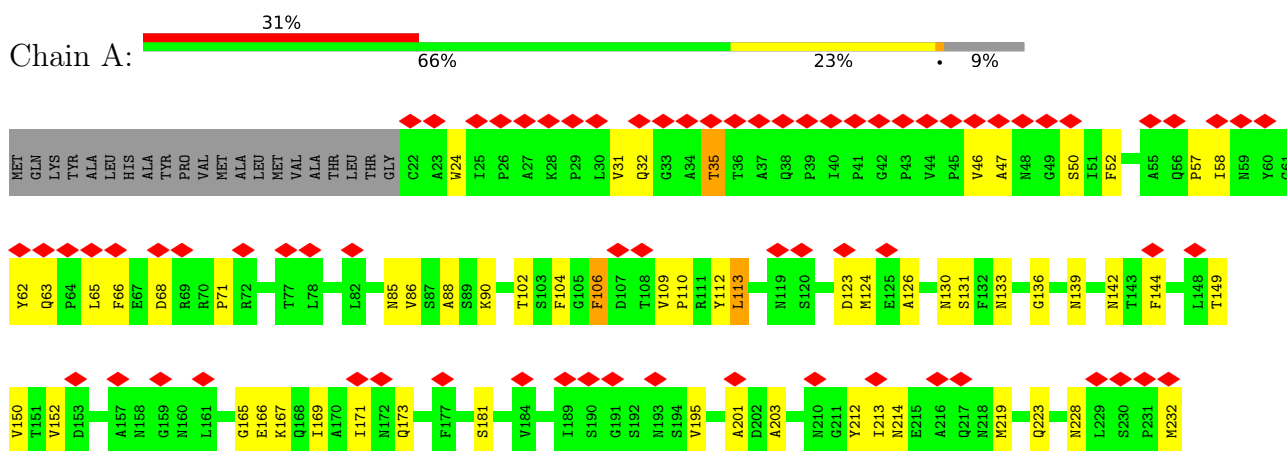
- Molecule 12 is a protein called Flagellar basal-body rod protein FlgC.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | BA    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 12  | BB    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |
| 12  | BC    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 12  | BD    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 12  | BE    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 956   | 595 | 165 | 191 | 5 |         |       |
| 12  | BF    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |

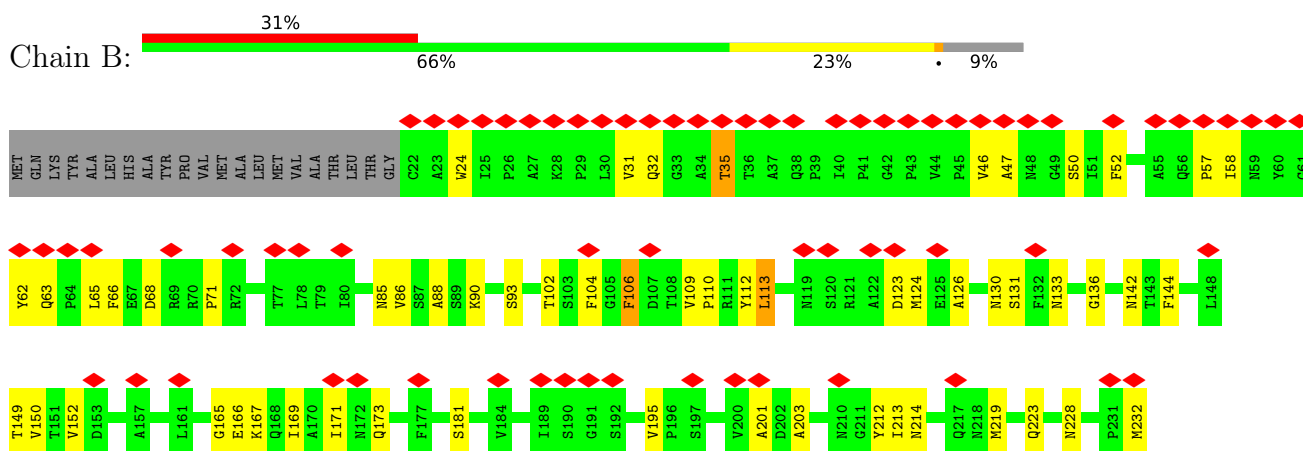
### 3 Residue-property plots

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.

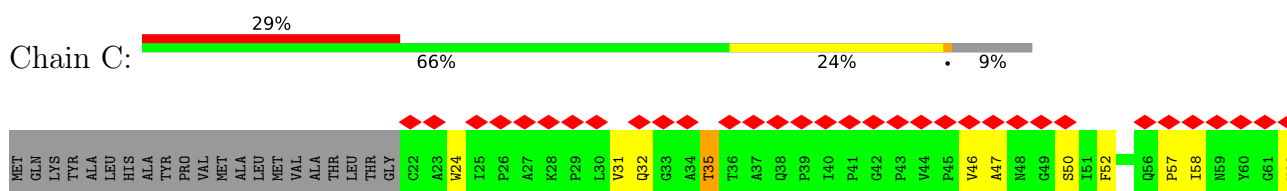
#### • Molecule 1: Flagellar L-ring protein



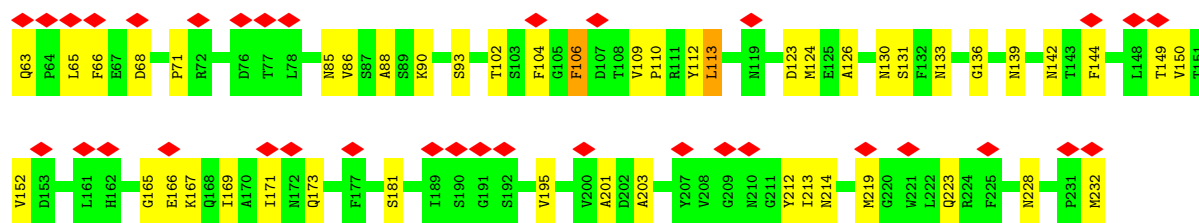
#### • Molecule 1: Flagellar L-ring protein



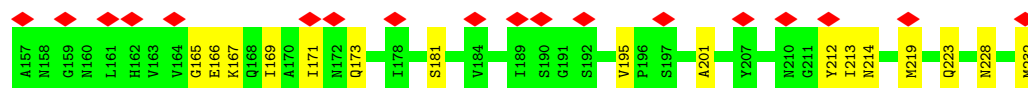
#### • Molecule 1: Flagellar L-ring protein



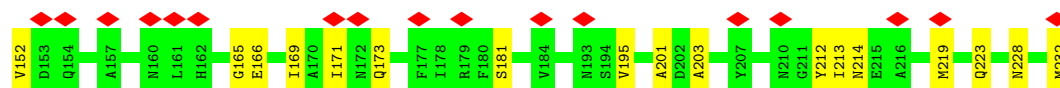




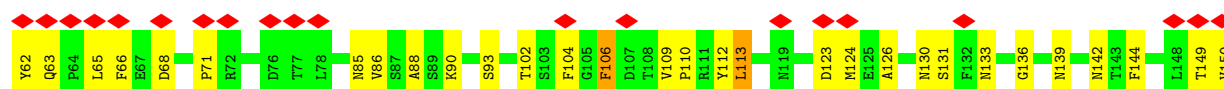
• Molecule 1: Flagellar L-ring protein

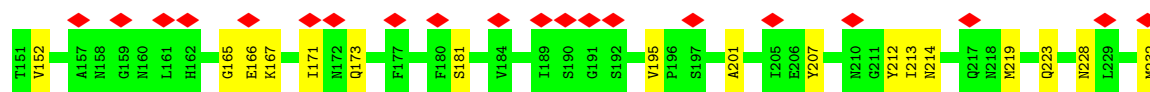


• Molecule 1: Flagellar L-ring protein

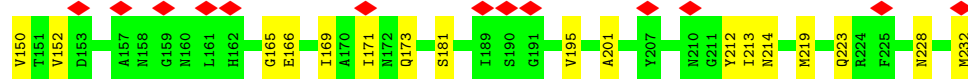
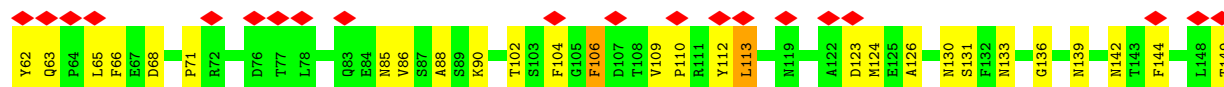
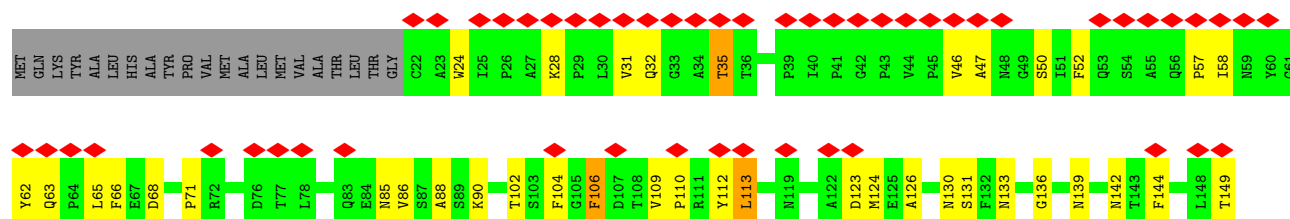


• Molecule 1: Flagellar L-ring protein

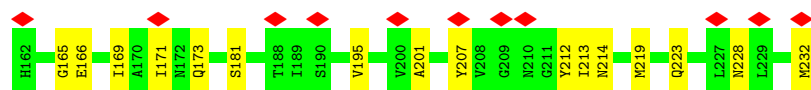
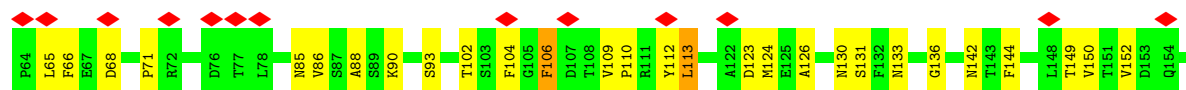




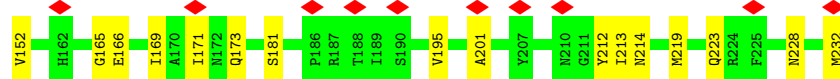
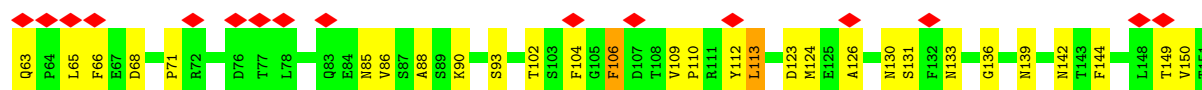
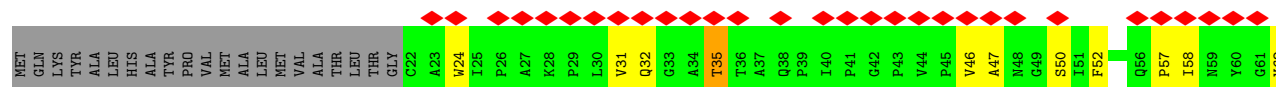
• Molecule 1: Flagellar L-ring protein



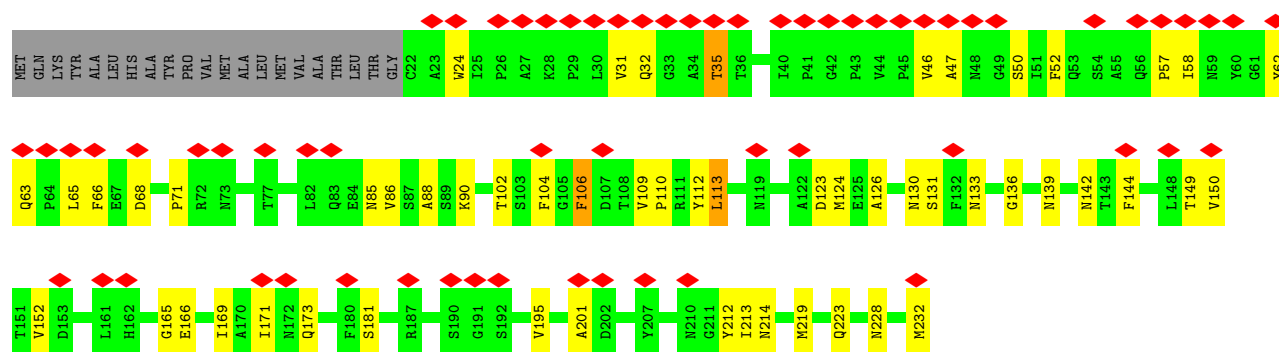
• Molecule 1: Flagellar L-ring protein



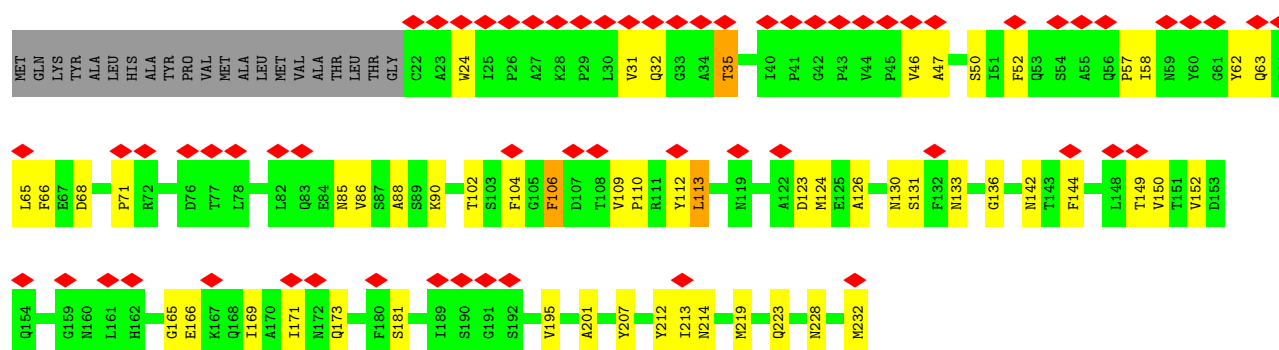
• Molecule 1: Flagellar L-ring protein



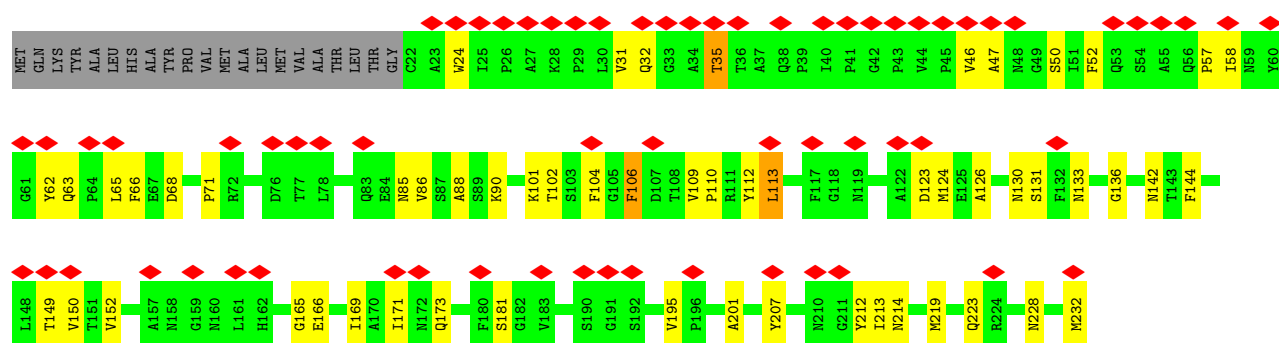
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

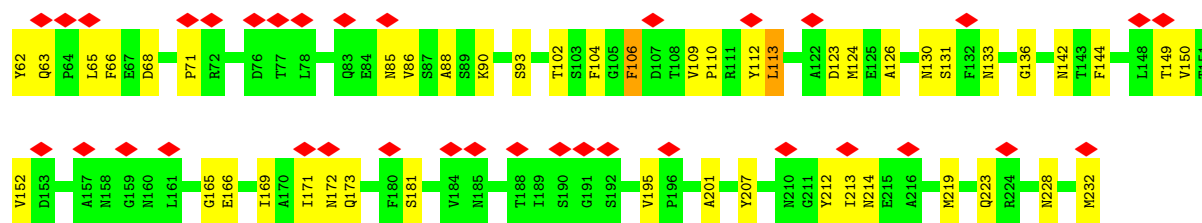


• Molecule 1: Flagellar L-ring protein

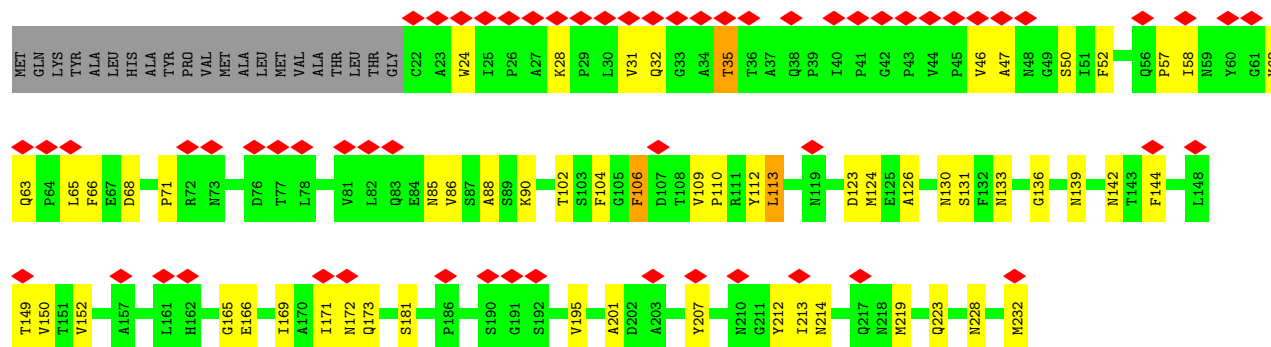


• Molecule 1: Flagellar L-ring protein

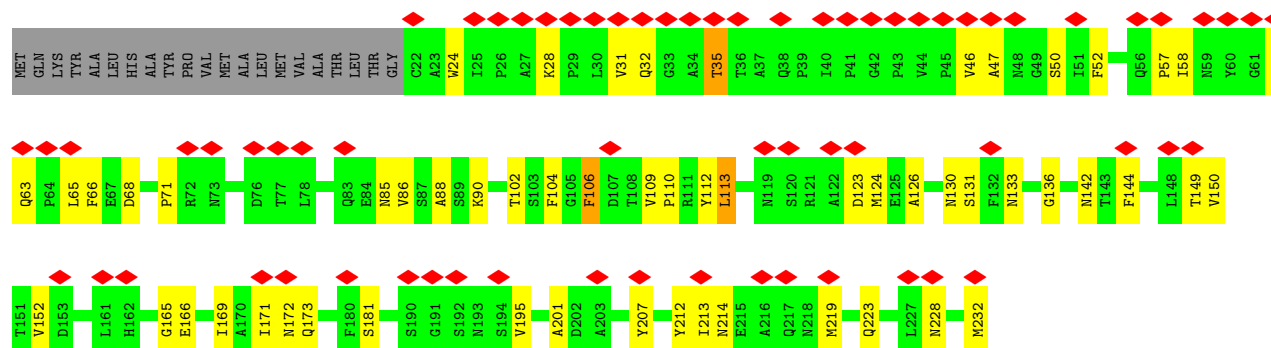




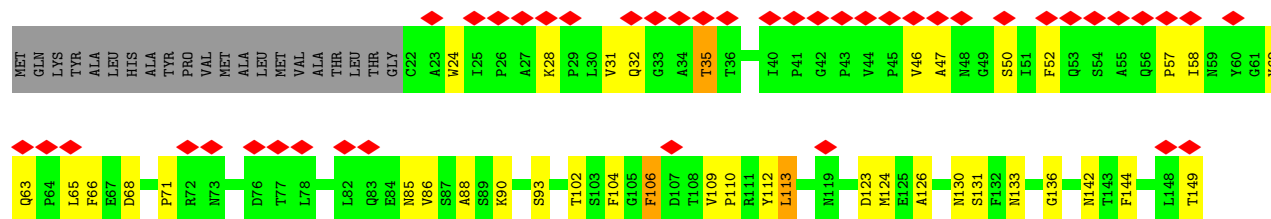
• Molecule 1: Flagellar L-ring protein

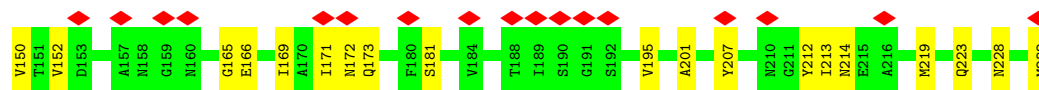


• Molecule 1: Flagellar L-ring protein

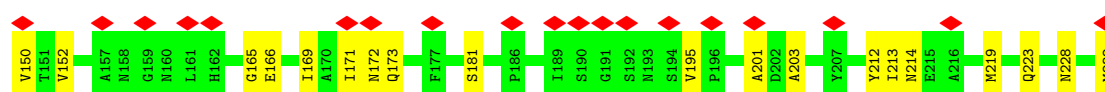
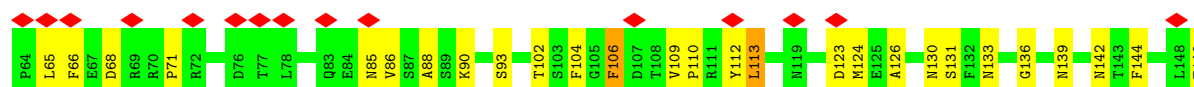


• Molecule 1: Flagellar L-ring protein

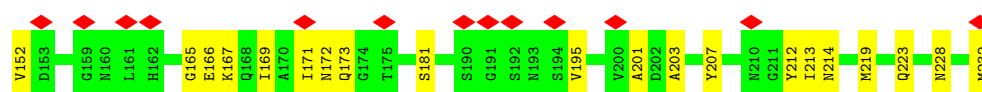
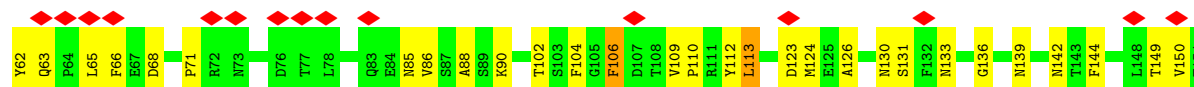
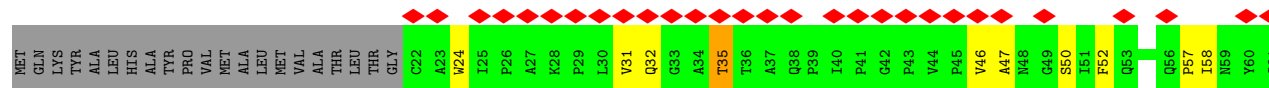




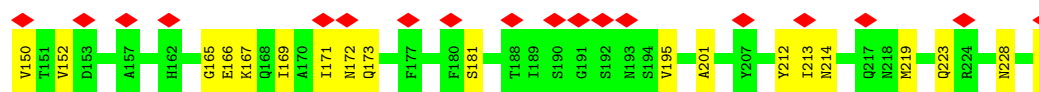
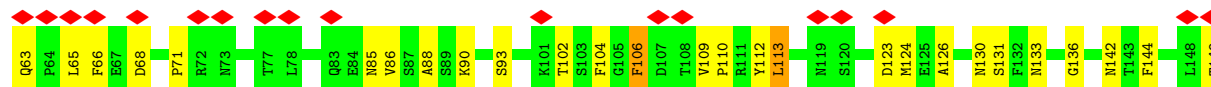
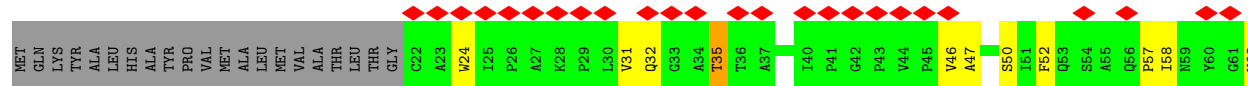
• Molecule 1: Flagellar L-ring protein



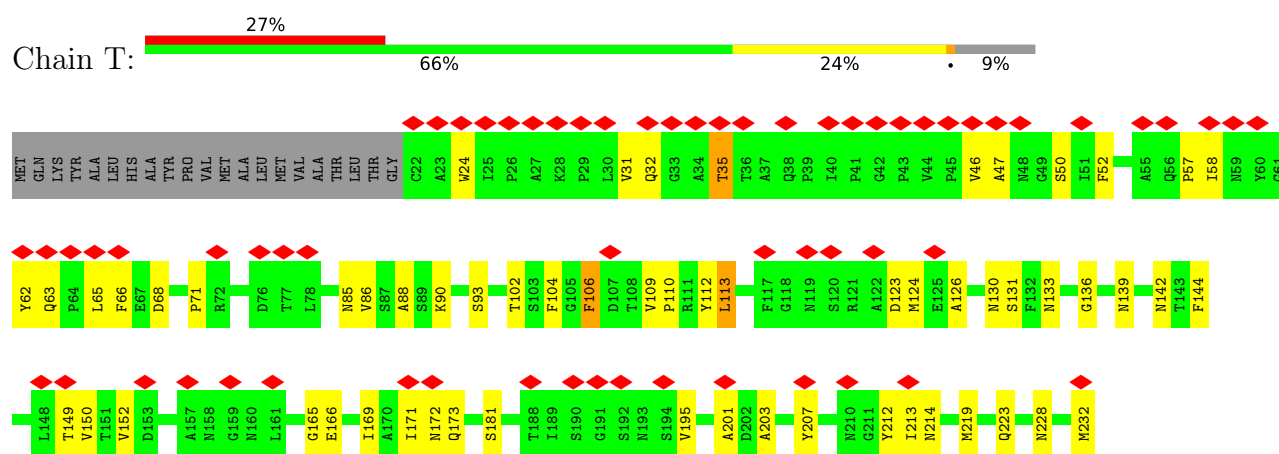
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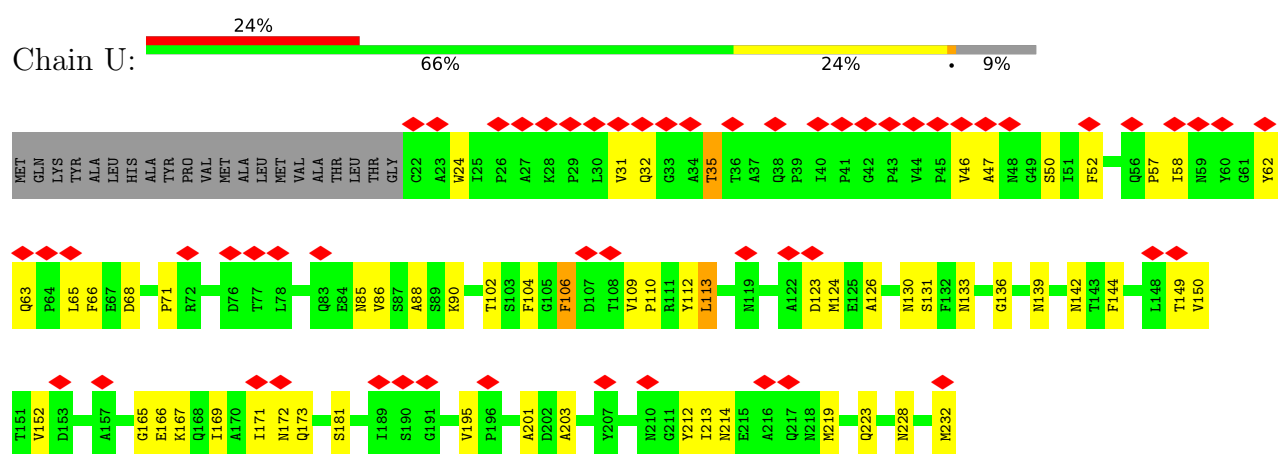
• Molecule 1: Flagellar L-ring protein



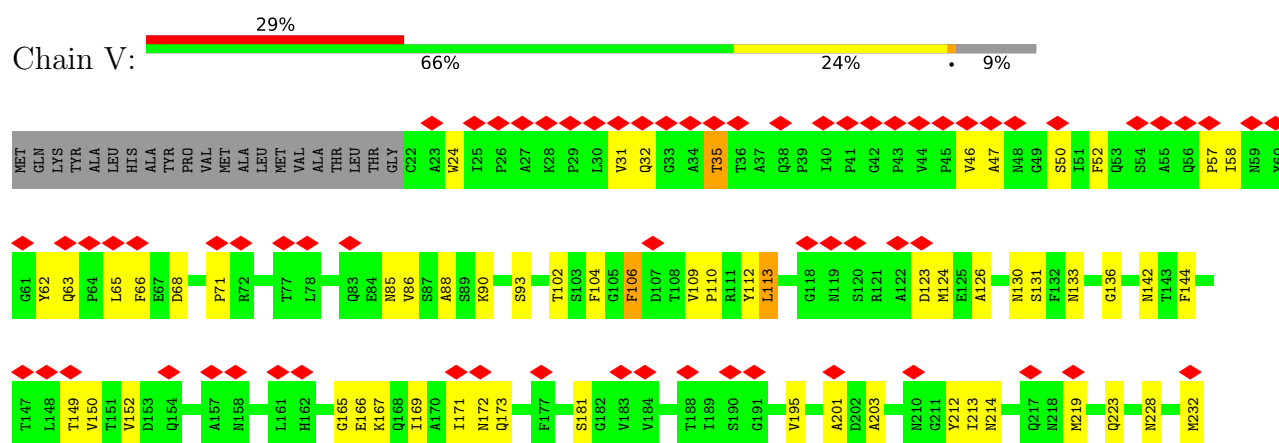
• Molecule 1: Flagellar L-ring protein



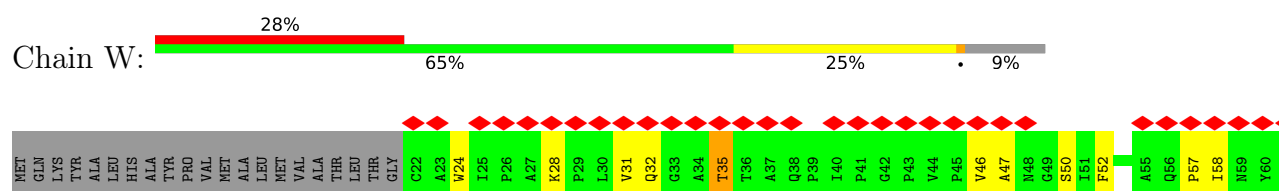
• Molecule 1: Flagellar L-ring protein

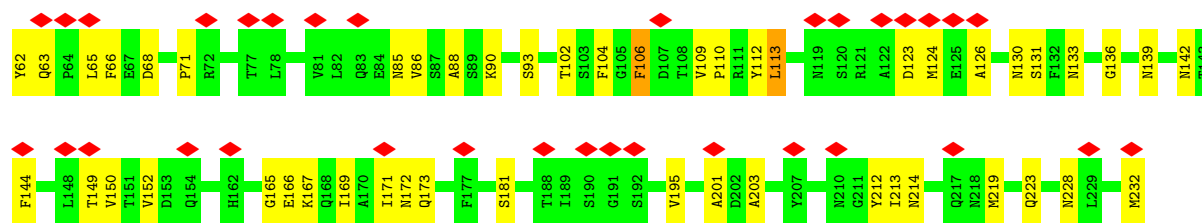


• Molecule 1: Flagellar L-ring protein

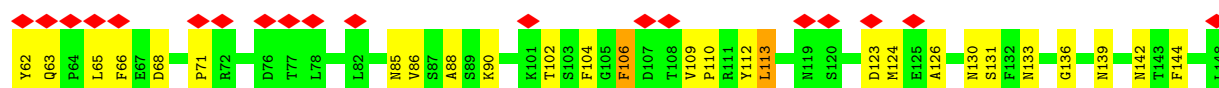


• Molecule 1: Flagellar L-ring protein

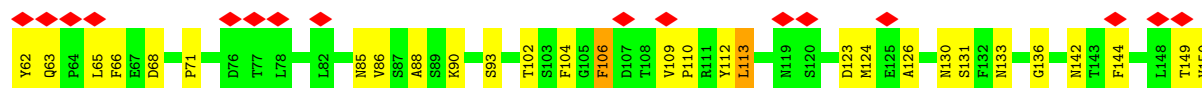




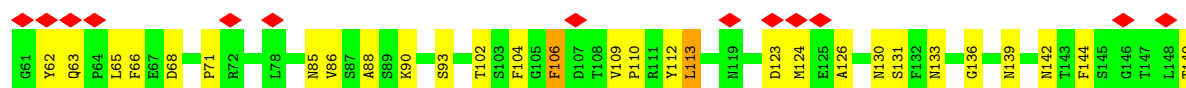
• Molecule 1: Flagellar L-ring protein

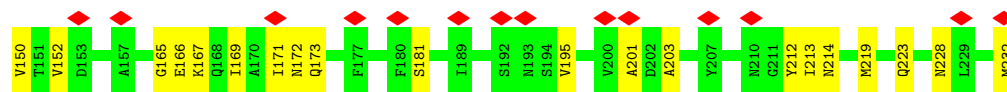


• Molecule 1: Flagellar L-ring protein

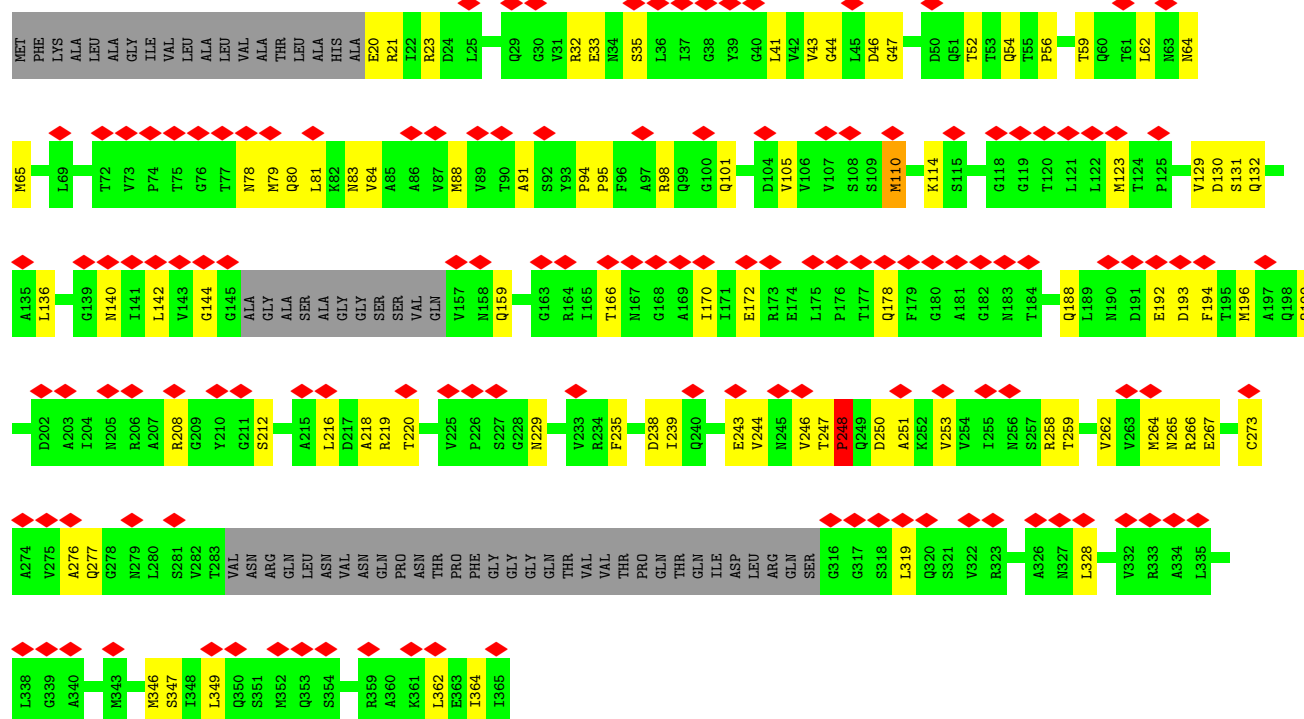


• Molecule 1: Flagellar L-ring protein

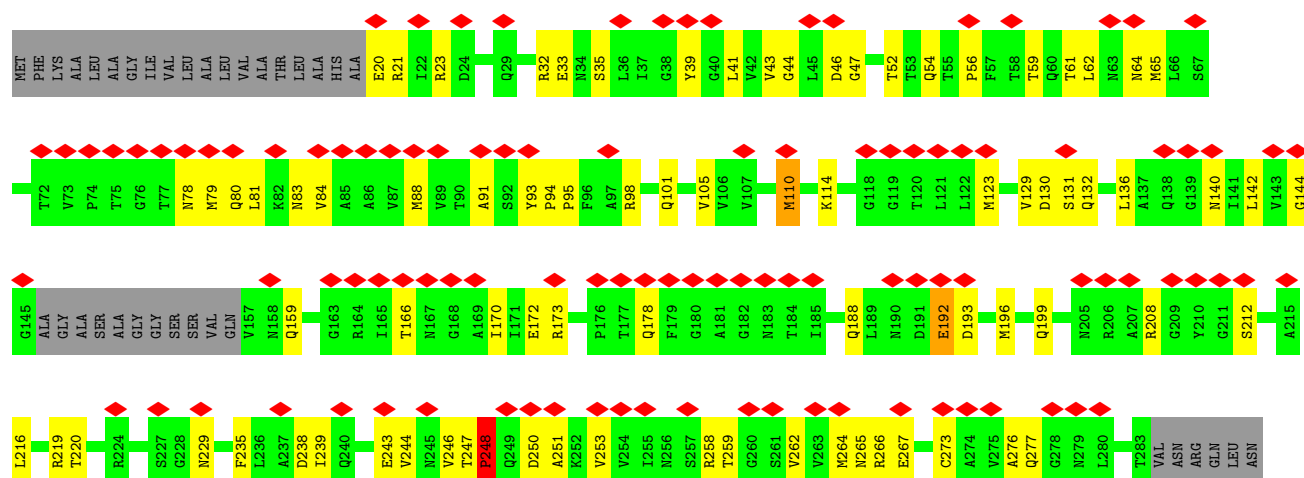




• Molecule 2: Flagellar P-ring protein



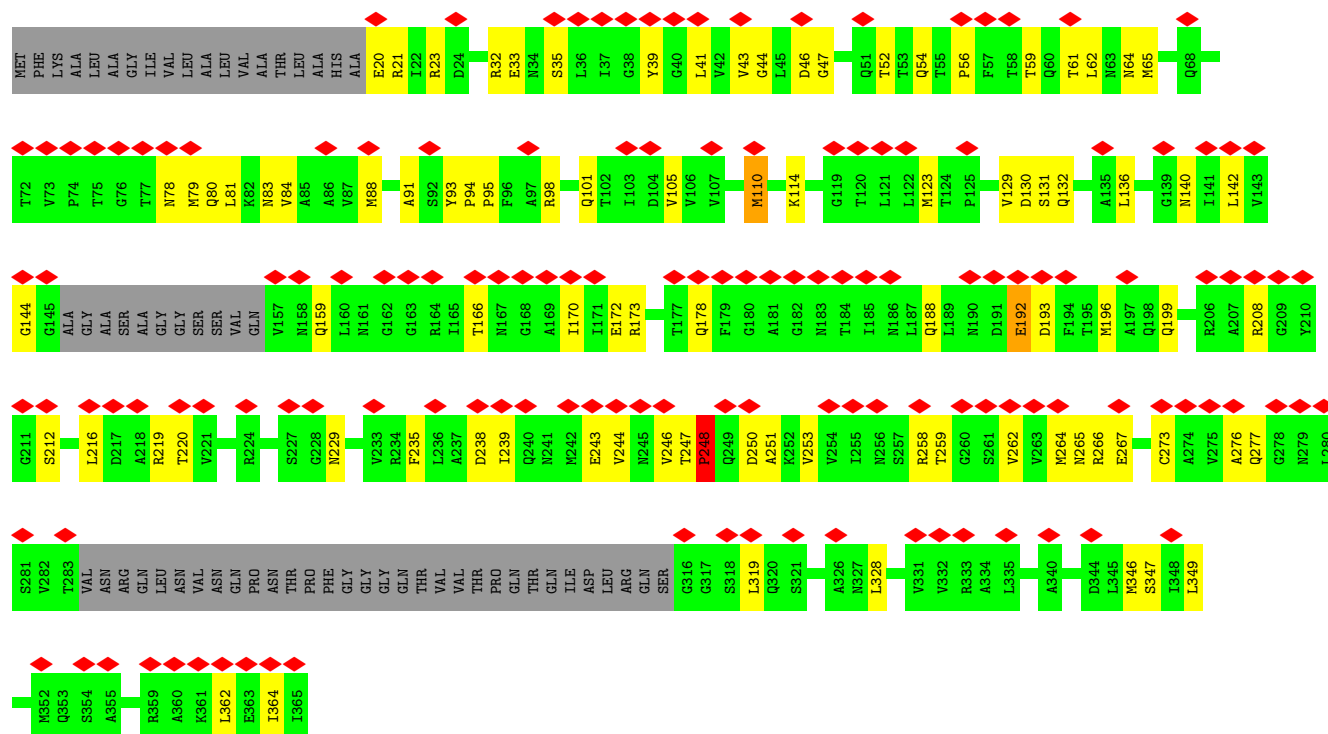
• Molecule 2: Flagellar P-ring protein



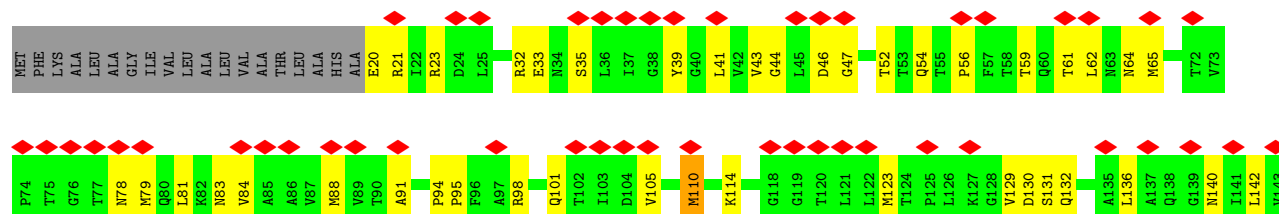


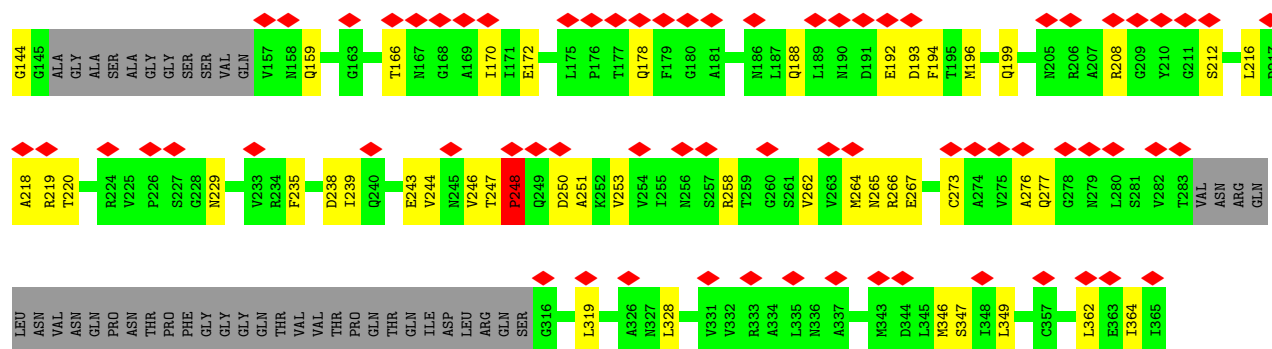


- Molecule 2: Flagellar P-ring protein

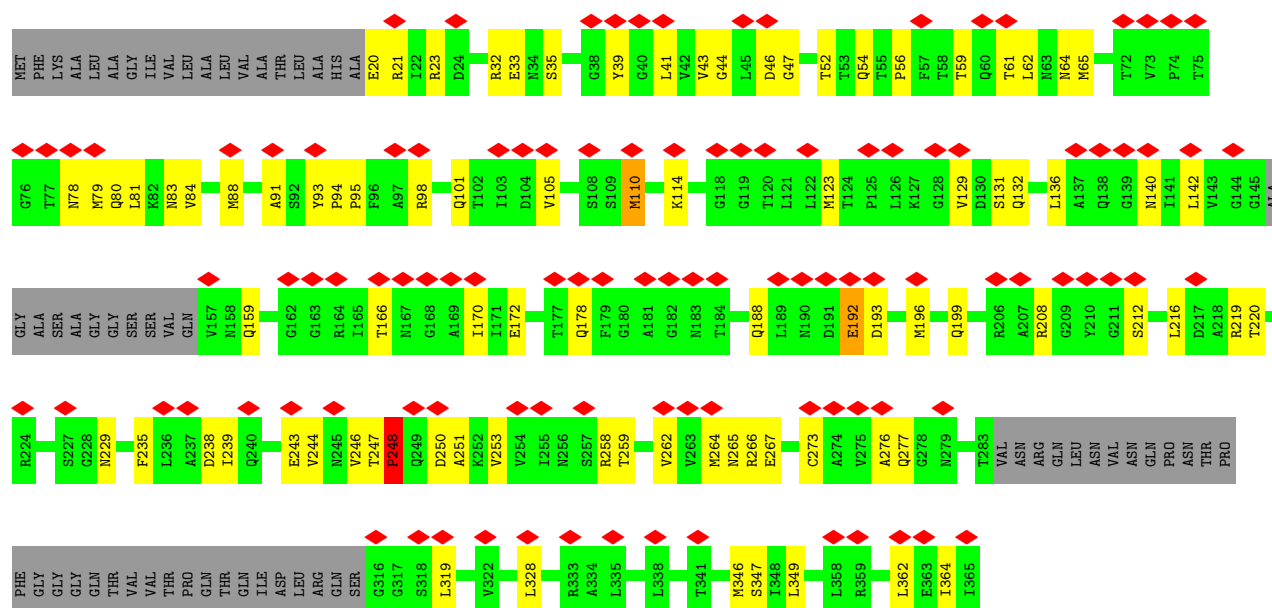


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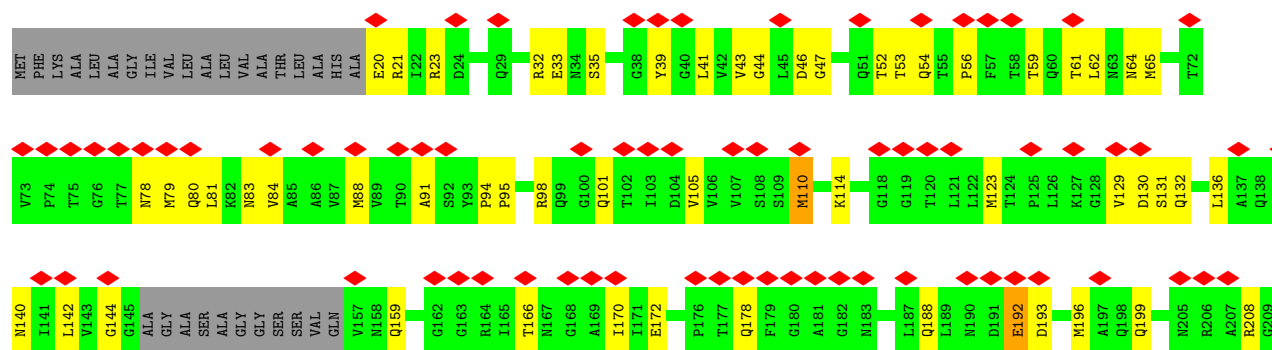


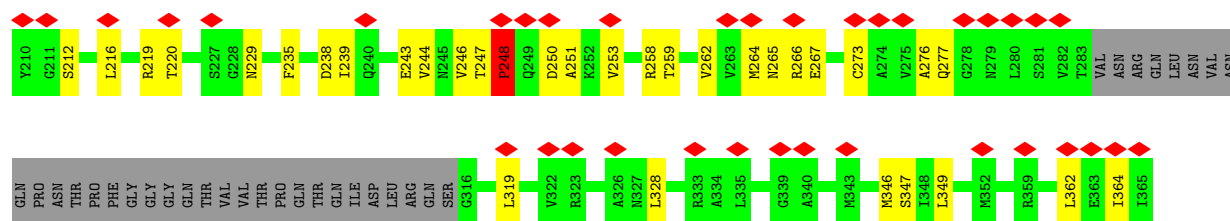


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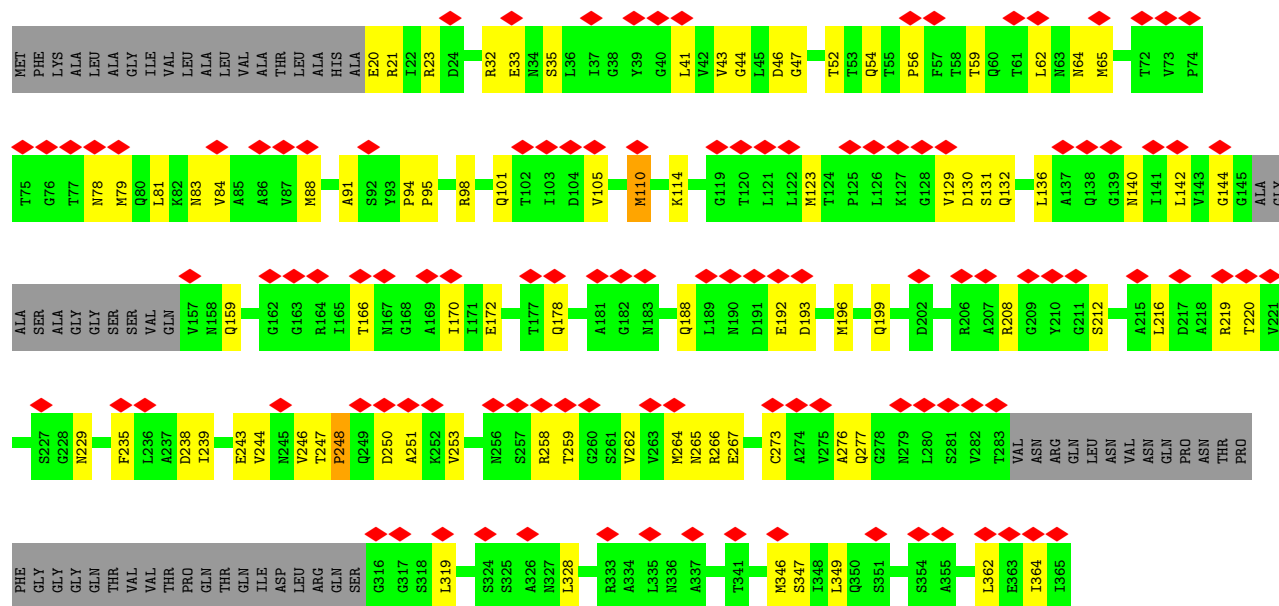


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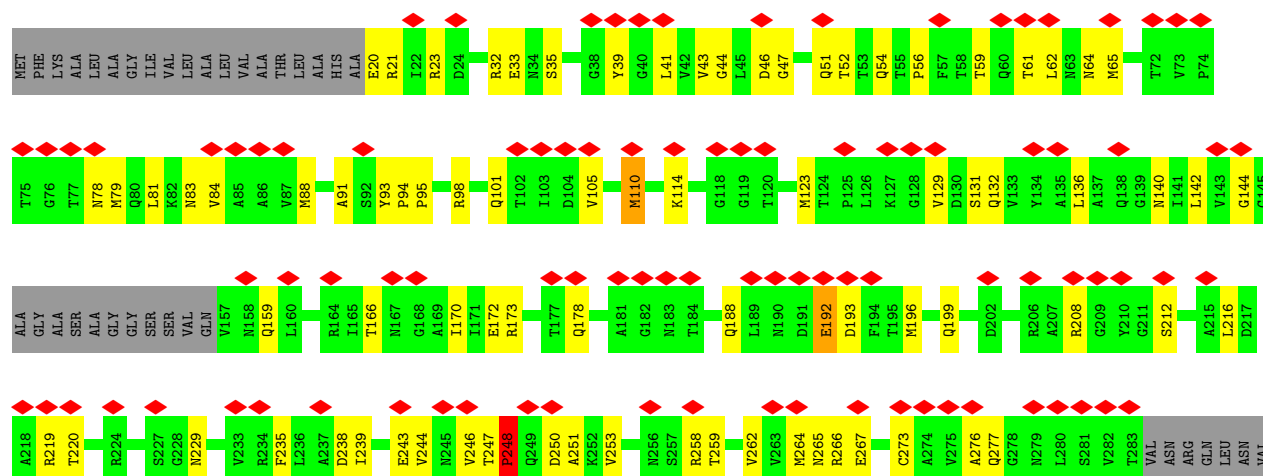


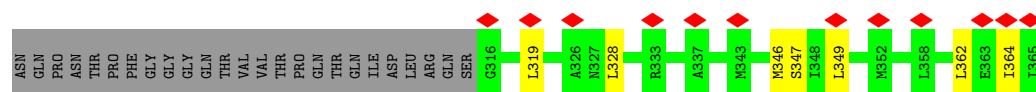


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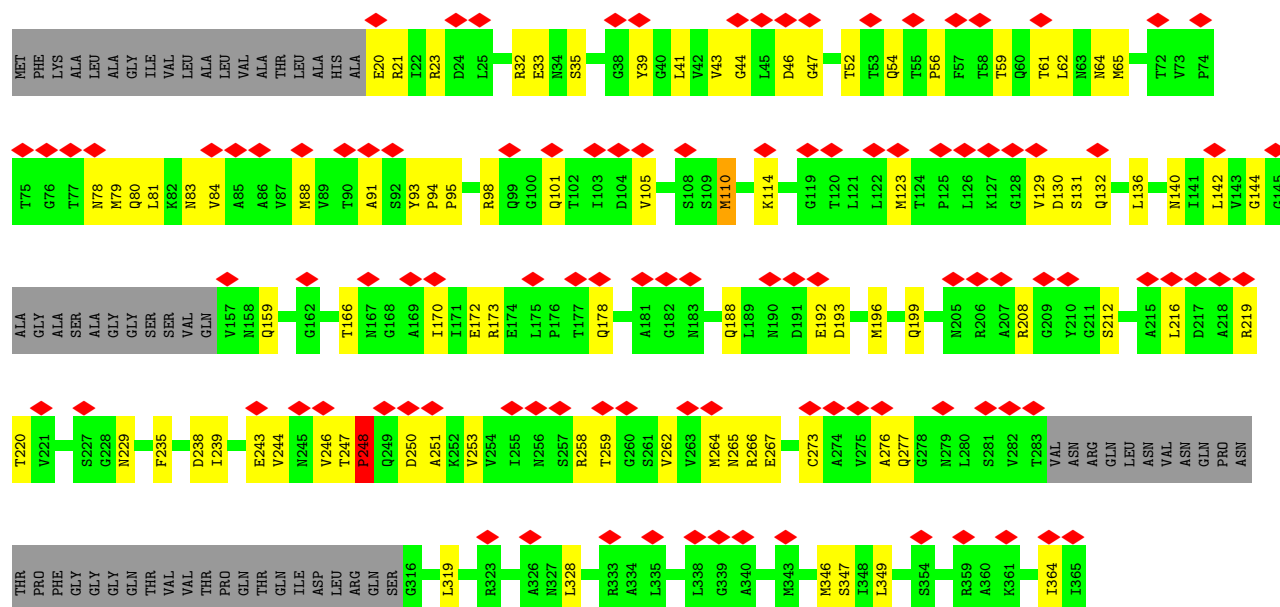


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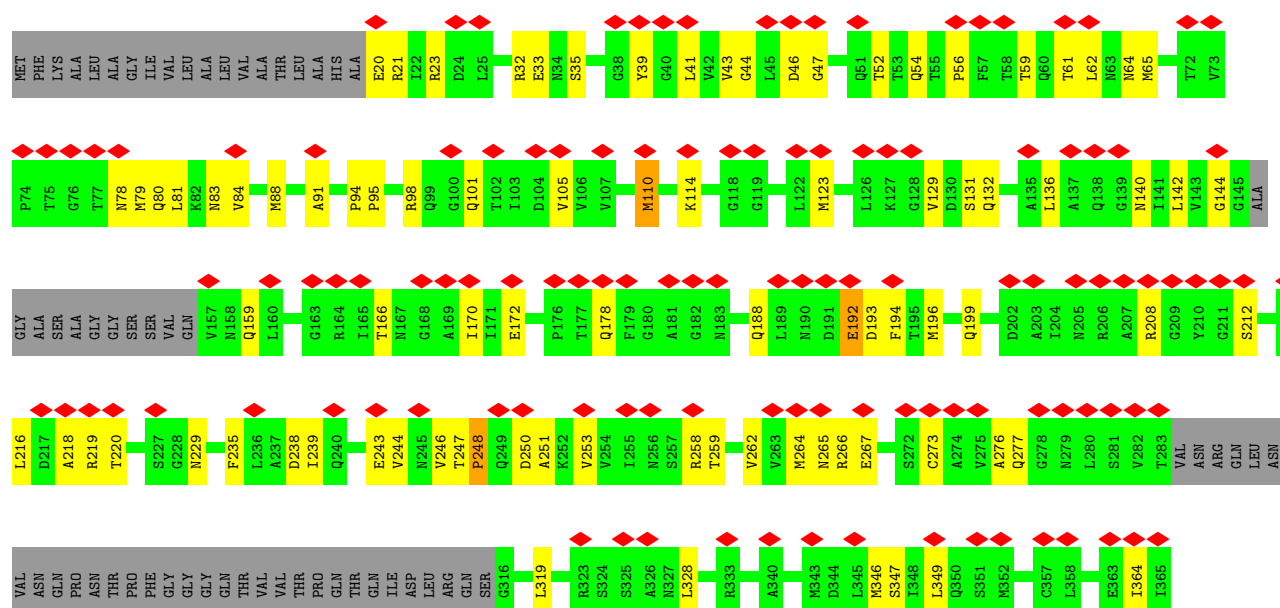




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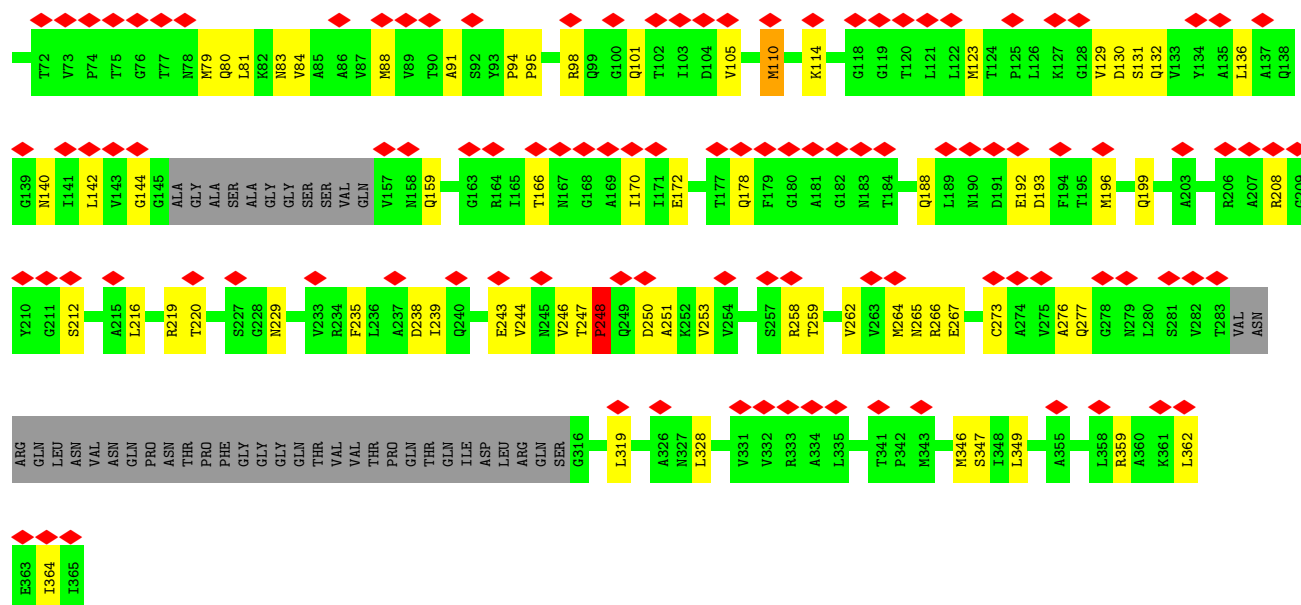
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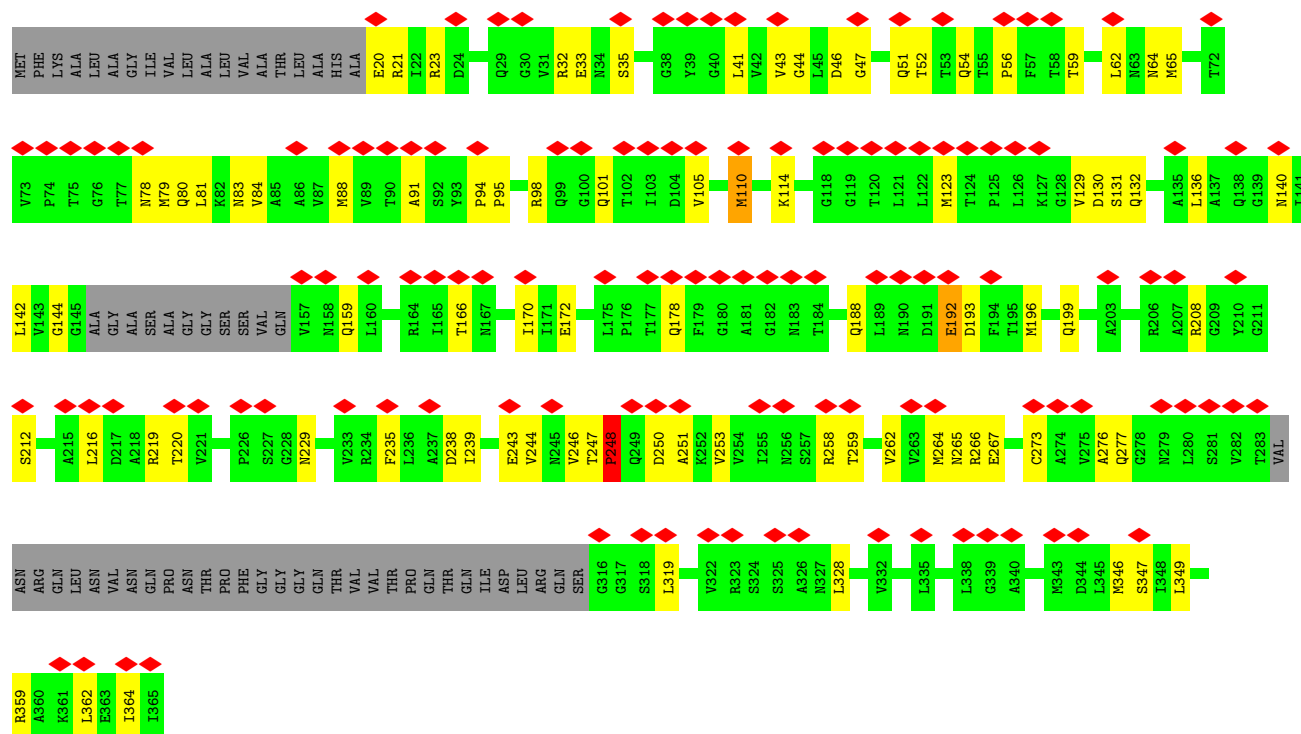
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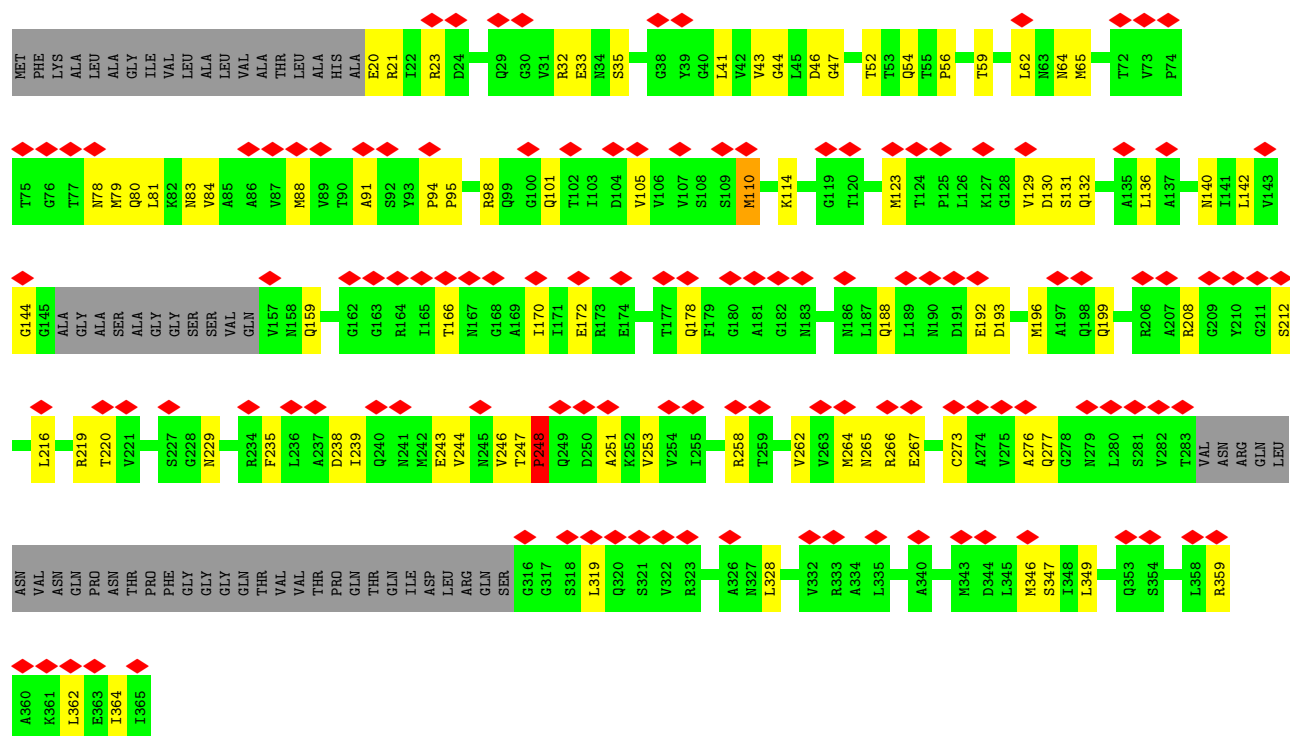
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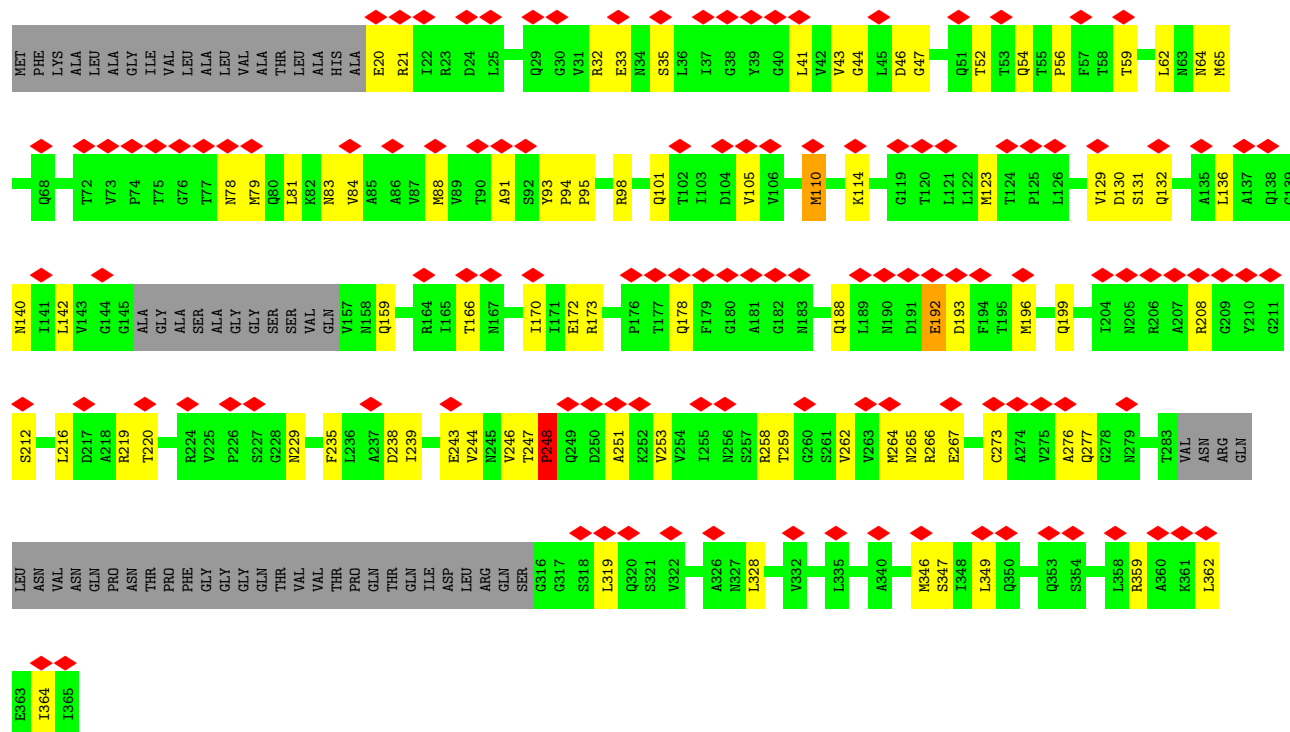
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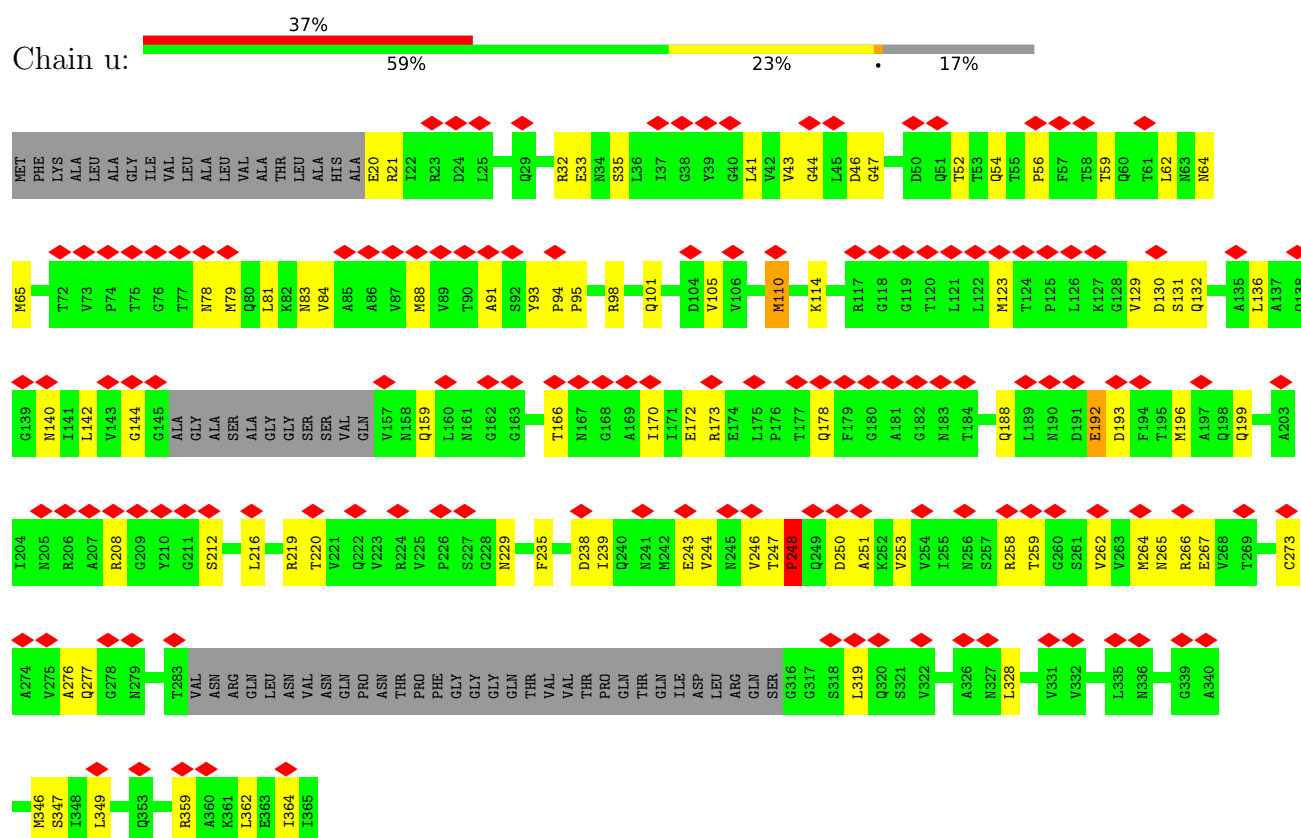




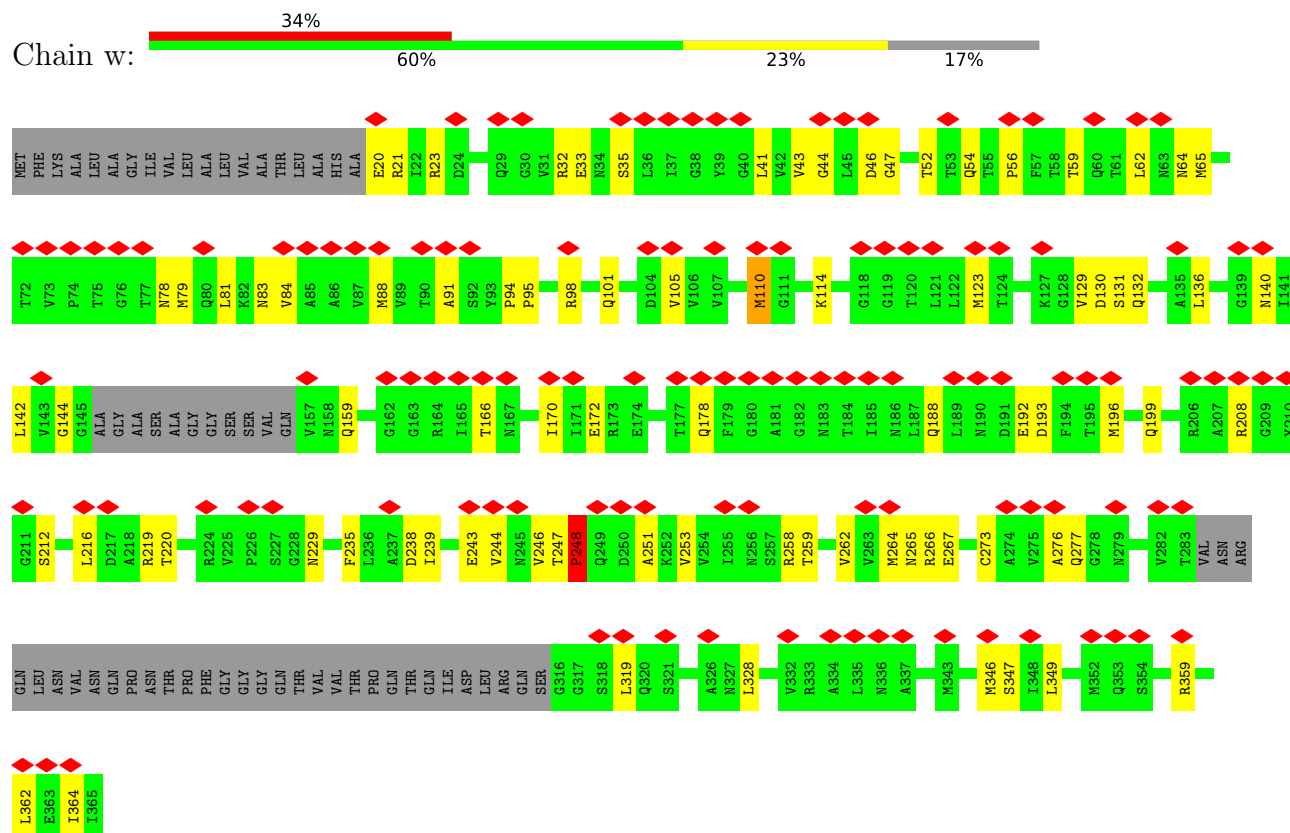
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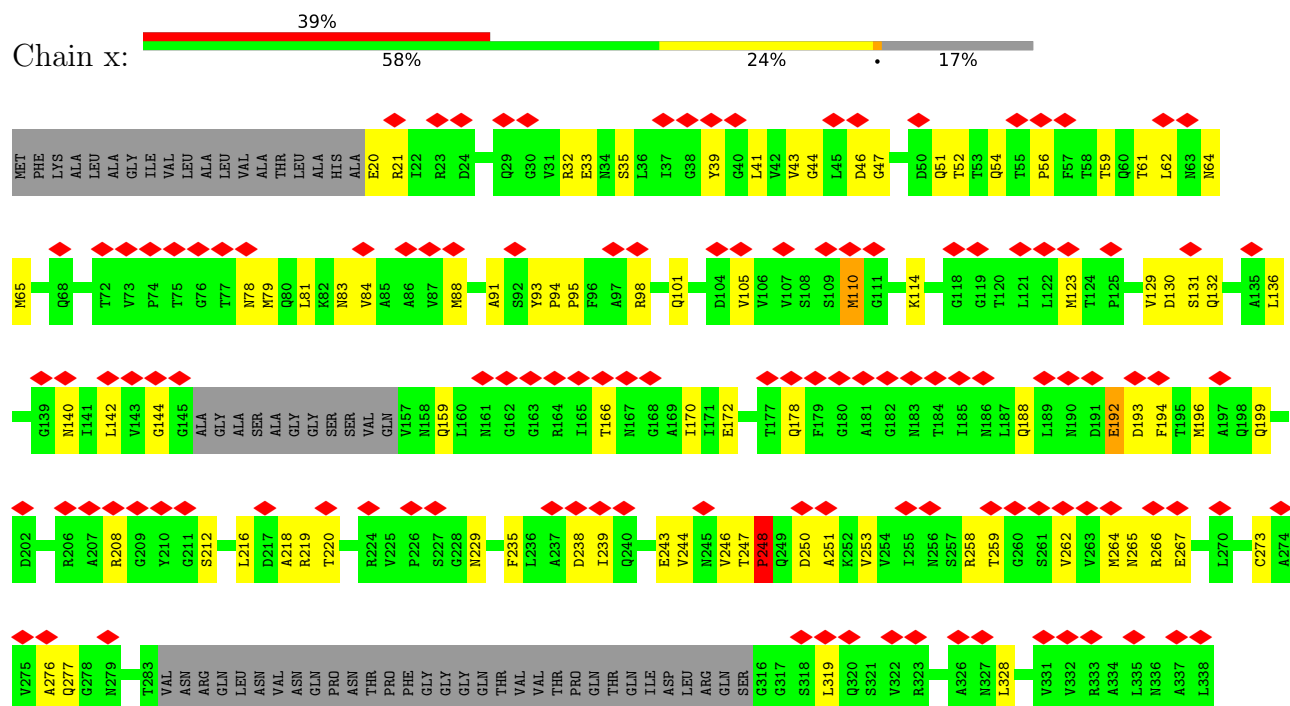
• Molecule 2: Flagellar P-ring protein

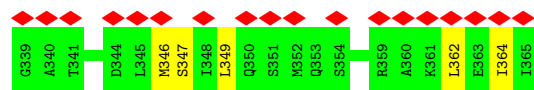


## Chain w:

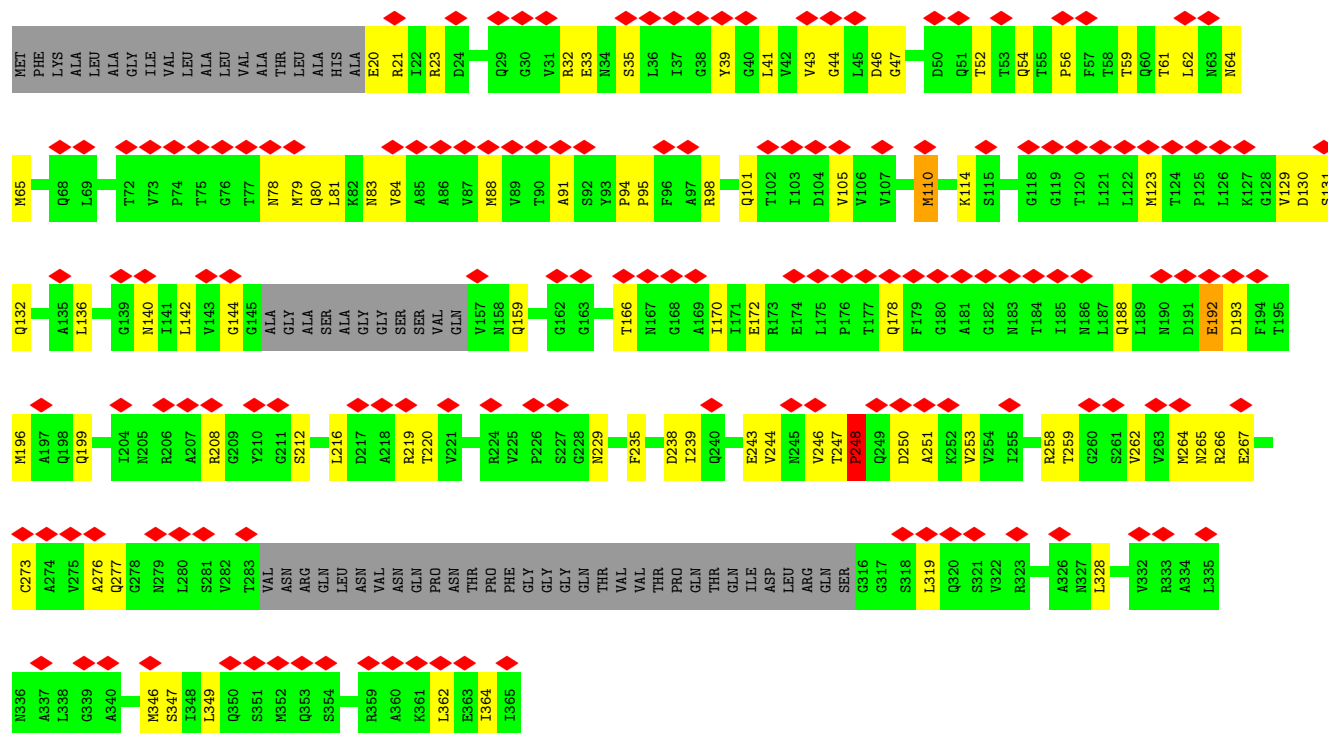
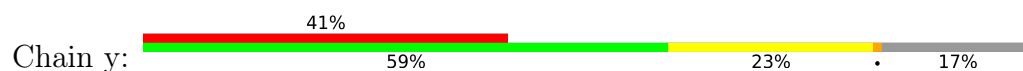


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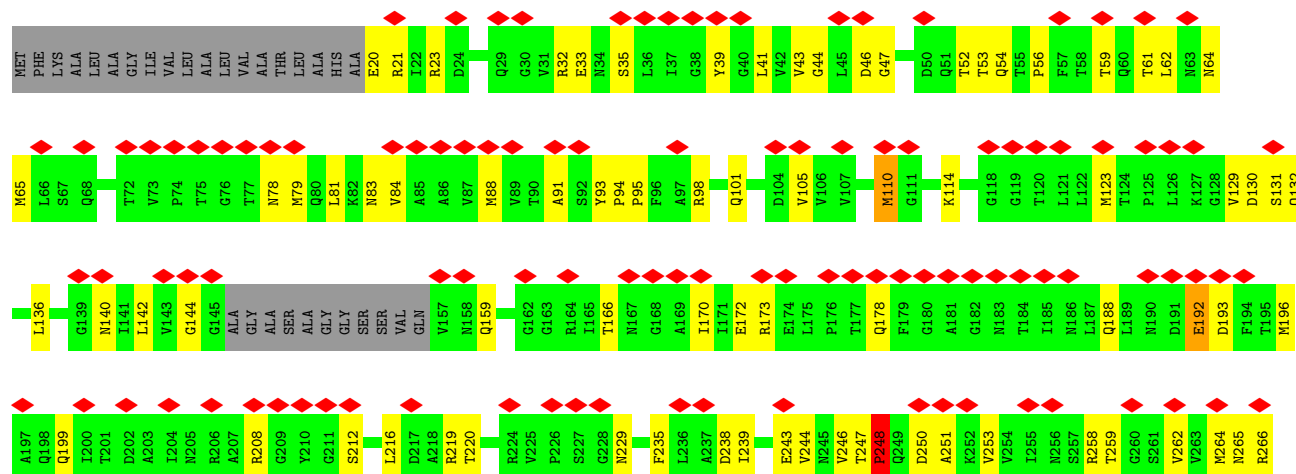


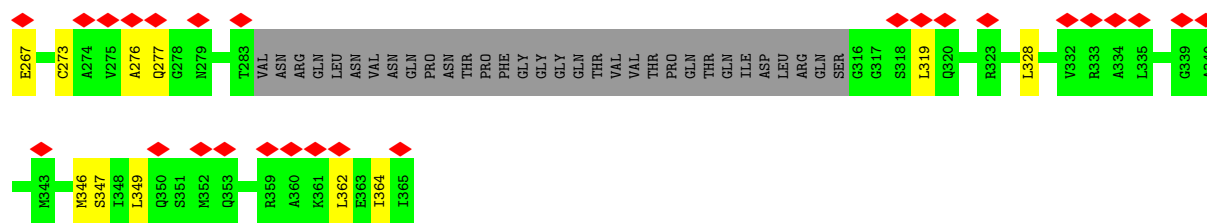


• Molecule 2: Flagellar P-ring protein



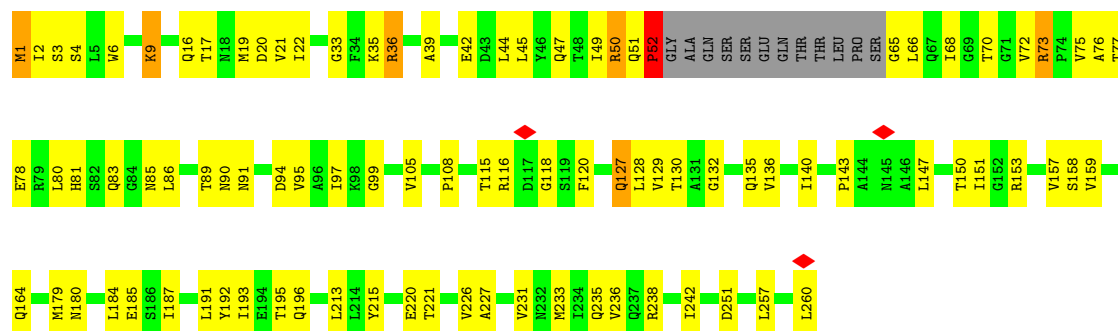
• Molecule 2: Flagellar P-ring protein





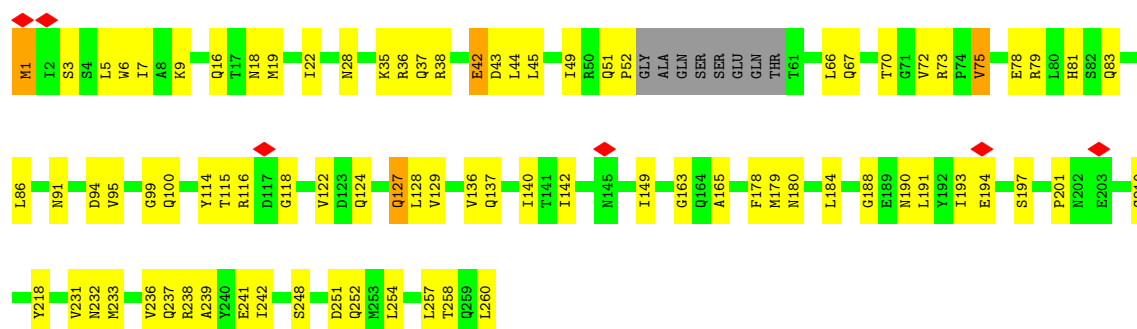
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 0: 59% 34% 5%



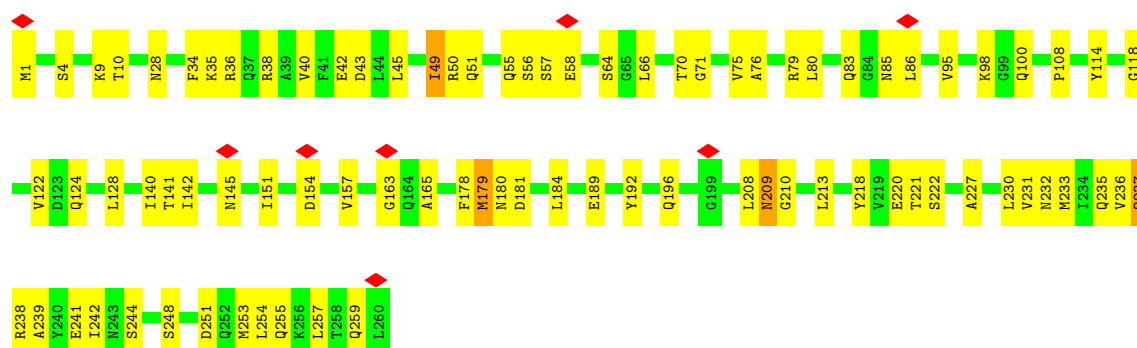
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 1: 65% 30% 5%

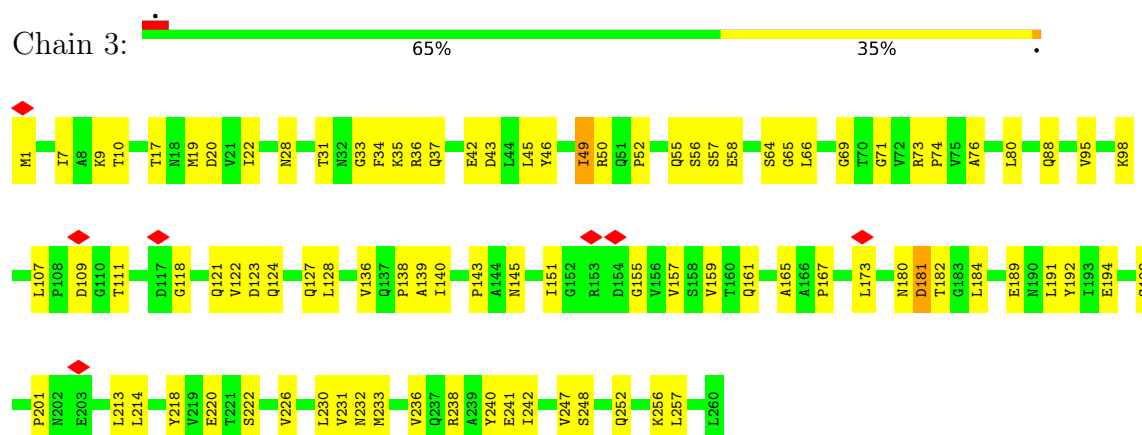


• Molecule 3: Flagellar basal-body rod protein FlgG

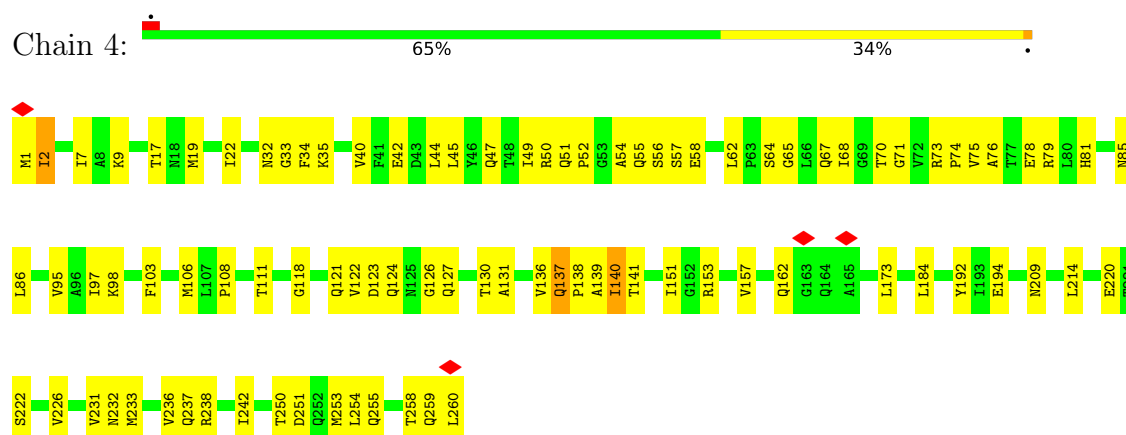
Chain 2: 67% 31% 2%



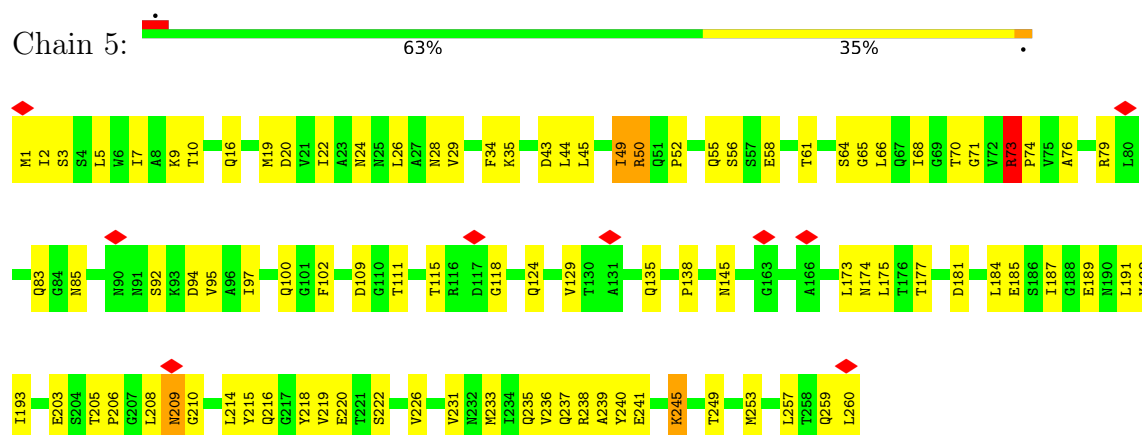
• Molecule 3: Flagellar basal-body rod protein FlgG



• Molecule 3: Flagellar basal-body rod protein FlgG

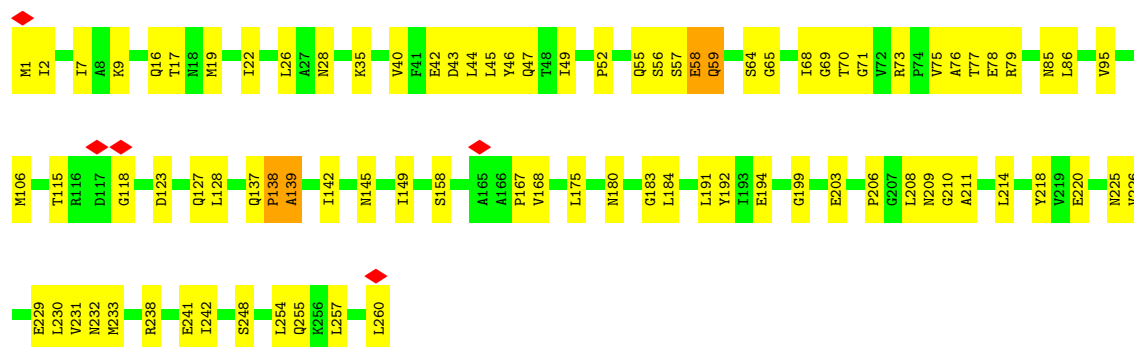


• Molecule 3: Flagellar basal-body rod protein FlgG



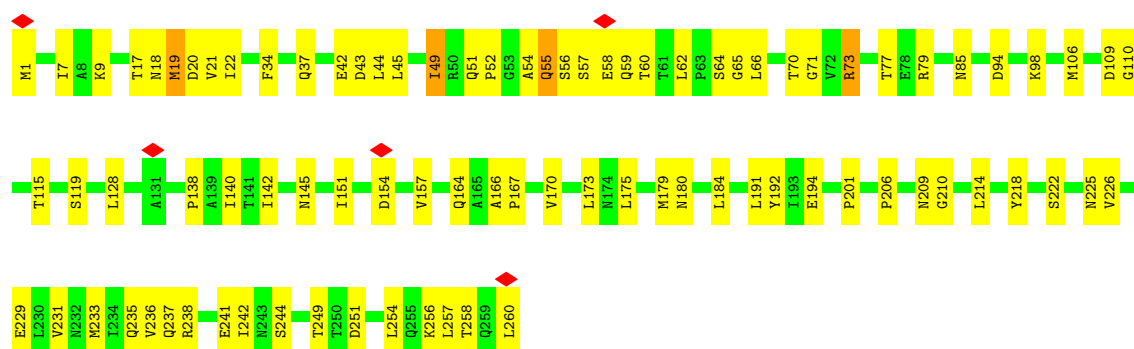
• Molecule 3: Flagellar basal-body rod protein FlgG





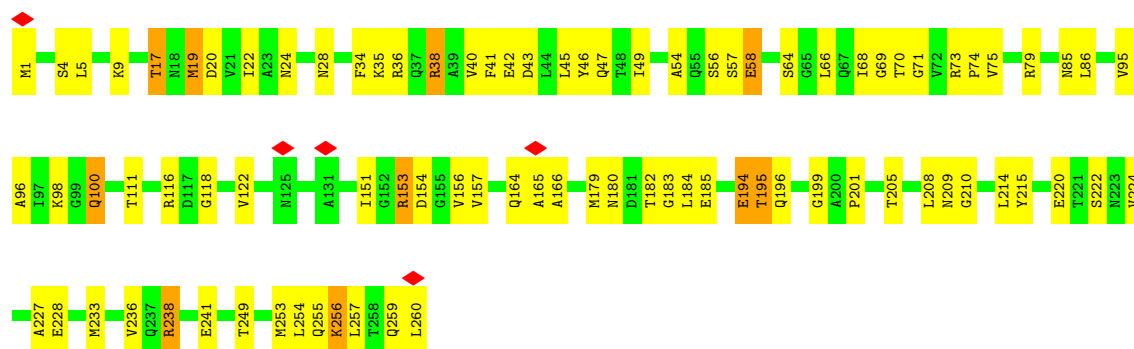
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 7: 66% 32%



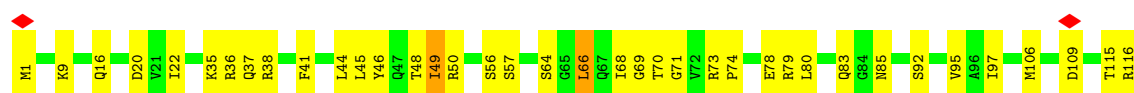
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 8: 66% 30%



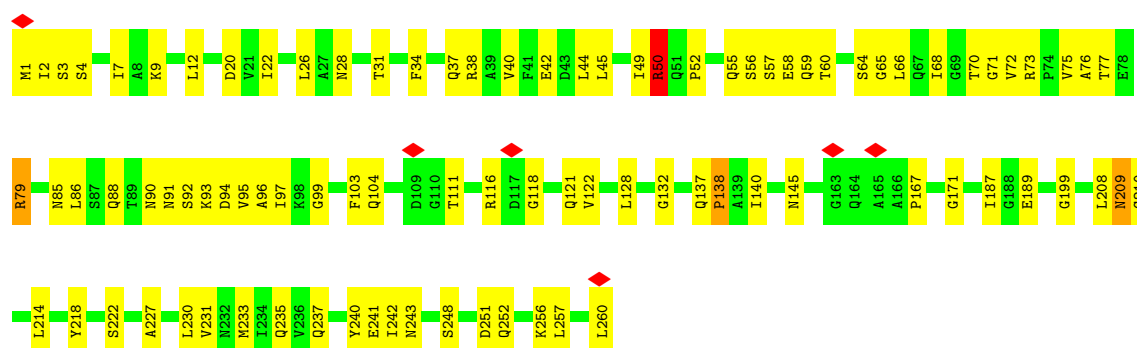
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 9: 71% 28%

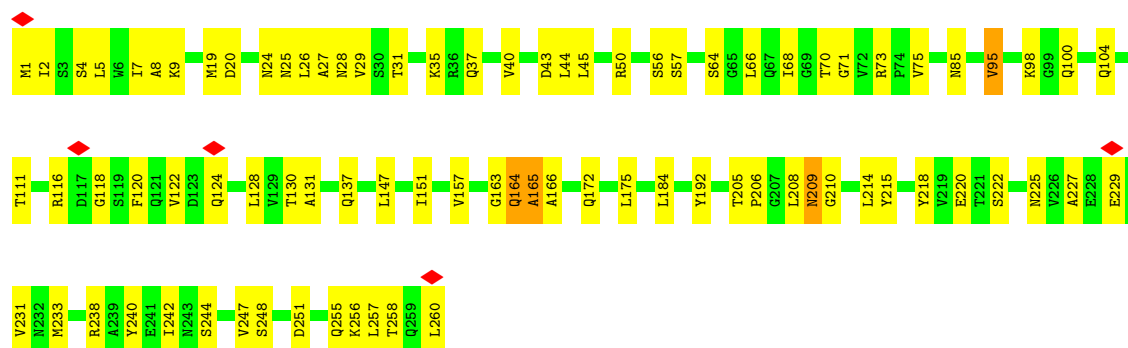




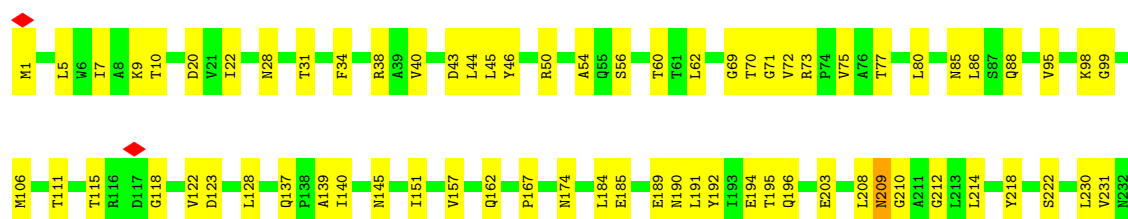
• Molecule 3: Flagellar basal-body rod protein FlgG



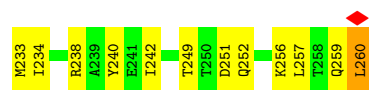
• Molecule 3: Flagellar basal-body rod protein FlgG



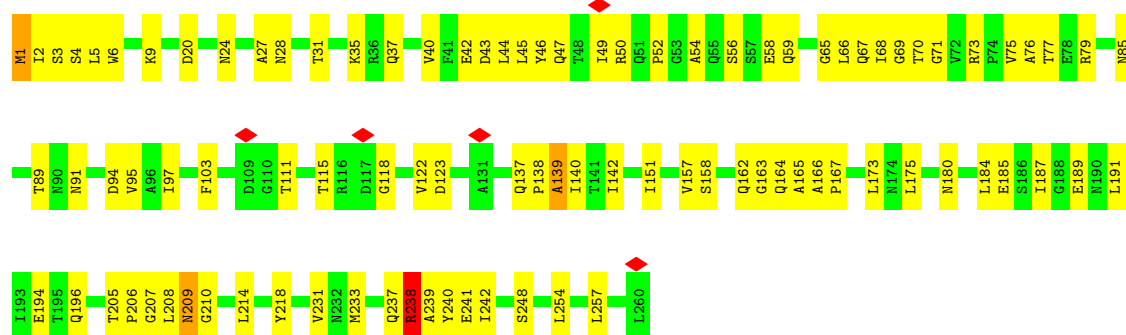
• Molecule 3: Flagellar basal-body rod protein FlgG



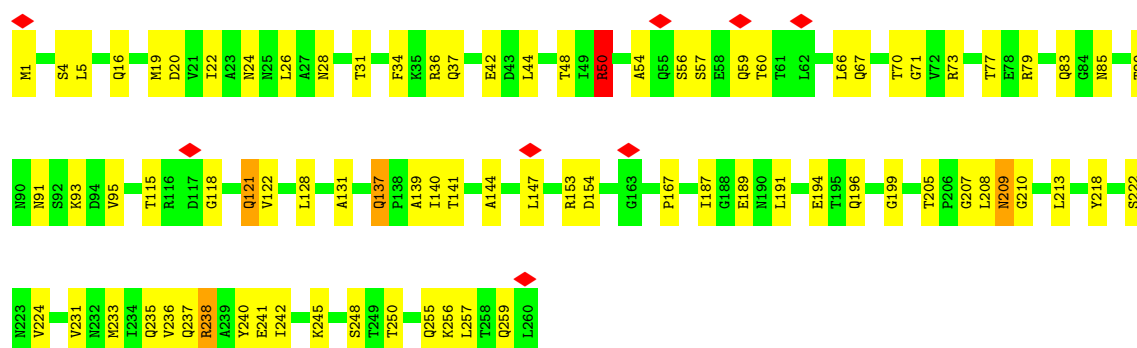




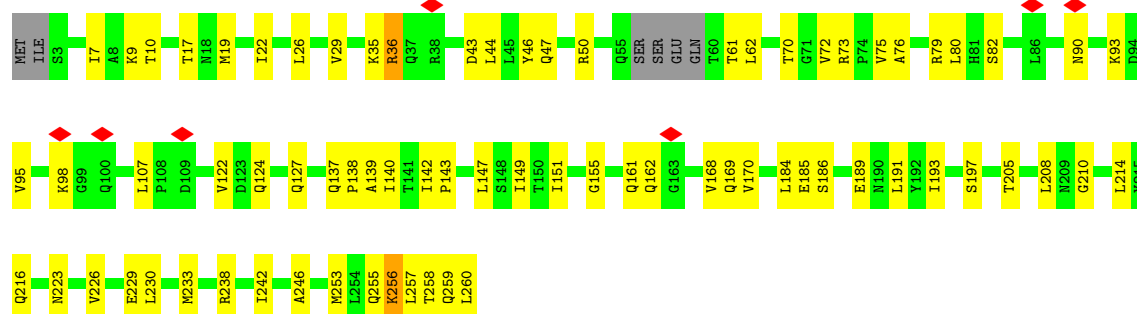
• Molecule 3: Flagellar basal-body rod protein FlgG



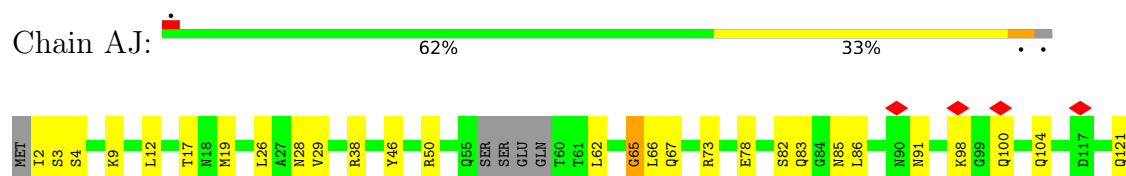
• Molecule 3: Flagellar basal-body rod protein FlgG

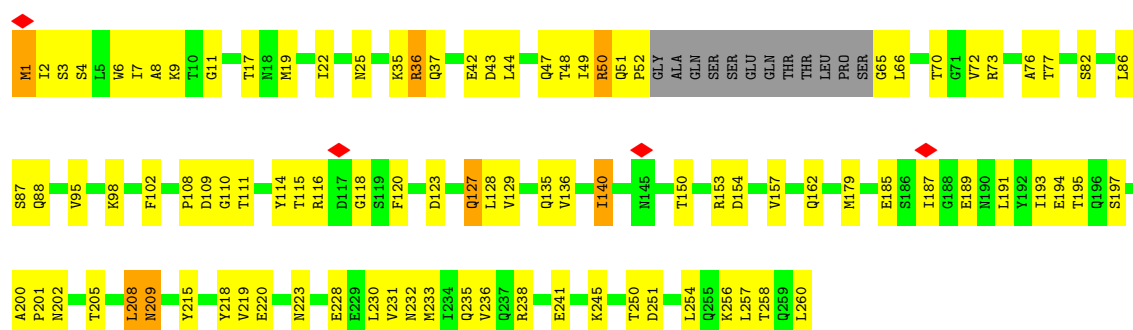


• Molecule 3: Flagellar basal-body rod protein FlgG

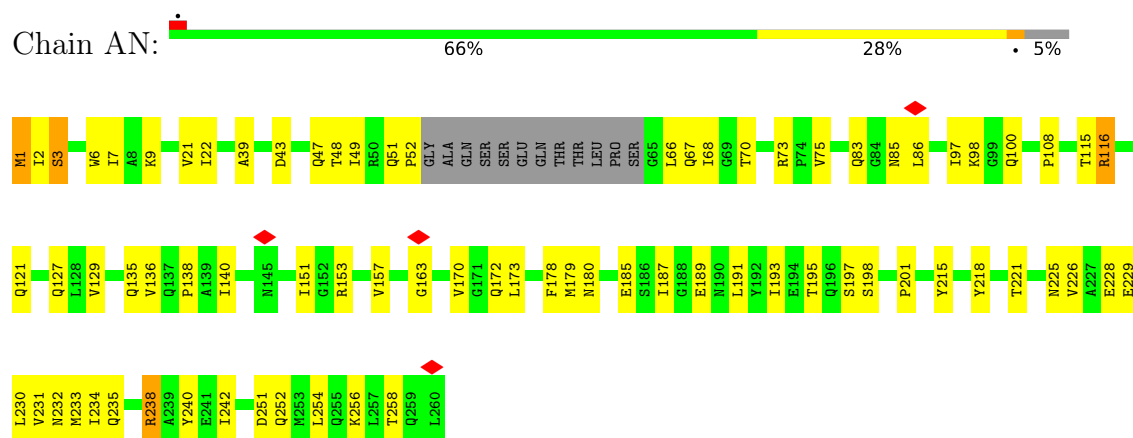


• Molecule 3: Flagellar basal-body rod protein FlgG

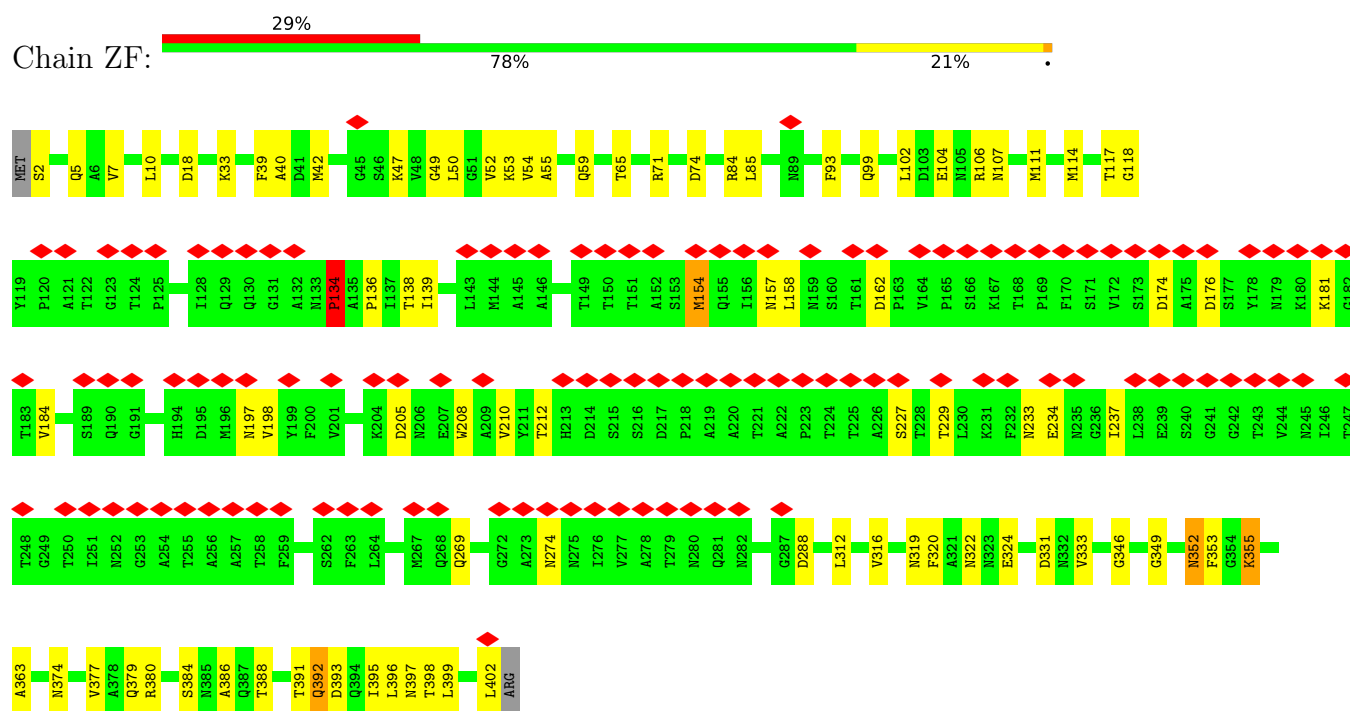




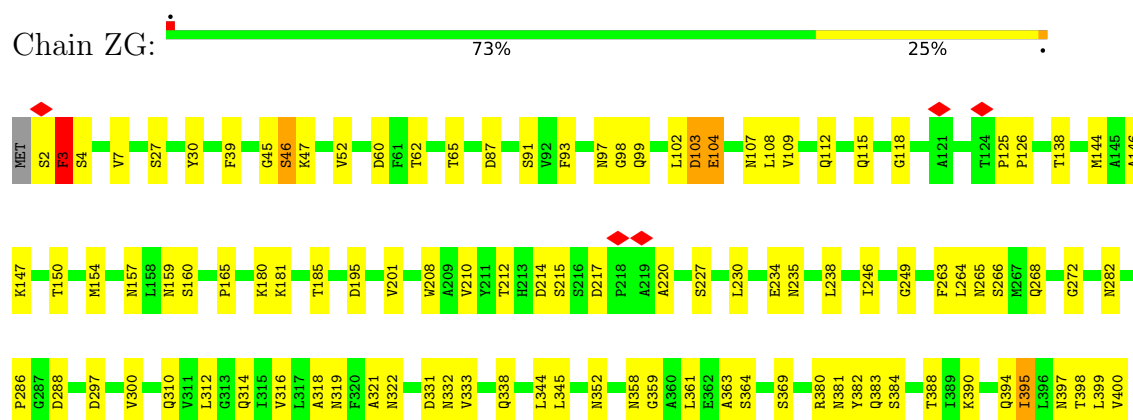
- Molecule 3: Flagellar basal-body rod protein FlgG



- Molecule 4: Flagellar hook protein FlgE



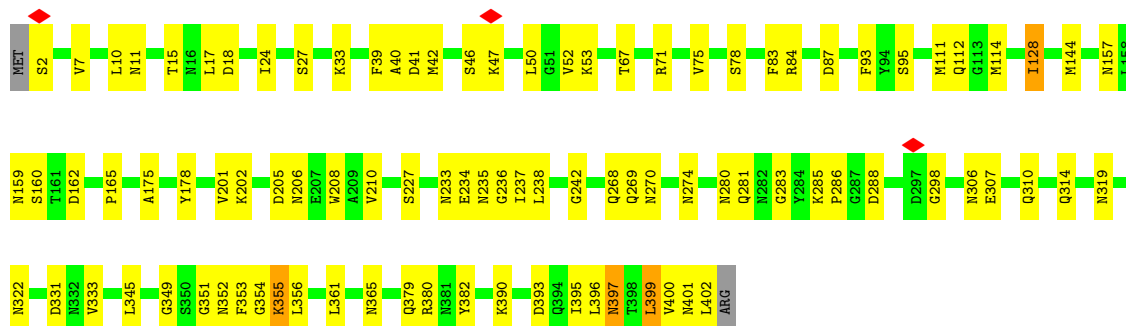
- Molecule 4: Flagellar hook protein FlgE





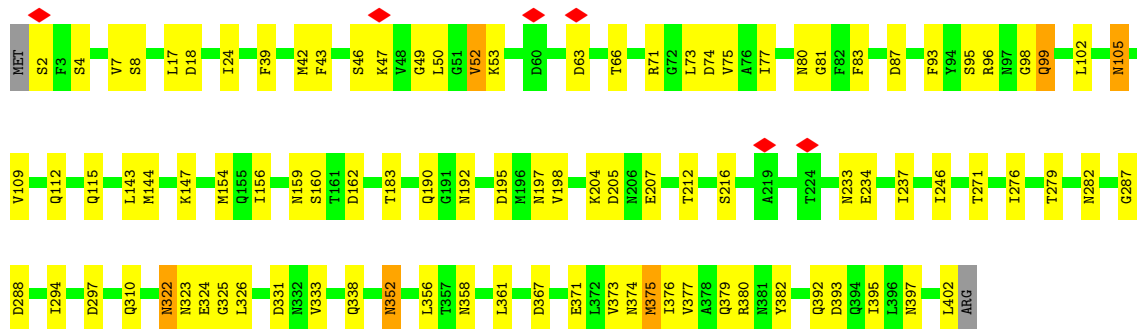
• Molecule 4: Flagellar hook protein FlgE

Chain ZH: 76% 23%



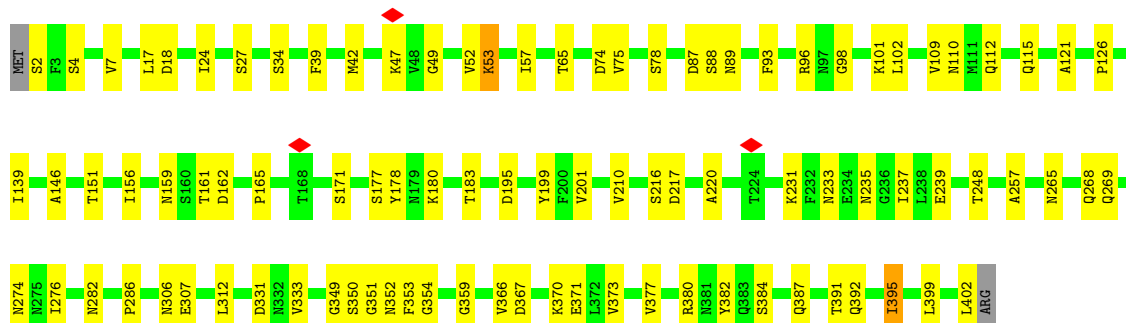
• Molecule 4: Flagellar hook protein FlgE

Chain ZI: 76% 22%



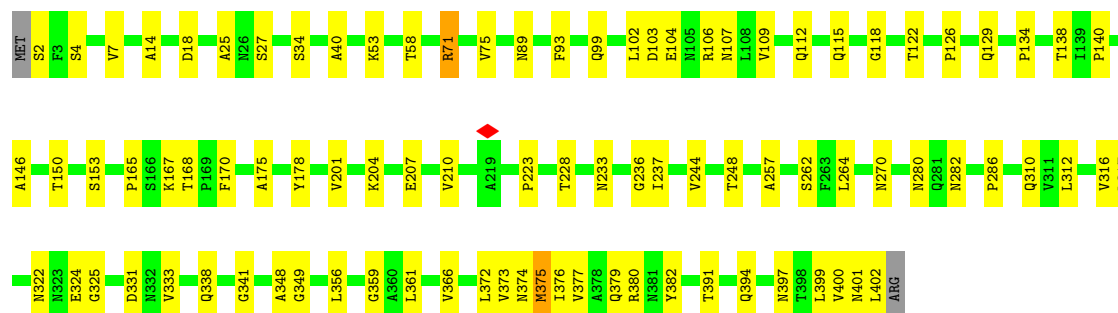
• Molecule 4: Flagellar hook protein FlgE

Chain ZJ: 76% 23%

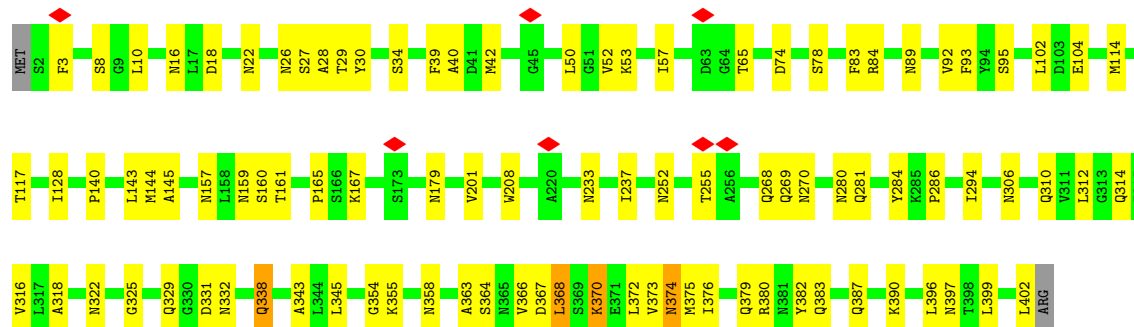
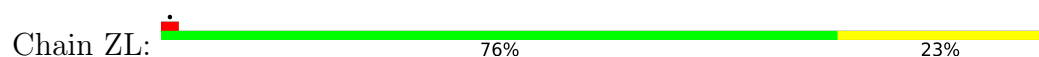


• Molecule 4: Flagellar hook protein FlgE

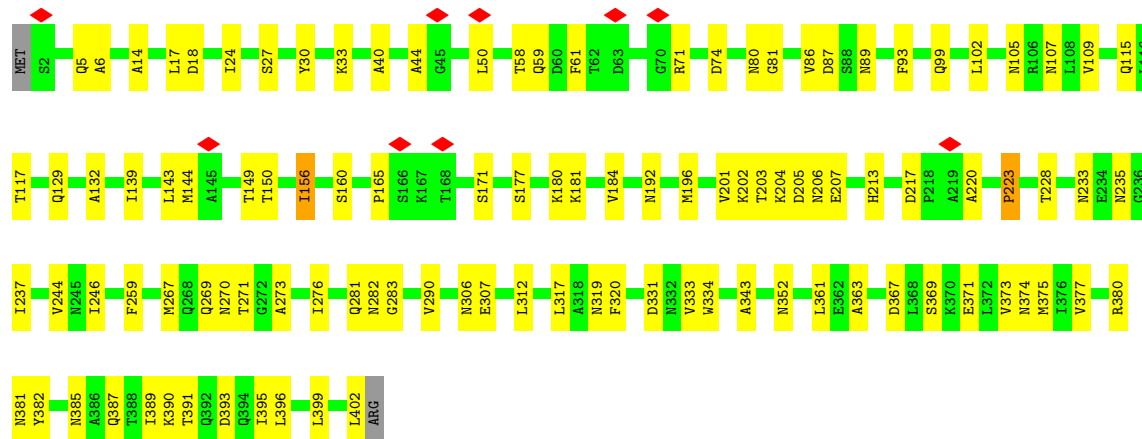
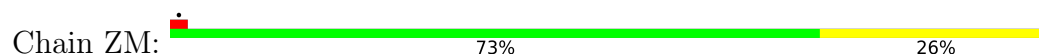
Chain ZK: 77% 22%



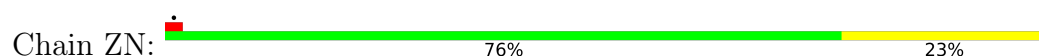
• Molecule 4: Flagellar hook protein FlgE

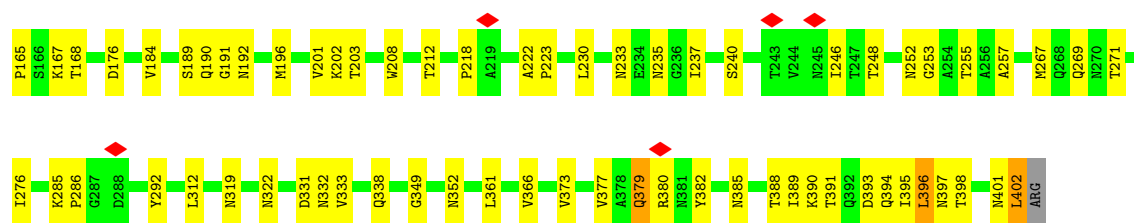


• Molecule 4: Flagellar hook protein FlgE

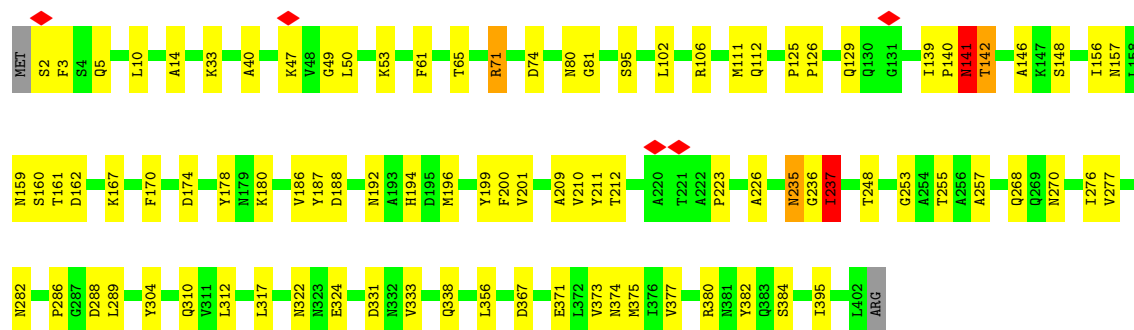
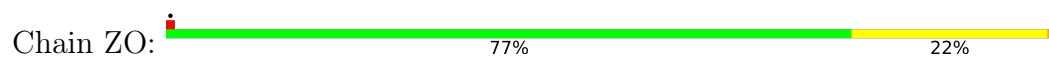


• Molecule 4: Flagellar hook protein FlgE

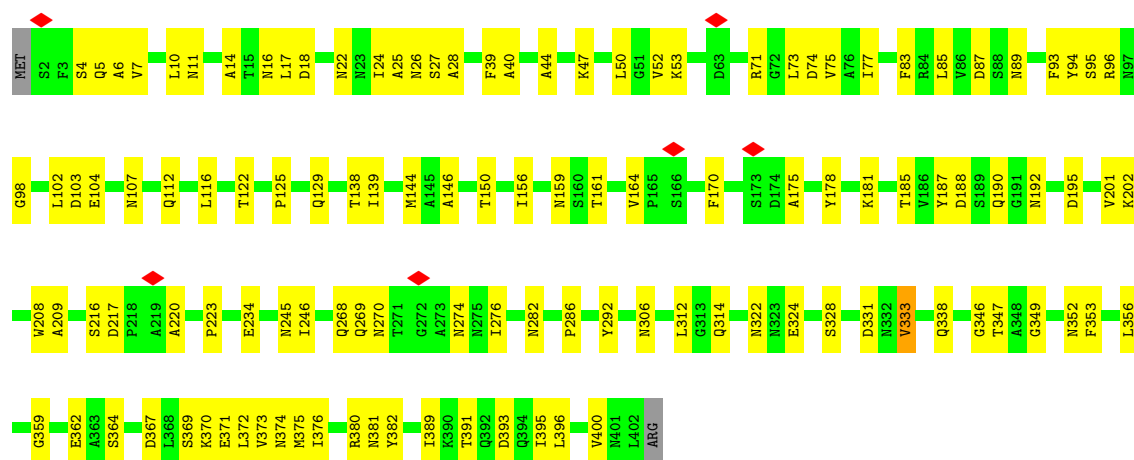




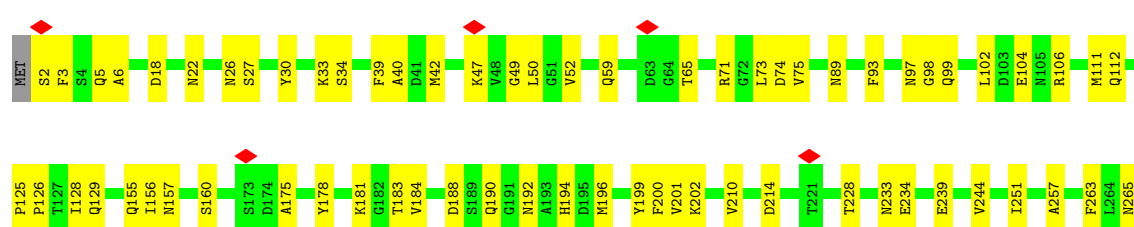
• Molecule 4: Flagellar hook protein FlgE

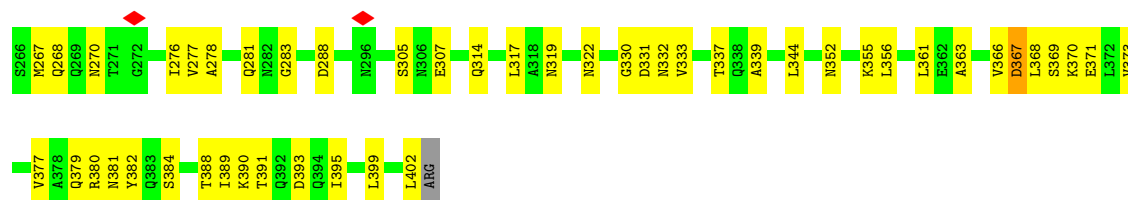


• Molecule 4: Flagellar hook protein FlgE

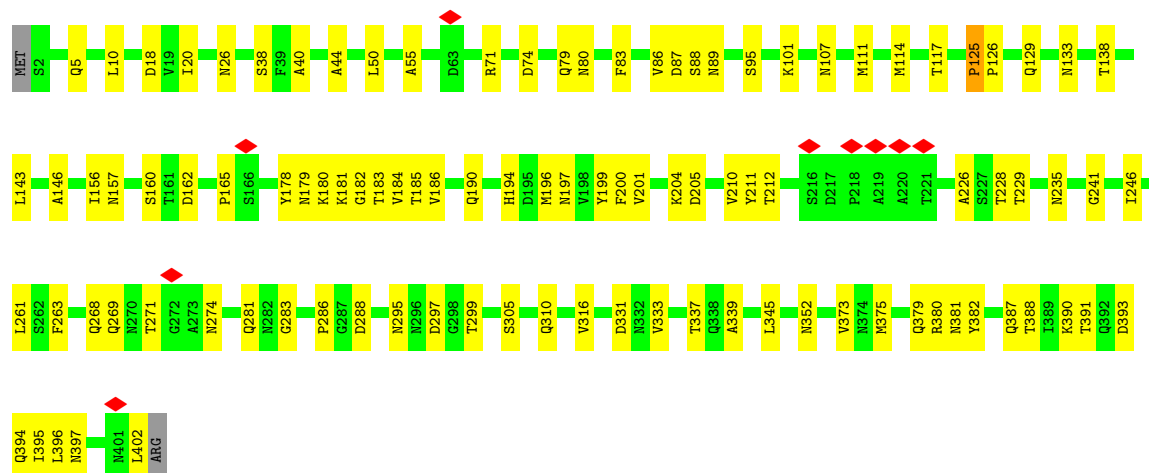
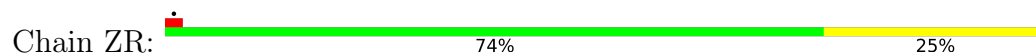


• Molecule 4: Flagellar hook protein FlgE

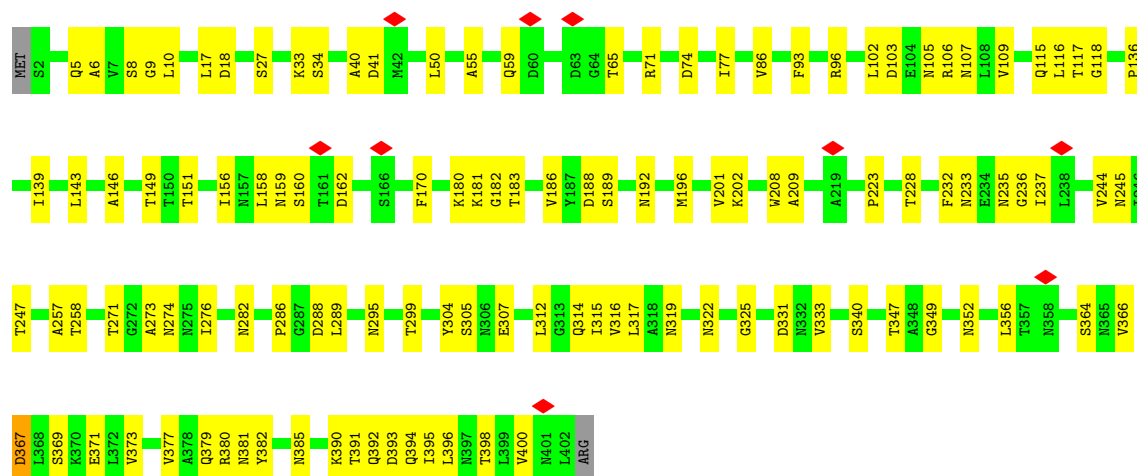




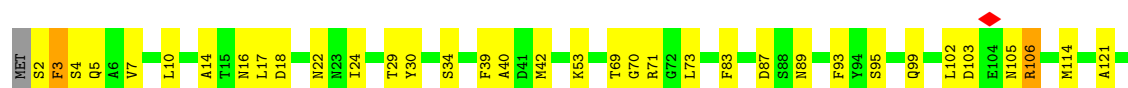
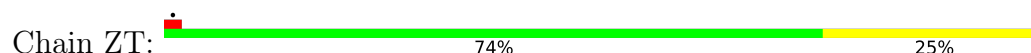
• Molecule 4: Flagellar hook protein FlgE



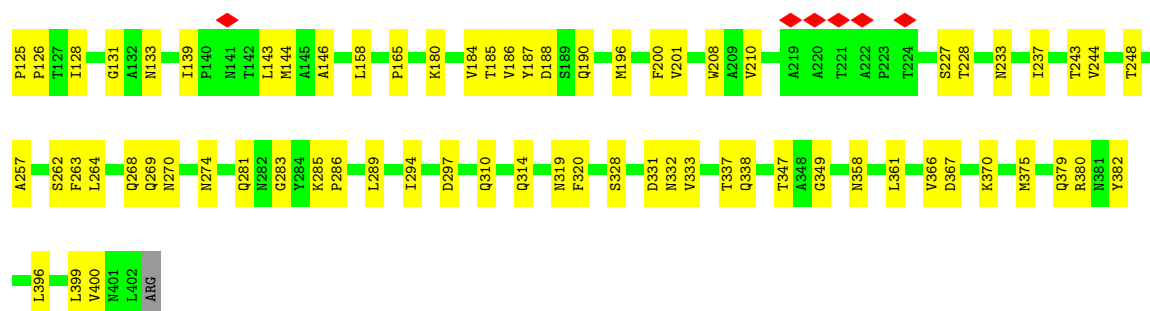
• Molecule 4: Flagellar hook protein FlgE



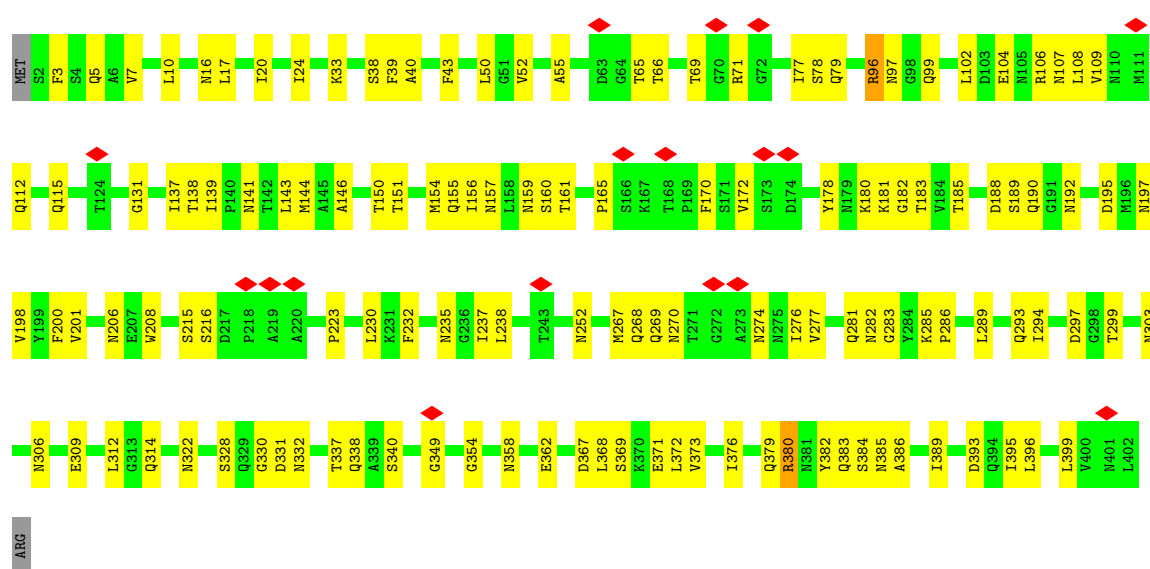
• Molecule 4: Flagellar hook protein FlgE



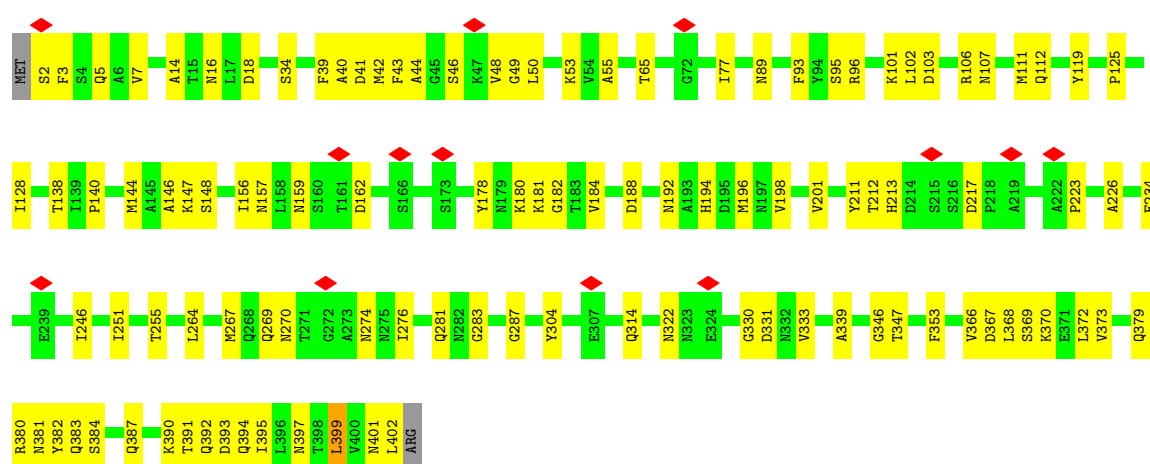
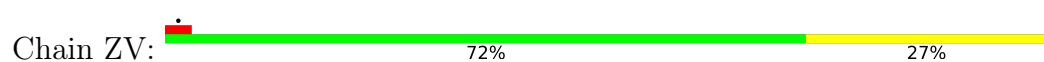




• Molecule 4: Flagellar hook protein FlgE

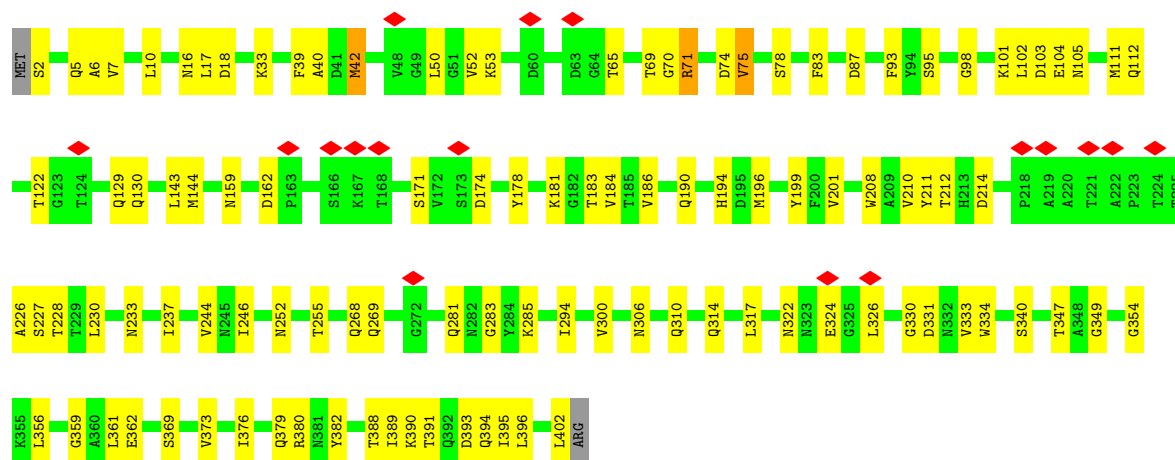


• Molecule 4: Flagellar hook protein FlgE



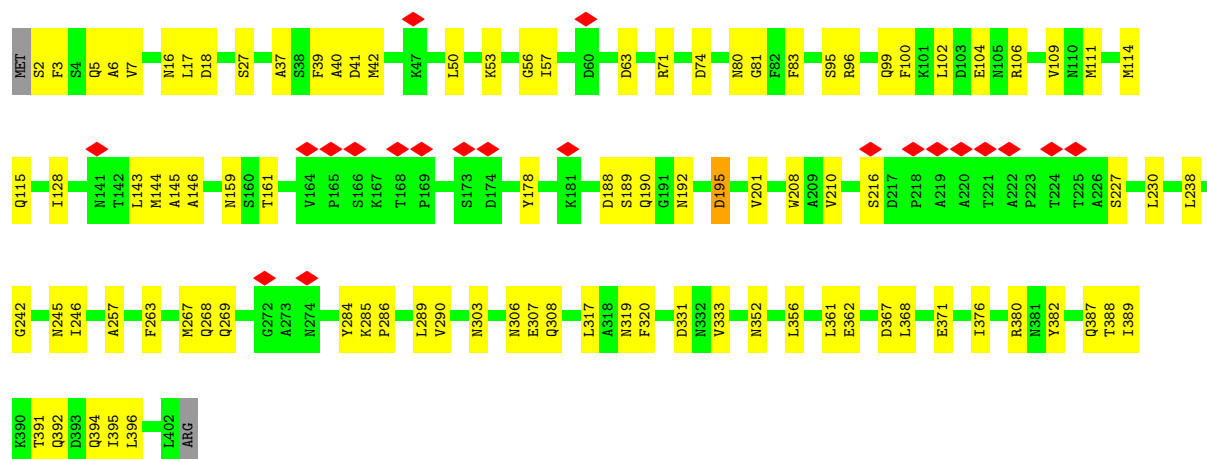
• Molecule 4: Flagellar hook protein FlgE

Chain ZW:  72% 26%



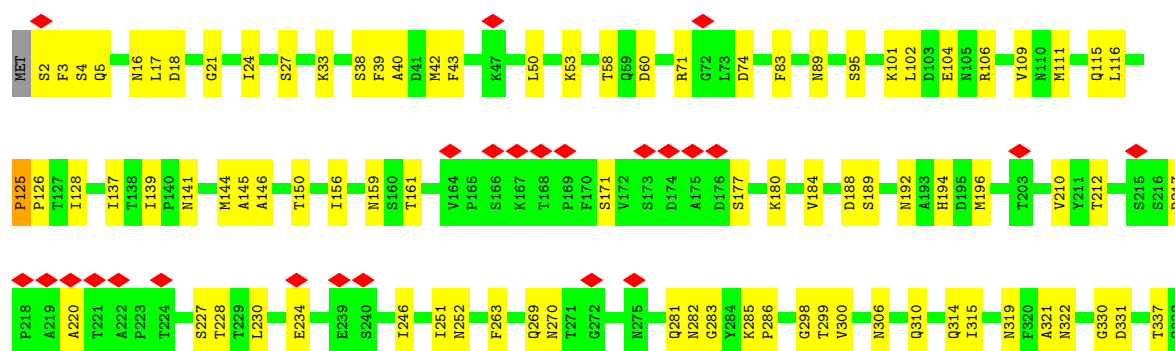
• Molecule 4: Flagellar hook protein FlgE

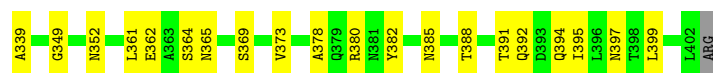
Chain ZX:  5% 76% 23%



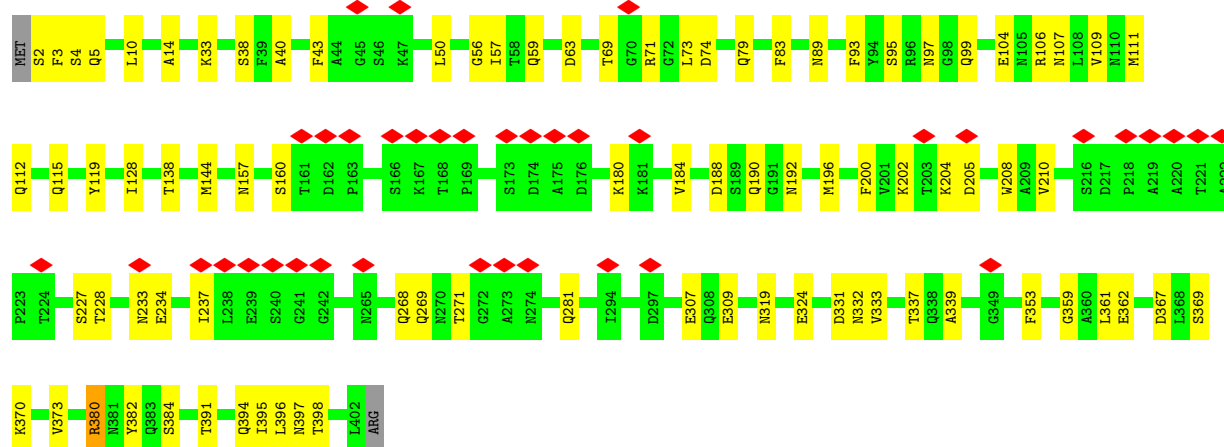
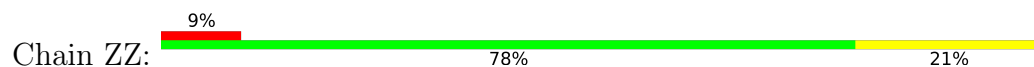
• Molecule 4: Flagellar hook protein FlgE

Chain ZY:  6% 73% 26%

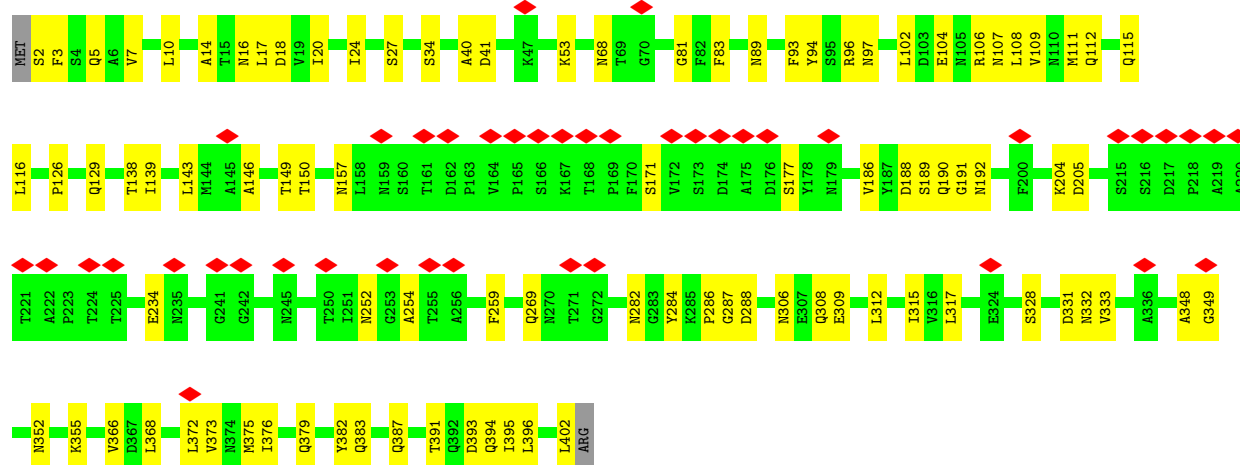
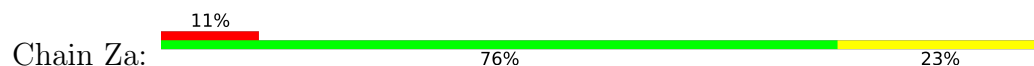




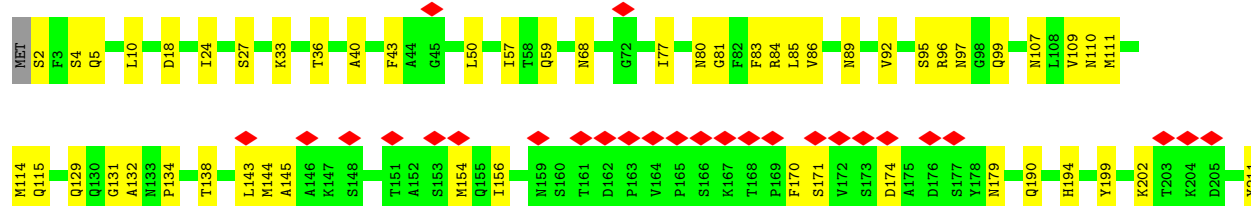
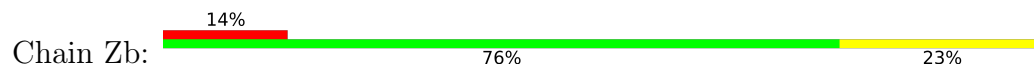
• Molecule 4: Flagellar hook protein FlgE

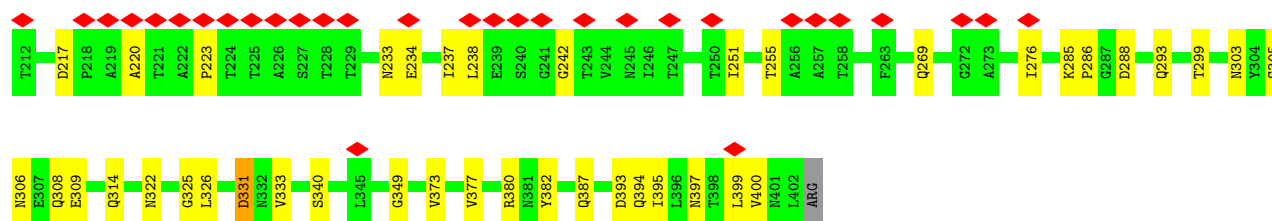


• Molecule 4: Flagellar hook protein FlgE

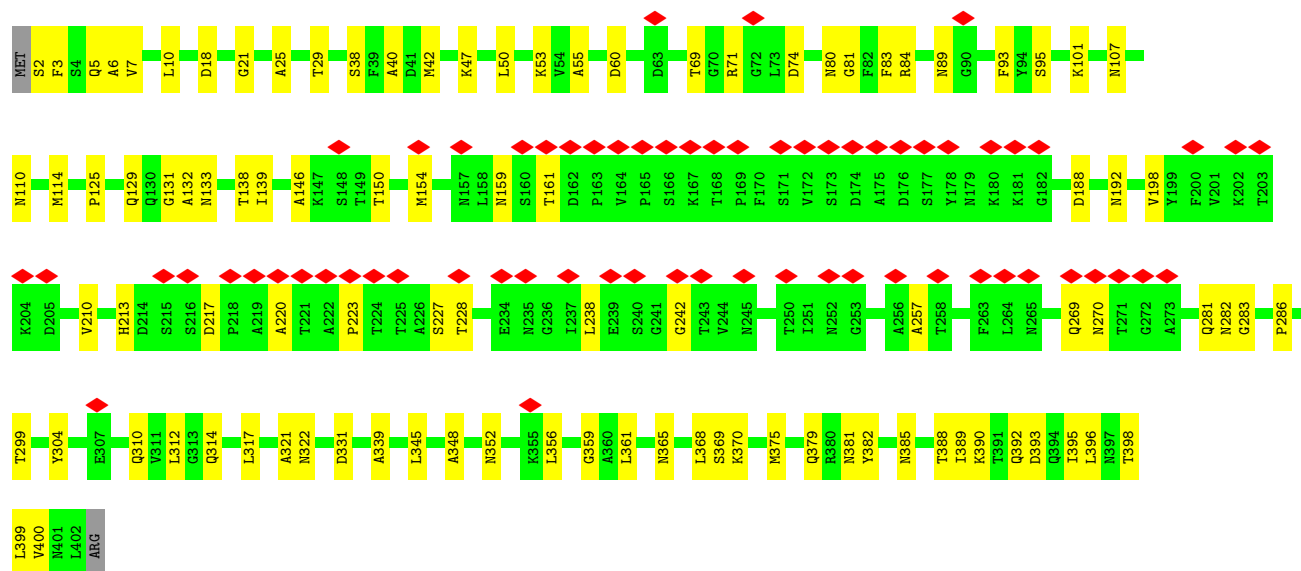
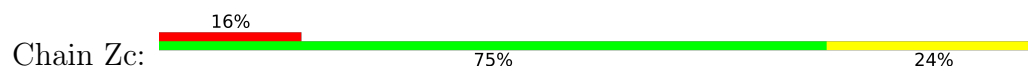


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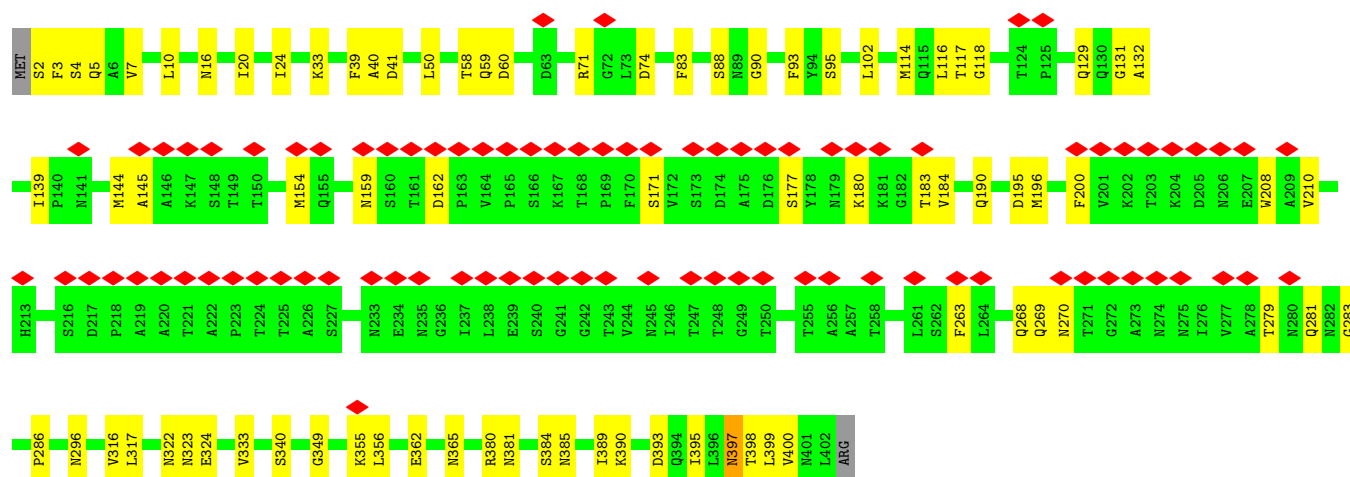
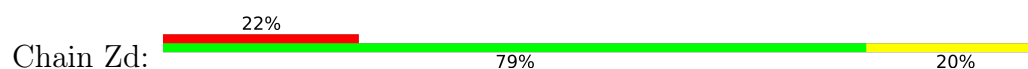




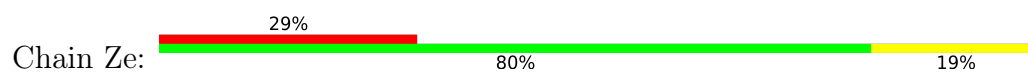
• Molecule 4: Flagellar hook protein FlgE

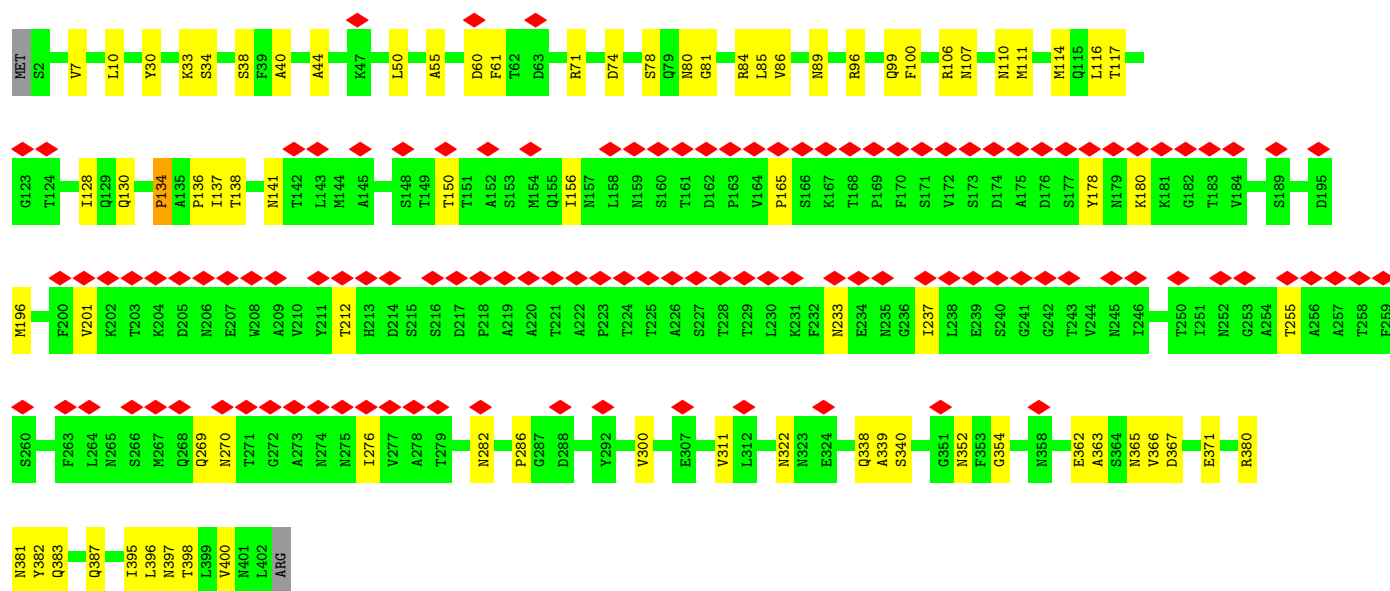


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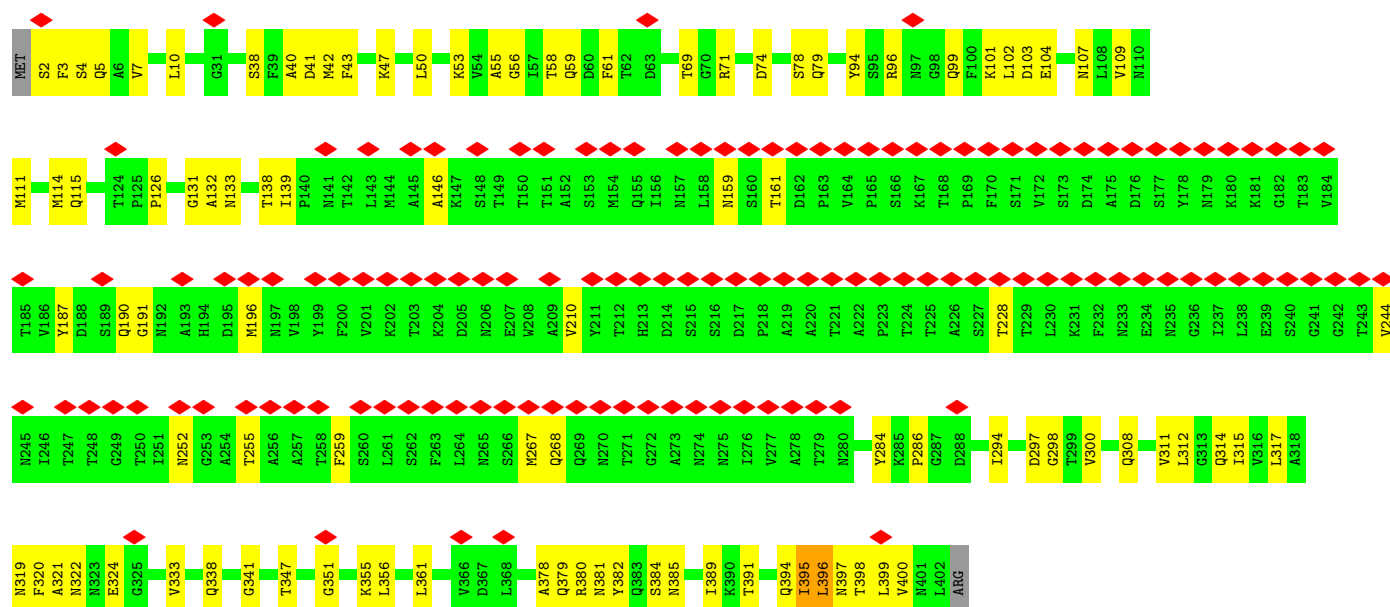
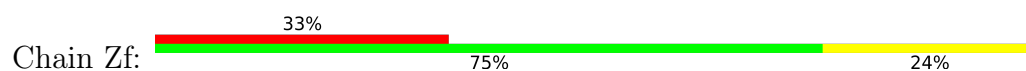


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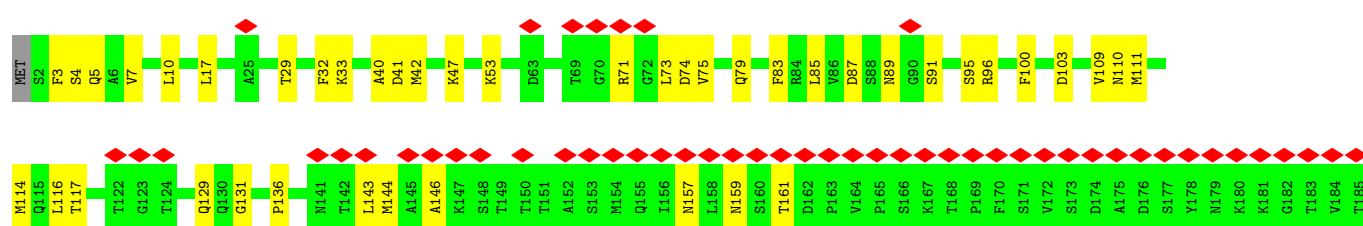
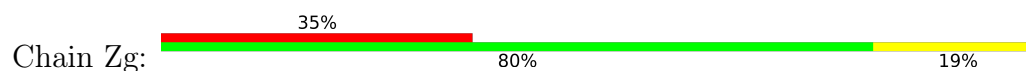


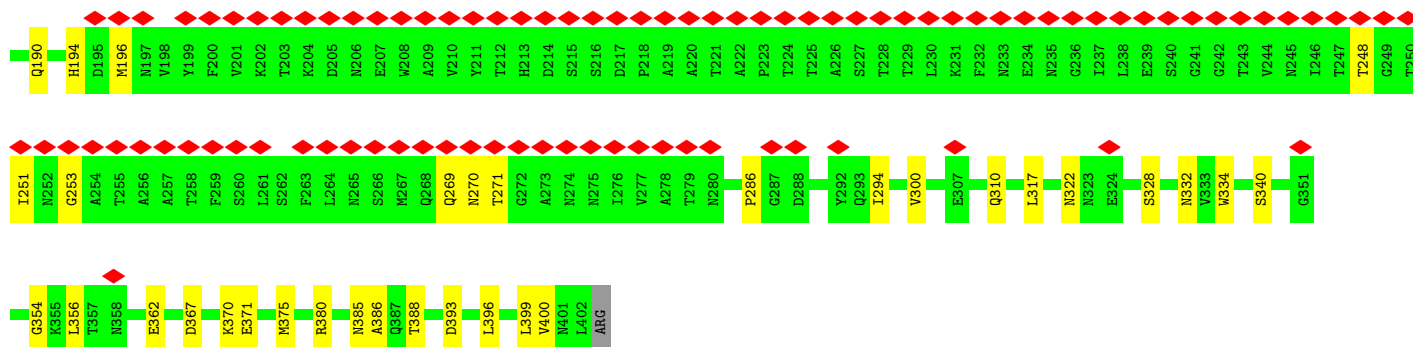


• Molecule 4: Flagellar hook protein FlgE

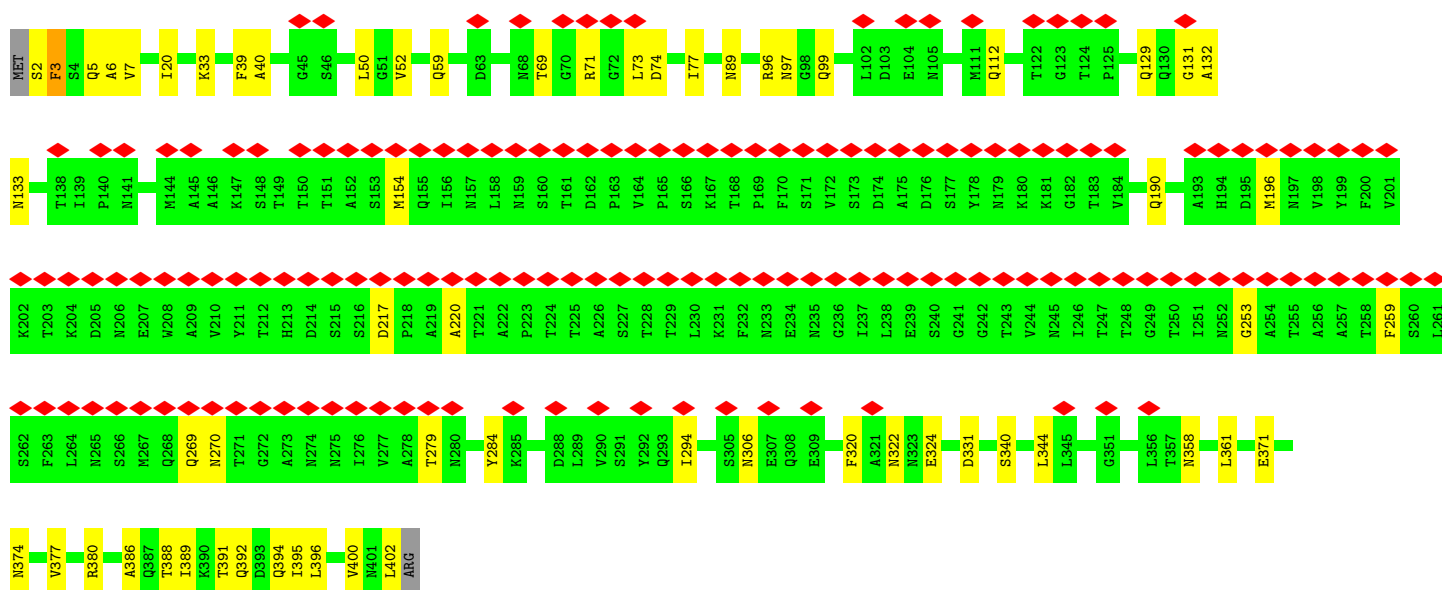
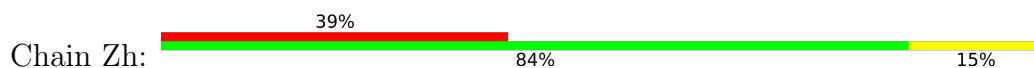


• Molecule 4: Flagellar hook protein FlgE

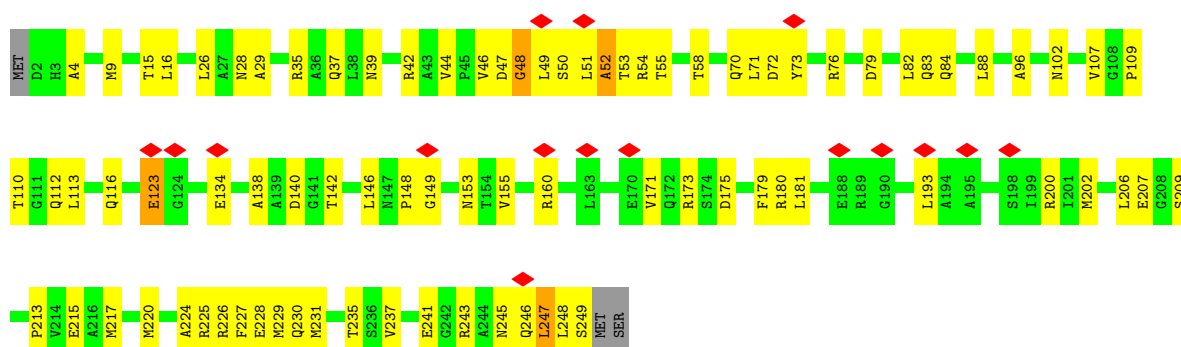




• Molecule 4: Flagellar hook protein FlgE

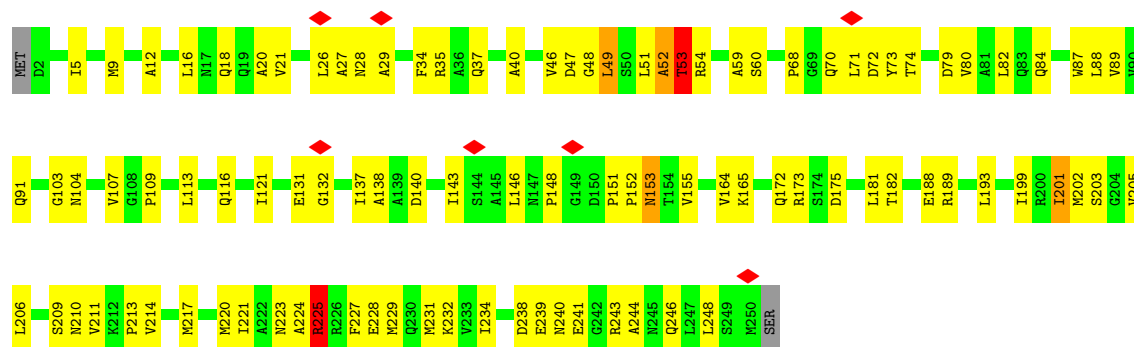


• Molecule 5: Flagellar basal-body rod protein FlgF

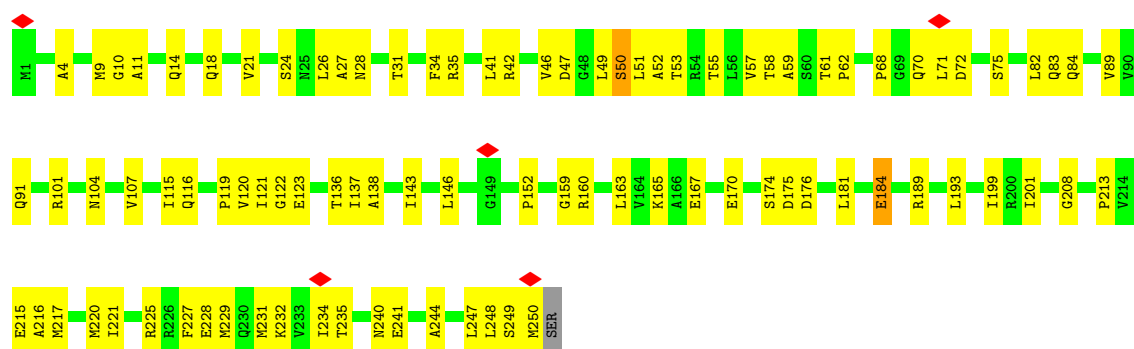


• Molecule 5: Flagellar basal-body rod protein FlgF

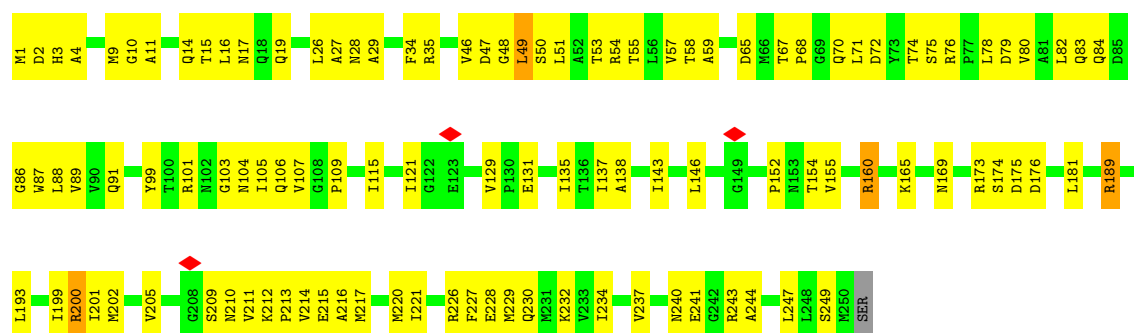




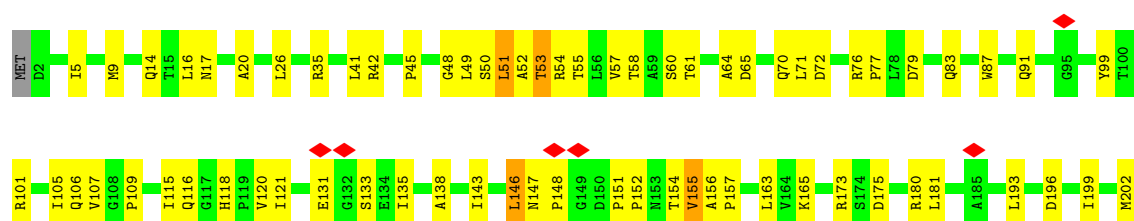
• Molecule 5: Flagellar basal-body rod protein FlgF

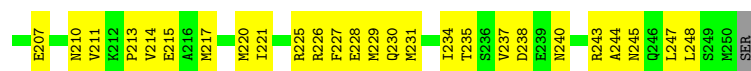


• Molecule 5: Flagellar basal-body rod protein FlgF

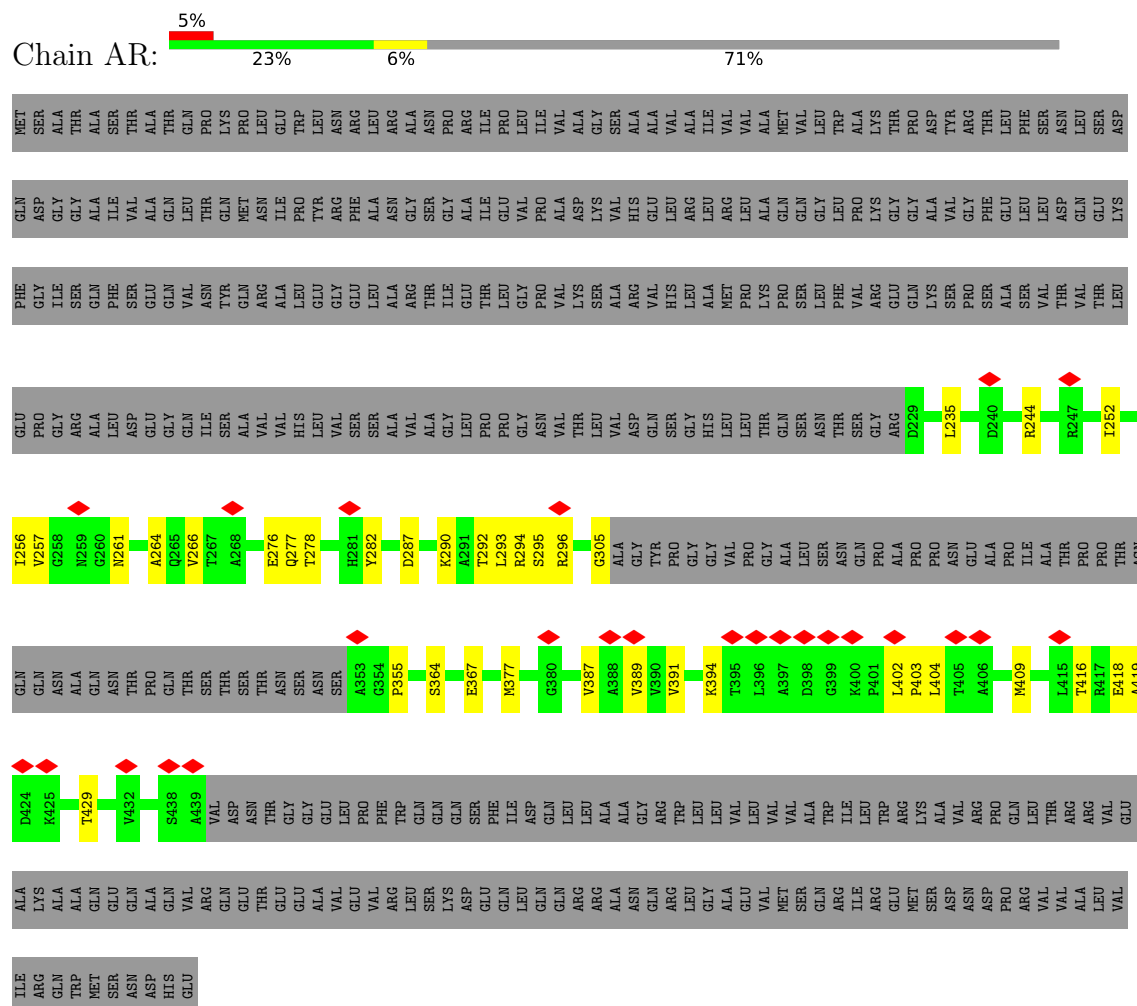


• Molecule 5: Flagellar basal-body rod protein FlgF

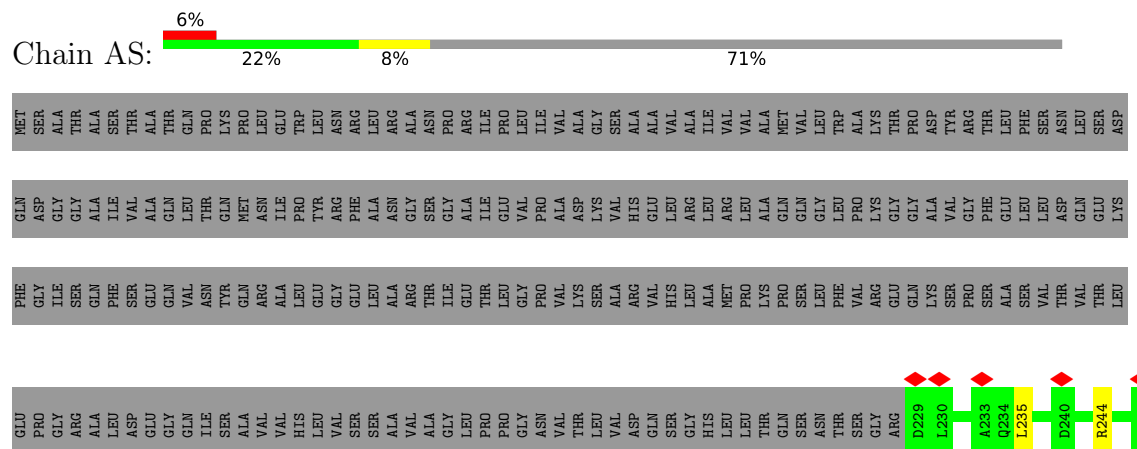




• Molecule 6: Flagellar M-ring protein



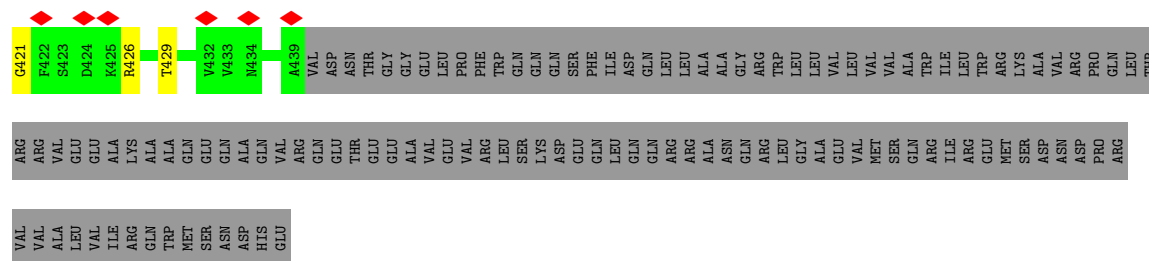
• Molecule 6: Flagellar M-ring protein



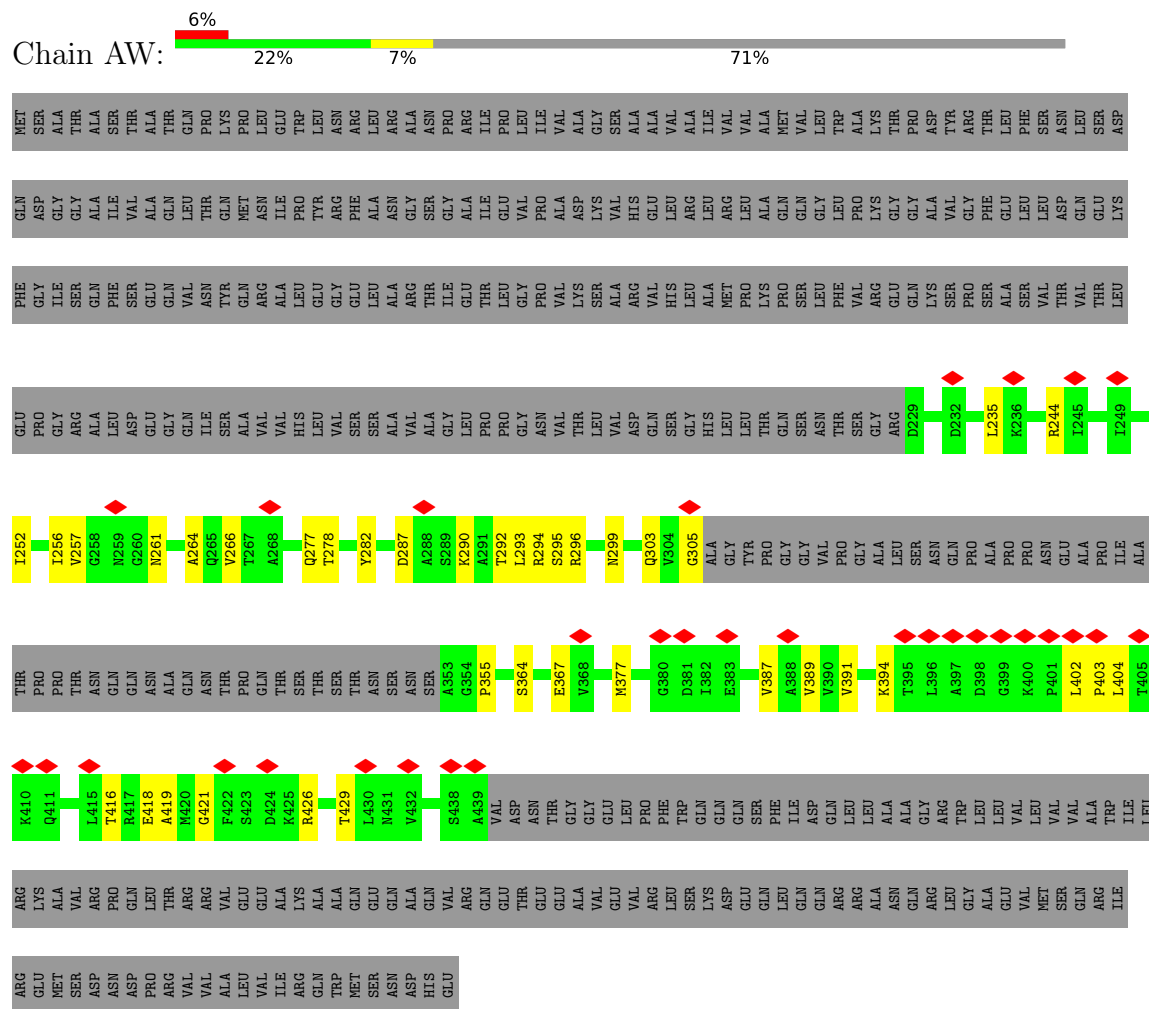




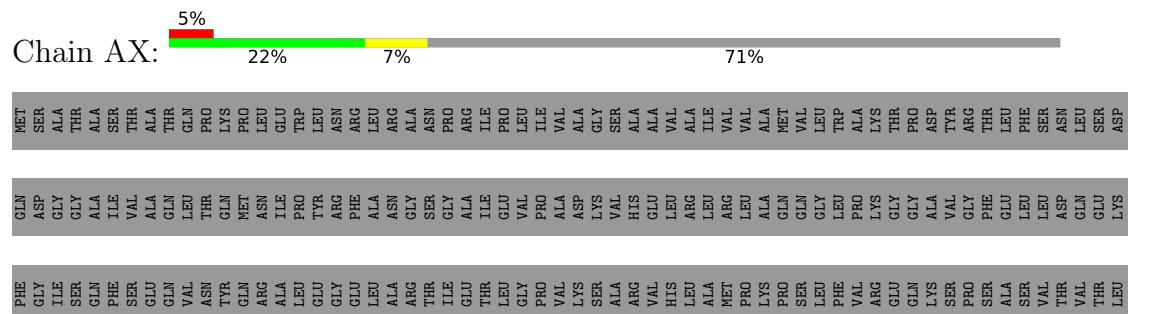




### • Molecule 6: Flagellar M-ring protein

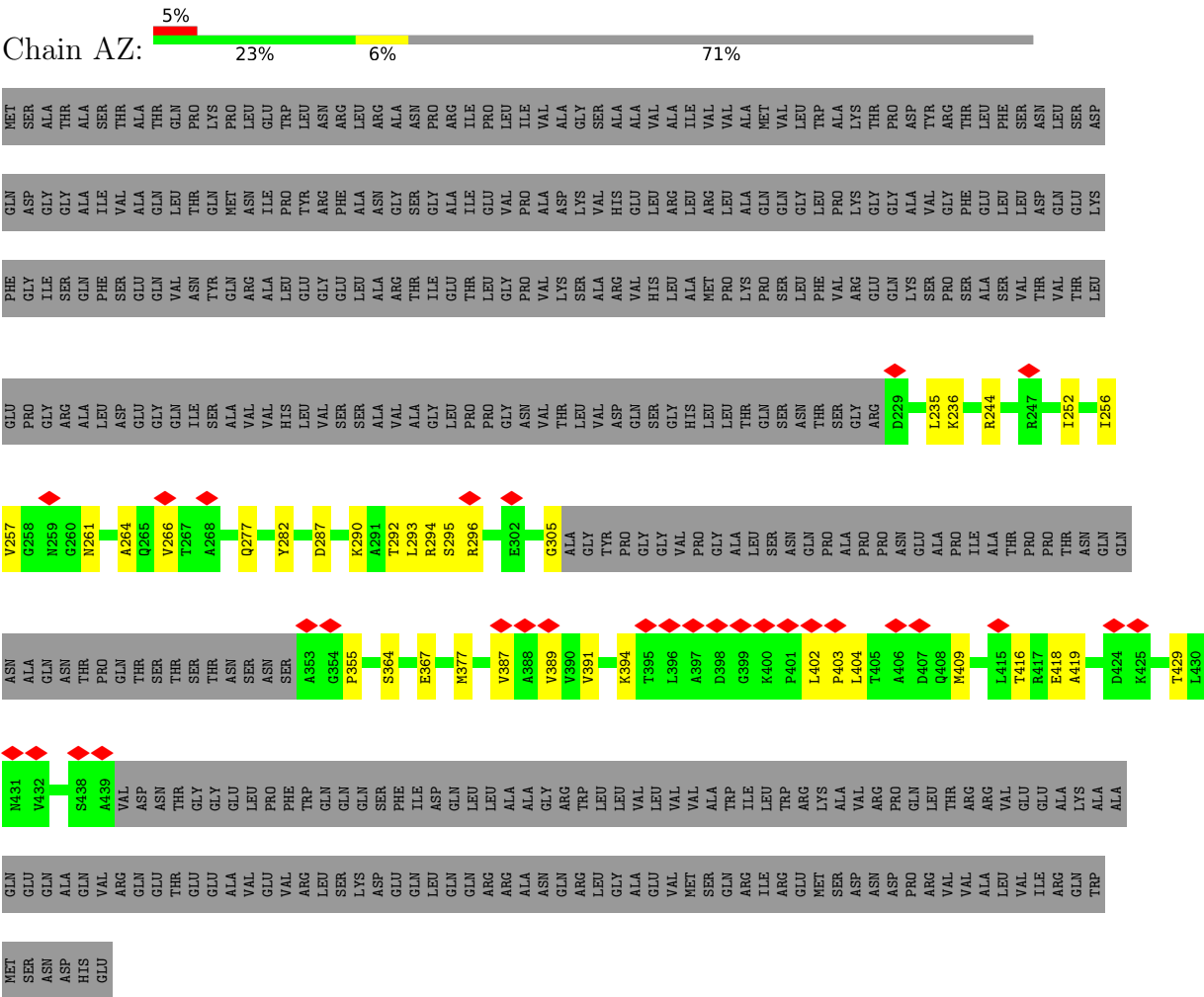


### • Molecule 6: Flagellar M-ring protein

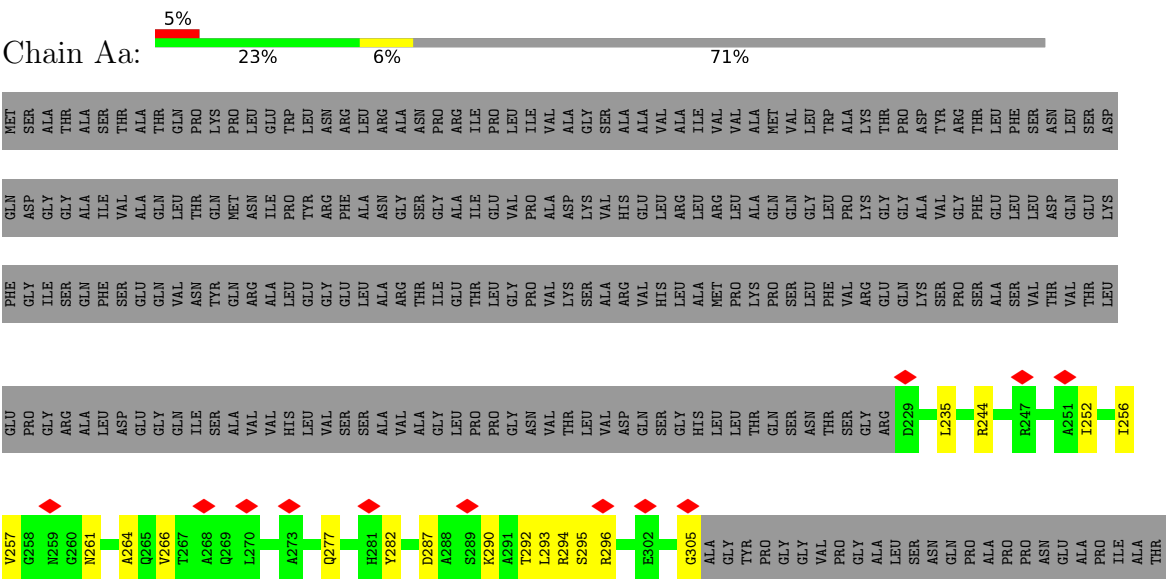




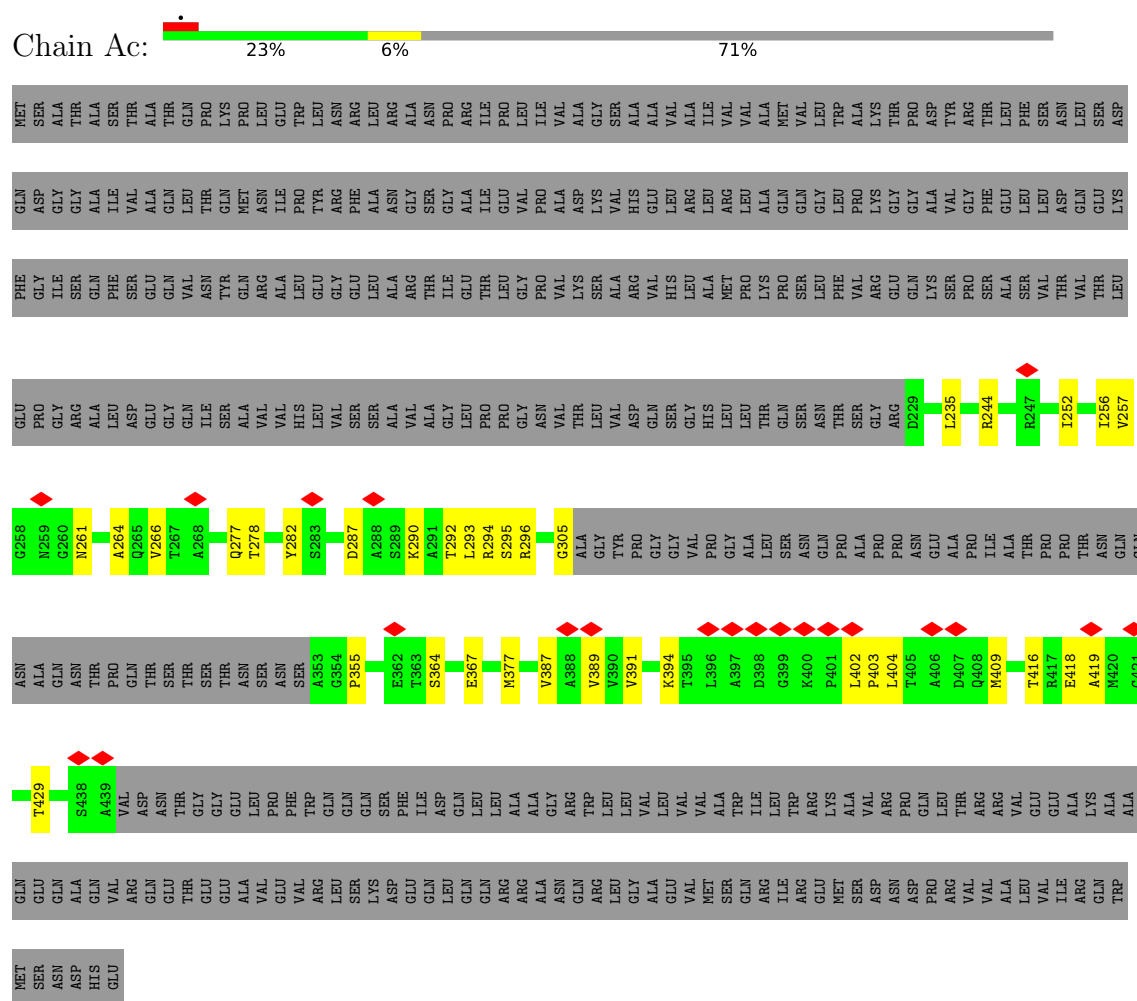
• Molecule 6: Flagellar M-ring protein



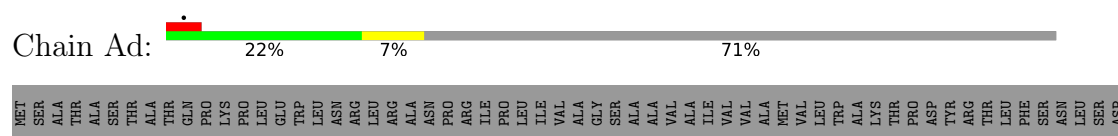
• Molecule 6: Flagellar M-ring protein

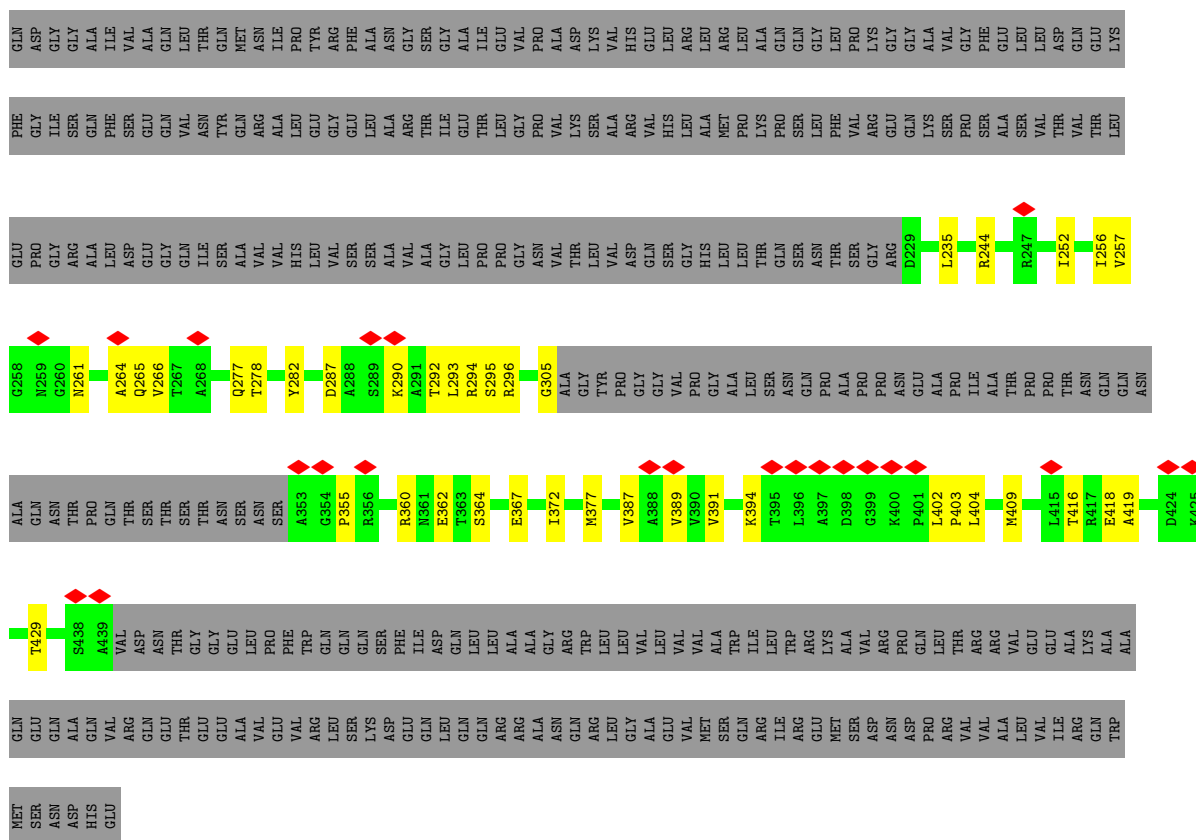


- Molecule 6: Flagellar M-ring protein

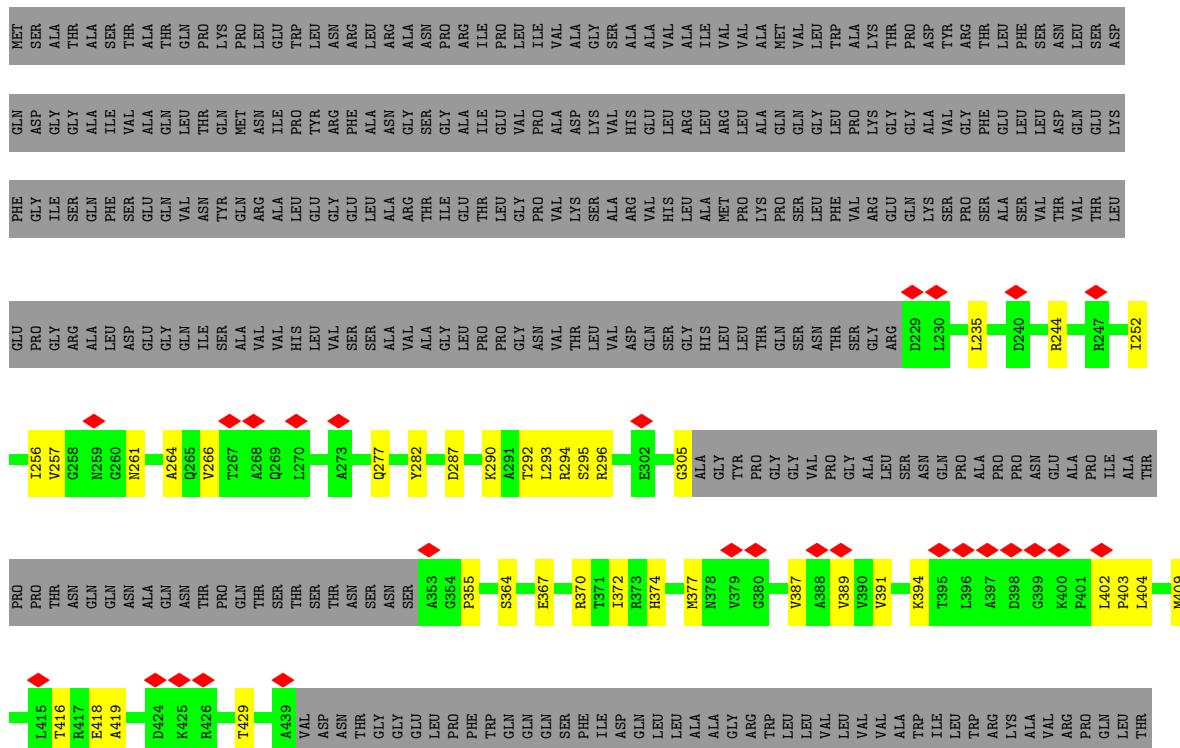


- Molecule 6: Flagellar M-ring protein





- Molecule 6: Flagellar M-ring protein



[illegible]

- Molecule 6: Flagellar M-ring protein



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

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| GLU | PRO | GLY | ARG | ALA | LEU | ASP | GLU | GLN | ILE | SER | VAL | ALA | VAL | VAL | HIS | LEU | VAL | SER | SER | ALA | VAL | GLY | LEU | PRO | PRO | GLY | ASN | VAL | THR | LEU | VAL | ASP | GLN | SER | GLY | HIS | LEU | THR | SER | GLY | ARG | D229 | L235 | D240 | V241 | E242 | S243 | R244 | I252 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| T256 | T257 | G258 | T259 | G260 | T261 | A264 | G265 | T267 | A268 | G269 | Q277 | Y282 | D287 | K290 | A291 | T292 | L293 | R294 | S295 | R296 | Q297 | G305 | ALA | GLY | TTR | PRO | GLY | GLY | VAL | PRO | GLY | ALA | LEU | SER | ASN | GLN | PRO | ALA | PRO | PRO | ASN | GLU | ALA | PRO | ILE | ALA | THR | PRO | PRO | THR | ASN |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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[illegible]

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- Molecule 6: Flagellar M-ring protein



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

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

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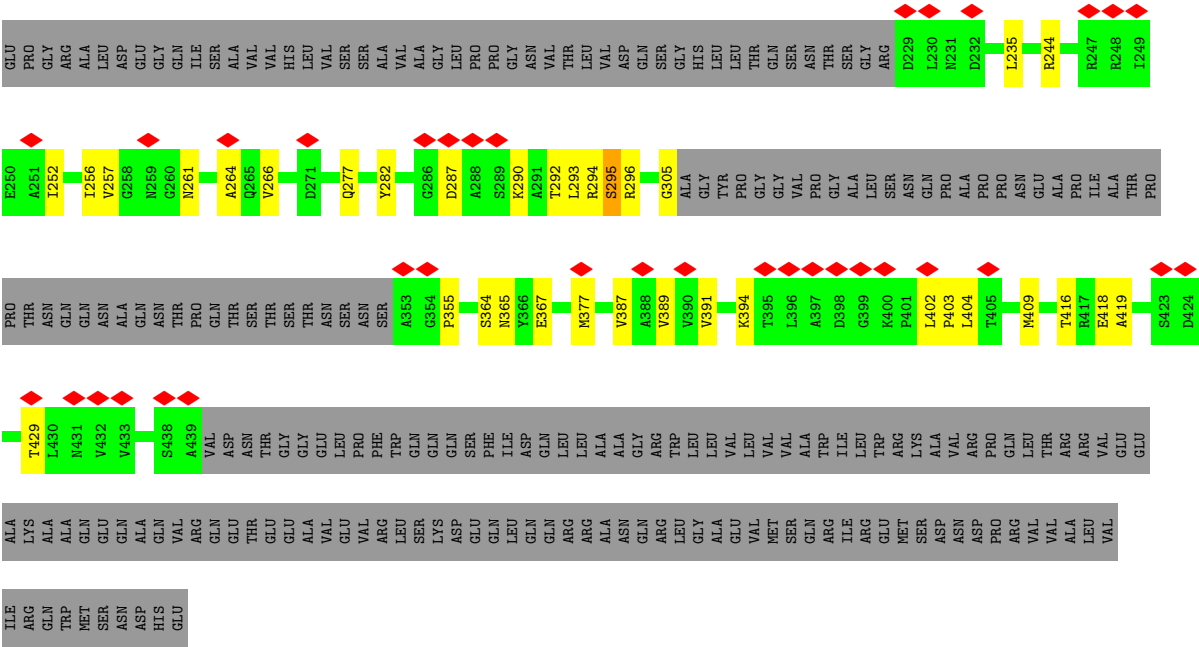
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|
| GLU | PRO | GLY | ARG | ALA | LEU | ASP | GLU | GLY | GLN | ILE | SER | ALA | VAL | VAL | HIS | LEU | VAL | SER | SER | ALA | VAL | VAL | ALA | GLY | LEU | PRO | PRO | GLY | ASN | VAL | THR | LEU | VAL | ASP | GLN | SER | GLY | HIS | LEU | THR | THR | GLN | SER | SER | ASN | THR | SER | GLY | ARG | D229 | L235 | R244 | I252 | I256 | V257 | G258 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|



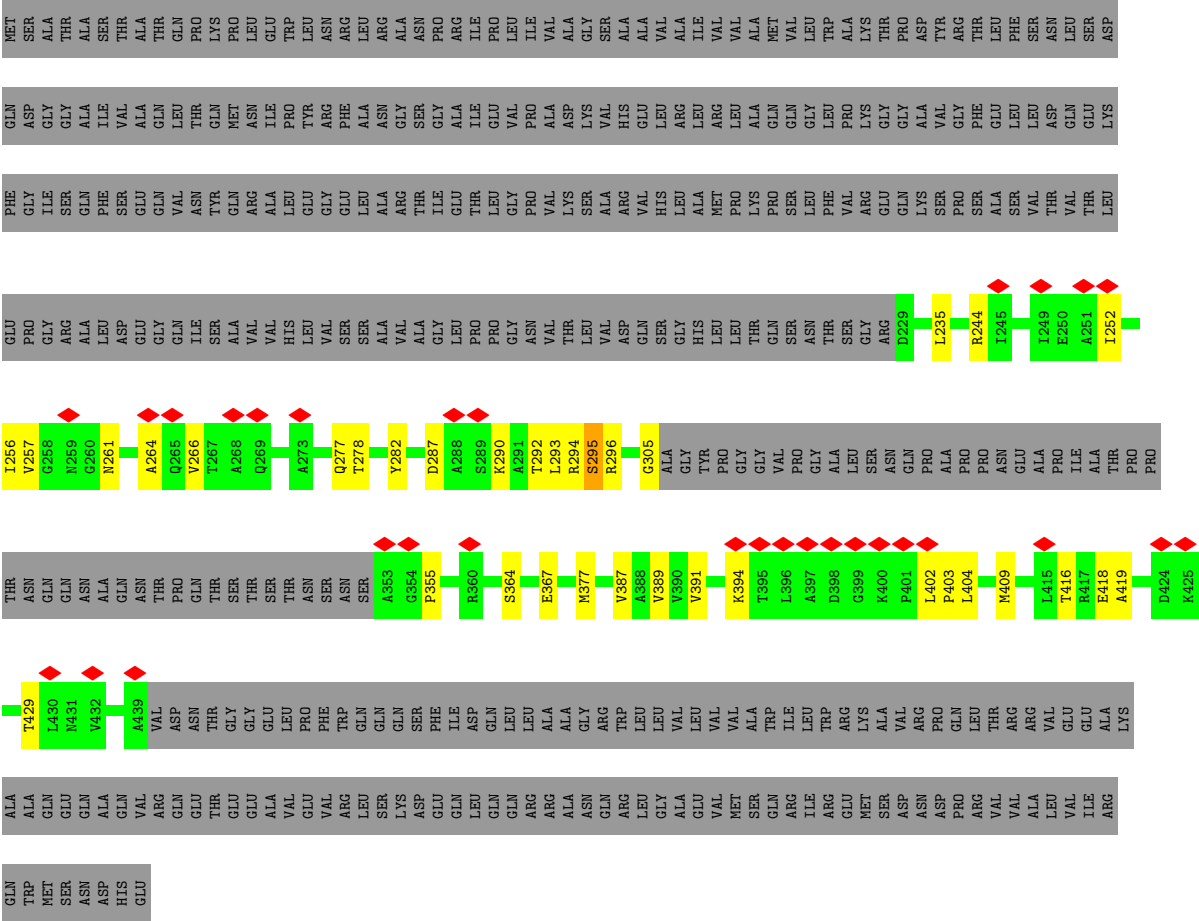








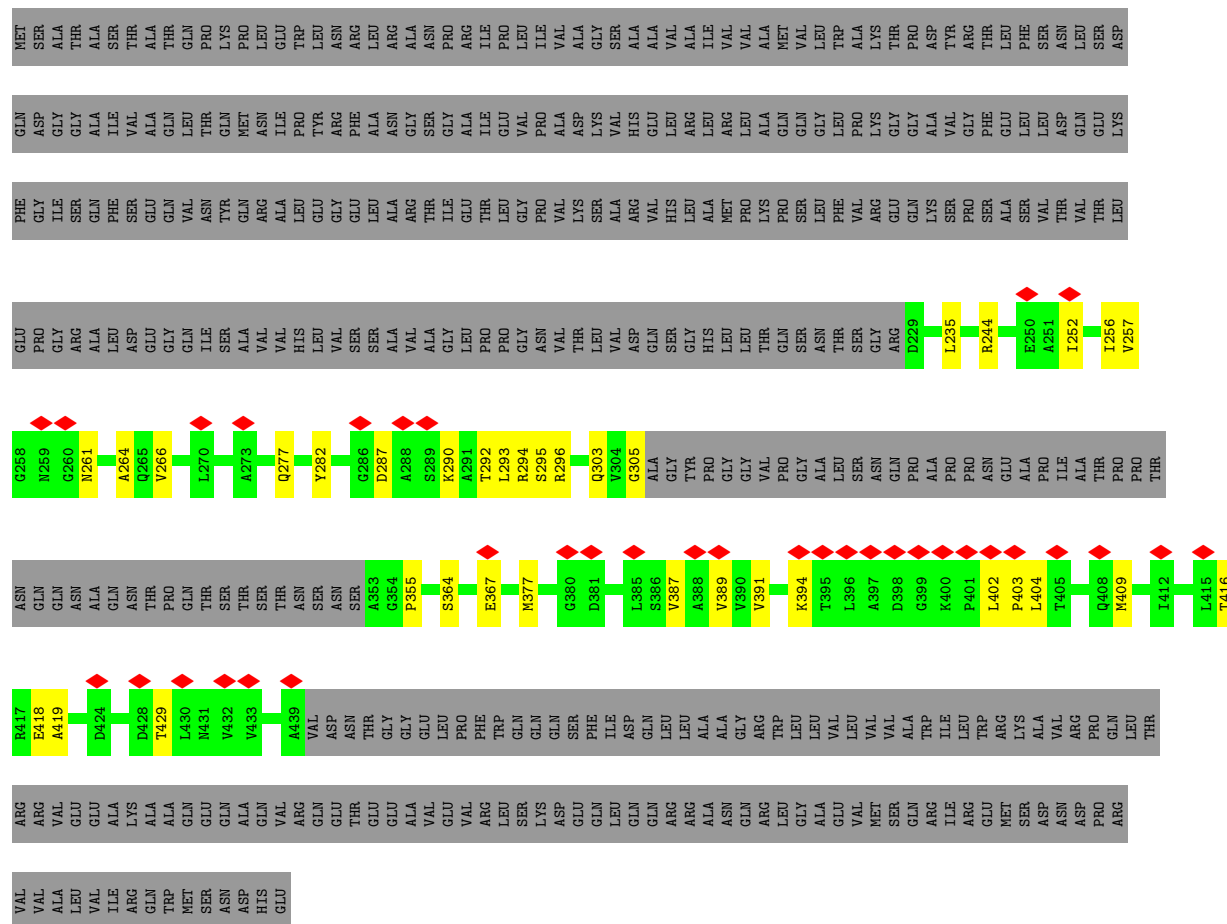
• Molecule 6: Flagellar M-ring protein



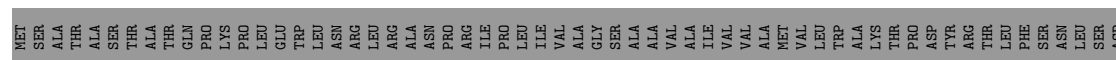


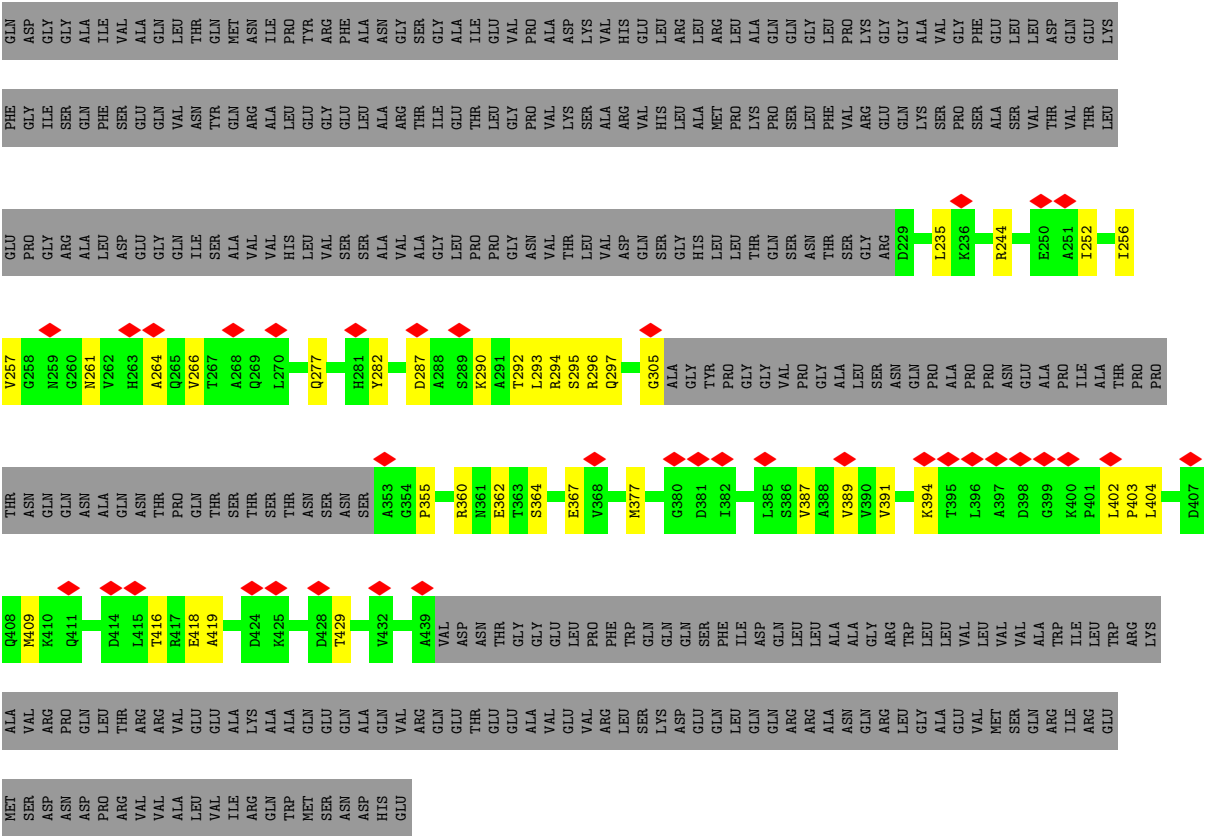
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- Molecule 6: Flagellar M-ring protein

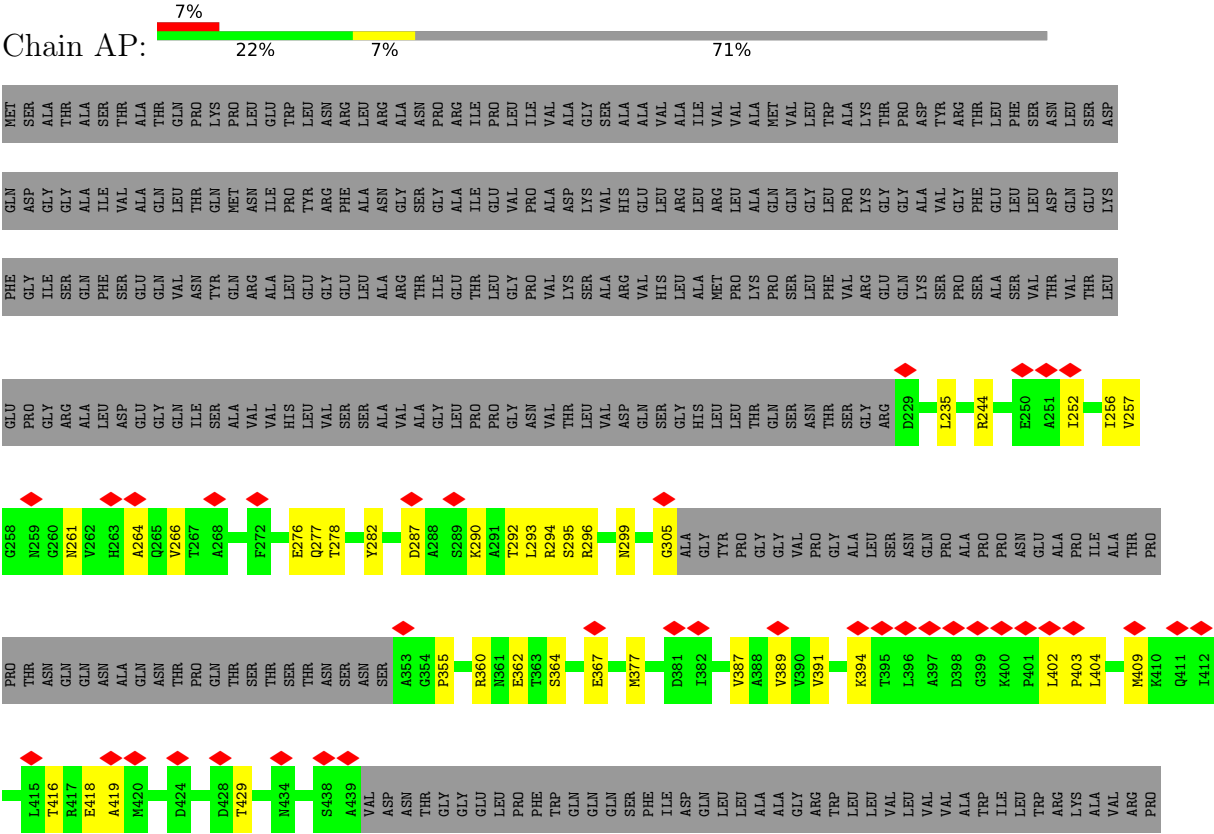


- Molecule 6: Flagellar M-ring protein



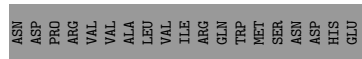


• Molecule 6: Flagellar M-ring protein

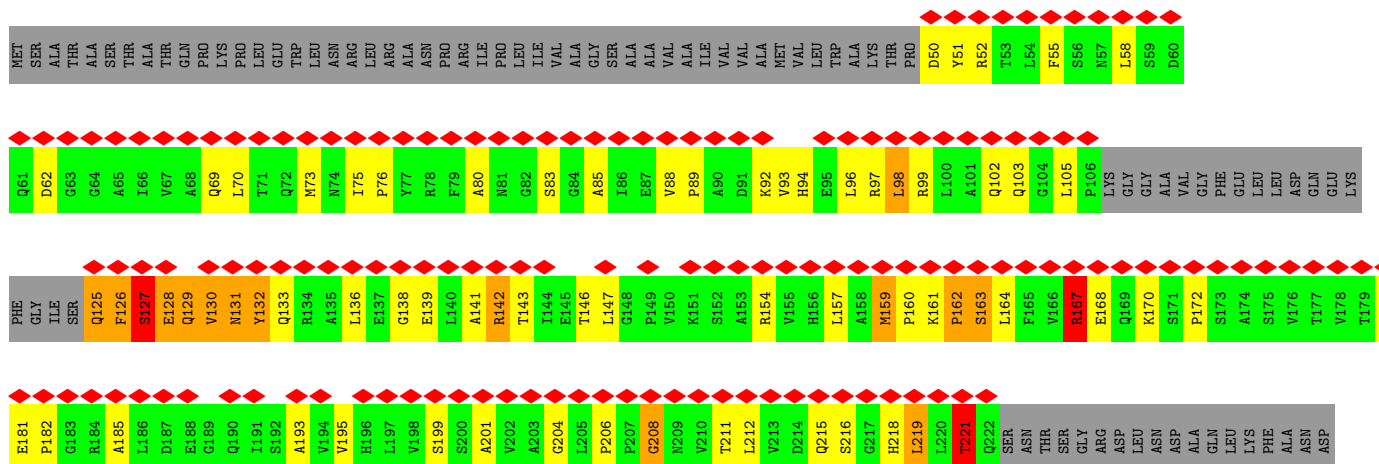








Chain UK: 25% 14% 11% 72%



- Molecule 6: Flagellar M-ring protein

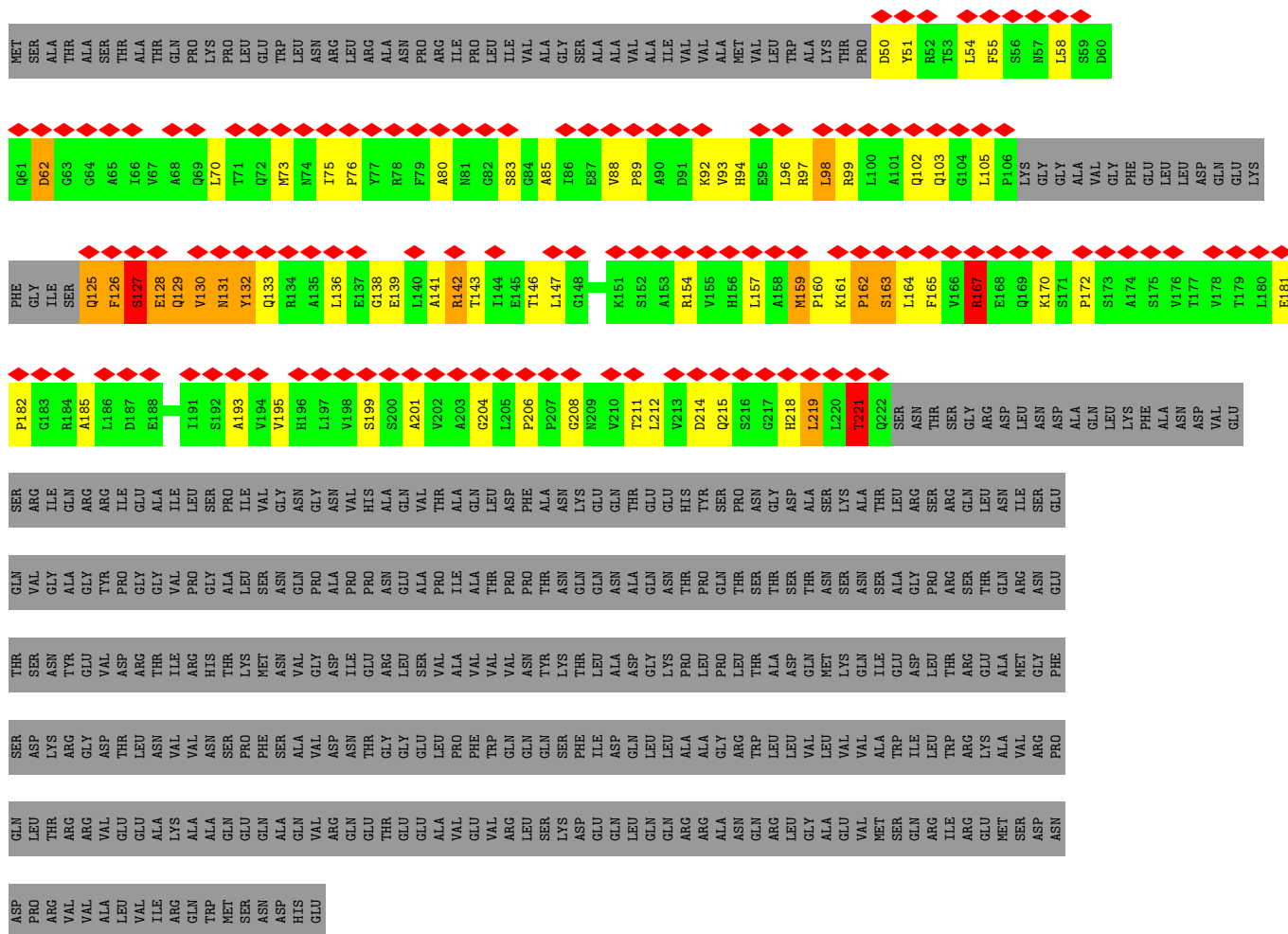


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|-----|-----|-----|-----|-----|-----|------|------|------|-----|
| ASP | ARG | GLY | ASN | SER | VAL | E181 | PHE  | G61  | MET |
| ASN | PRO | PHE | THR | GLN | GLU | P182 | GLY  | D62  | SER |
| ASP | GLN | SER | GLN | SER | VAL | G183 | SER  | G63  | ALA |
| PRO | LEU | LYS | ASN | ASN | GLY | R184 | Q125 | G64  | ALA |
| ARG | THR | ARG | THR | ALA | GLN | A185 | F126 | A65  | SER |
| VAL | ARG | GLY | GLU | GLY | ARG | L186 | S127 | I66  | THR |
| VAL | VAL | ASP | VAL | VAL | ARG | D187 | E128 | I67  | ALA |
| ALA | GLU | THR | GLU | GLY | GLU | E188 | Q129 | A68  | GLN |
| VAL | GLU | LEU | ARG | GLY | ALA | E189 | V130 | G69  | PRO |
| ILE | ALA | ASN | THR | GLY | VAL | Q190 | N131 | L70  | LYS |
| ARG | LYS | VAL | ILE | VAL | ILE | Q191 | Y132 | T71  | PRO |
| GLN | ALA | ASN | SER | GLY | SER | I191 | Q133 | Q72  | LEU |
| TRP | GLN | SER | THR | ALA | PRO | S192 | Q133 | M73  | LEU |
| ASN | GLN | PHE | LYS | ILE | ILE | A193 | R134 | I74  | TRP |
| ASN | ALA | SER | ASN | SER | VAL | V194 | A135 | I75  | ASN |
| ASP | ALA | SER | ASN | ASN | GLY | V195 | L136 | P76  | ARG |
| HIS | GLN | VAL | VAL | PRO | GLY | H196 | E137 | I77  | ARG |
| GLU | VAL | VAL | GLY | ALA | ASN | L197 | G138 | I78  | ALA |
| GLN | GLN | ASN | ASP | PRO | VAL | V198 | E139 | I79  | ASN |
| GLU | GLU | THR | GLU | PRO | HIS | S199 | A140 | I80  | PRO |
| THR | THR | GLY | ARG | ASN | GLN | S200 | L141 | A80  | ARG |
| GLU | GLU | GLY | LEU | GLU | VAL | A201 | R142 | N81  | PRO |
| GLU | GLU | LEU | SER | ALA | THR | T202 | T143 | G82  | ILE |
| ALA | ALA | PRO | VAL | ILE | ALA | V203 | I144 | S83  | LEU |
| PHE | PHE | THR | VAL | ALA | GLN | A203 | E145 | G84  | VAL |
| VAL | VAL | TRP | VAL | THR | LEU | G204 | T146 | A85  | ALA |
| ARG | ARG | GLN | VAL | PRO | ASP | L205 | Y146 | I86  | GLY |
| LEU | LEU | GLN | ASN | PRO | PHE | T206 | L147 | I87  | SER |
| GLN | GLN | GLN | VAL | THR | ALA | P207 | G148 | I88  | ALA |
| SER | SER | SER | LYS | ASN | ASN | G208 | P149 | E87  | ALA |
| LYS | ASP | PHE | THR | GLN | LYS | P209 | V150 | V88  | ALA |
| GLU | GLU | ILE | LEU | GLN | GLU | G210 | K151 | P89  | VAL |
| ASP | GLN | ASP | ALA | ASN | GLN | N209 | S152 | A90  | ILE |
| GLN | GLN | LEU | GLY | ALA | GLU | V210 | A153 | D91  | VAL |
| GLN | GLN | LEU | LEU | ASN | GLU | T211 | R154 | K92  | VAL |
| ARG | ARG | ALA | PRO | THR | HIS | L212 | V155 | V93  | ALA |
| ALA | ALA | GLY | LEU | PRO | TYR | V213 | I156 | H94  | MET |
| GLY | GLY | ARG | PRO | GLN | SER | D214 | H156 | I95  | VAL |
| ARG | ARG | GLY | THR | GLN | THR | Q215 | L157 | E95  | LEU |
| TRP | TRP | LEU | THR | SER | ASN | S216 | A158 | I96  | TRP |
| LEU | LEU | LEU | ASP | THR | GLY | G217 | M159 | A97  | LYS |
| VAL | VAL | VAL | GLN | THR | ALA | H218 | P160 | L98  | PRO |
| ALA | ALA | GLN | LYS | SER | LYS | L219 | K161 | R99  | LYS |
| VAL | VAL | VAL | GLN | ASN | ALA | L220 | P162 | I100 | PRO |
| MET | MET | ALA | ILE | ASN | THR | T221 | S163 | A101 | LYS |
| SER | SER | TRP | GLU | ALA | LEU | Q222 | L164 | Q102 | THR |
| ILE | ILE | ILE | ASP | GLY | ARG | SER  | F165 | Q103 | ALA |
| LEU | LEU | LEU | LEU | PRO | SER | ASN  | V166 | I104 | F55 |
| TRP | TRP | TRP | THR | ARG | ARG | THR  | R167 | L105 | S56 |
| ARG | ARG | ARG | ARG | SER | GLN | SER  | E168 | P106 | S57 |
| LYS | LYS | LYS | GLU | THR | LEU | GLY  | Q169 | I57  | S58 |
| ALA | ALA | ALA | ALA | GLN | ASN | ARG  | K170 | L58  | S59 |
| VAL | VAL | VAL | MET | ASN | LEU | ASP  | I171 | D60  |     |
| SER | SER | SER | SER | ASN | ILE | ASP  | Y172 |      |     |
|     |     |     |     | ALA |     | ALA  |      |      |     |
|     |     |     |     | GLN |     | GLN  |      |      |     |
|     |     |     |     | LYS |     | LYS  |      |      |     |
|     |     |     |     | PHE |     | PHE  |      |      |     |
|     |     |     |     | LEU |     | LEU  |      |      |     |
|     |     |     |     | LEU |     | LEU  |      |      |     |
|     |     |     |     | ASP |     | ASP  |      |      |     |
|     |     |     |     | ALA |     | ALA  |      |      |     |
|     |     |     |     | GLN |     | GLN  |      |      |     |
|     |     |     |     | GLY |     | GLY  |      |      |     |
|     |     |     |     | THR |     | THR  |      |      |     |
|     |     |     |     | GLU |     | GLU  |      |      |     |
|     |     |     |     | GLN |     | GLN  |      |      |     |
|     |     |     |     | ASP |     | ASP  |      |      |     |
|     |     |     |     | LYS |     | LYS  |      |      |     |
|     |     |     |     | TRP |     | TRP  |      |      |     |
|     |     |     |     | VAL |     | VAL  |      |      |     |
|     |     |     |     | GLN |     | GLN  |      |      |     |
|     |     |     |     | ARG |     | ARG  |      |      |     |
|     |     |     |     | LEU |     | LEU  |      |      |     |
|     |     |     |     | GLY |     | GLY  |      |      |     |
|     |     |     |     | ALA |     | ALA  |      |      |     |
|     |     |     |     | VAL |     | VAL  |      |      |     |
|     |     |     |     | TRP |     | TRP  |      |      |     |
|     |     |     |     | SER |     | SER  |      |      |     |
|     |     |     |     | THR |     | THR  |      |      |     |
|     |     |     |     | LEU |     | LEU  |      |      |     |
|     |     |     |     | GLN |     | GLN  |      |      |     |
|     |     |     |     | ASN |     | ASN  |      |      |     |
|     |     |     |     | ASP |     | ASP  |      |      |     |
|     |     |     |     | HIS |     | HIS  |      |      |     |
|     |     |     |     | GLU |     | GLU  |      |      |     |

- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein

| Frequency | Percentage |
|-----------|------------|
| Daily     | 11%        |
| Weekly    | 8%         |
| Monthly   | 80%        |
| Other     | 1%         |

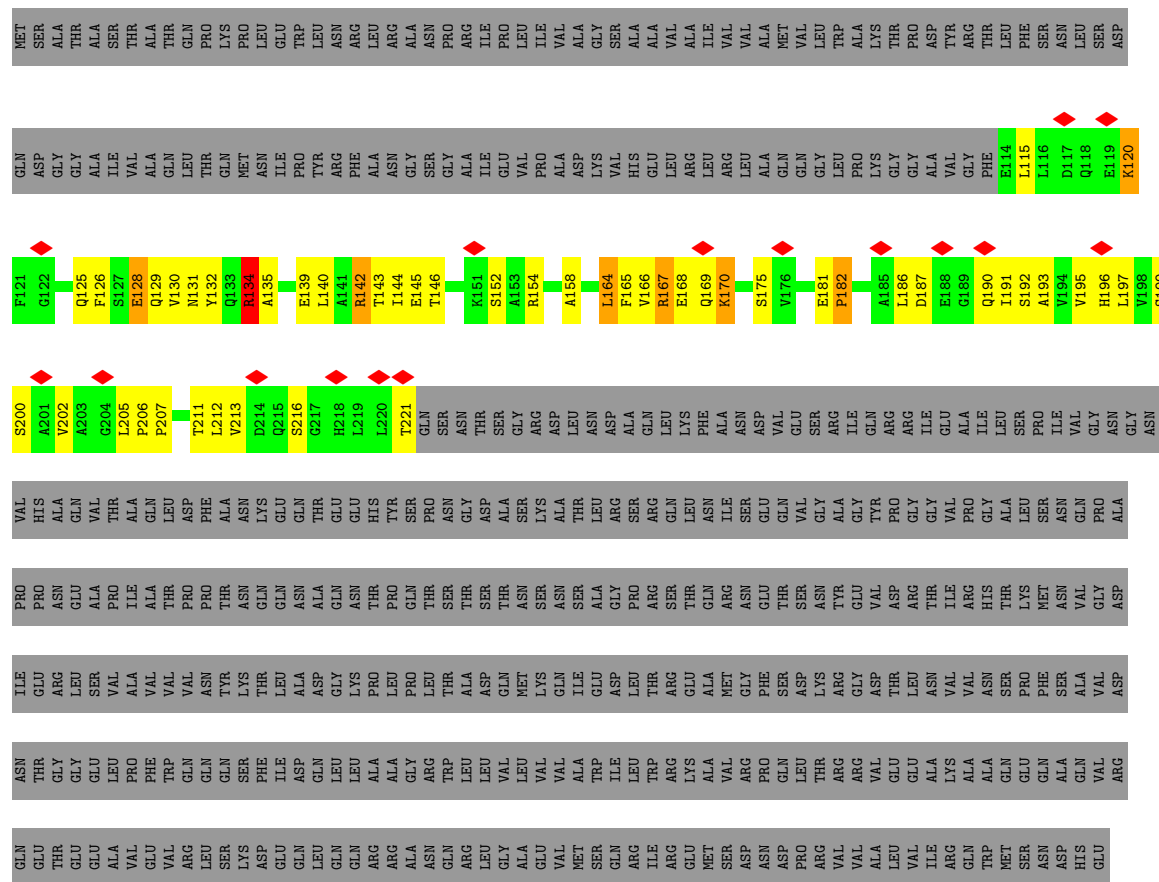


| Category            | Percentage |
|---------------------|------------|
| Category 1 (Red)    | 10%        |
| Category 2 (Green)  | 8%         |
| Category 3 (Yellow) | 80%        |

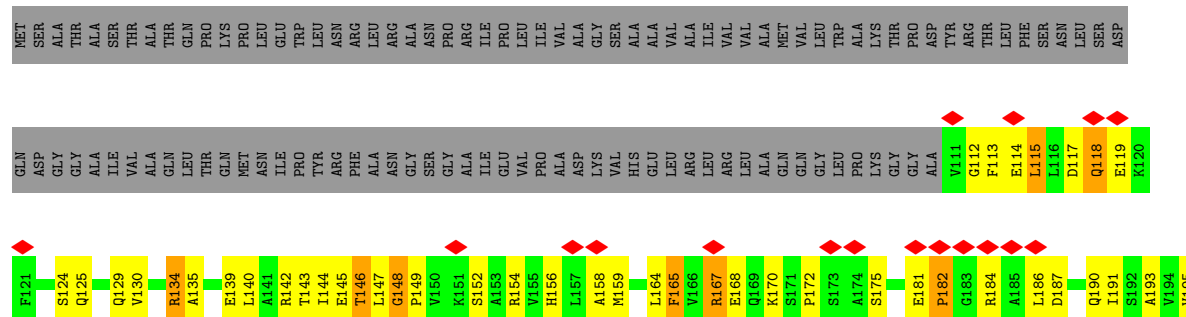




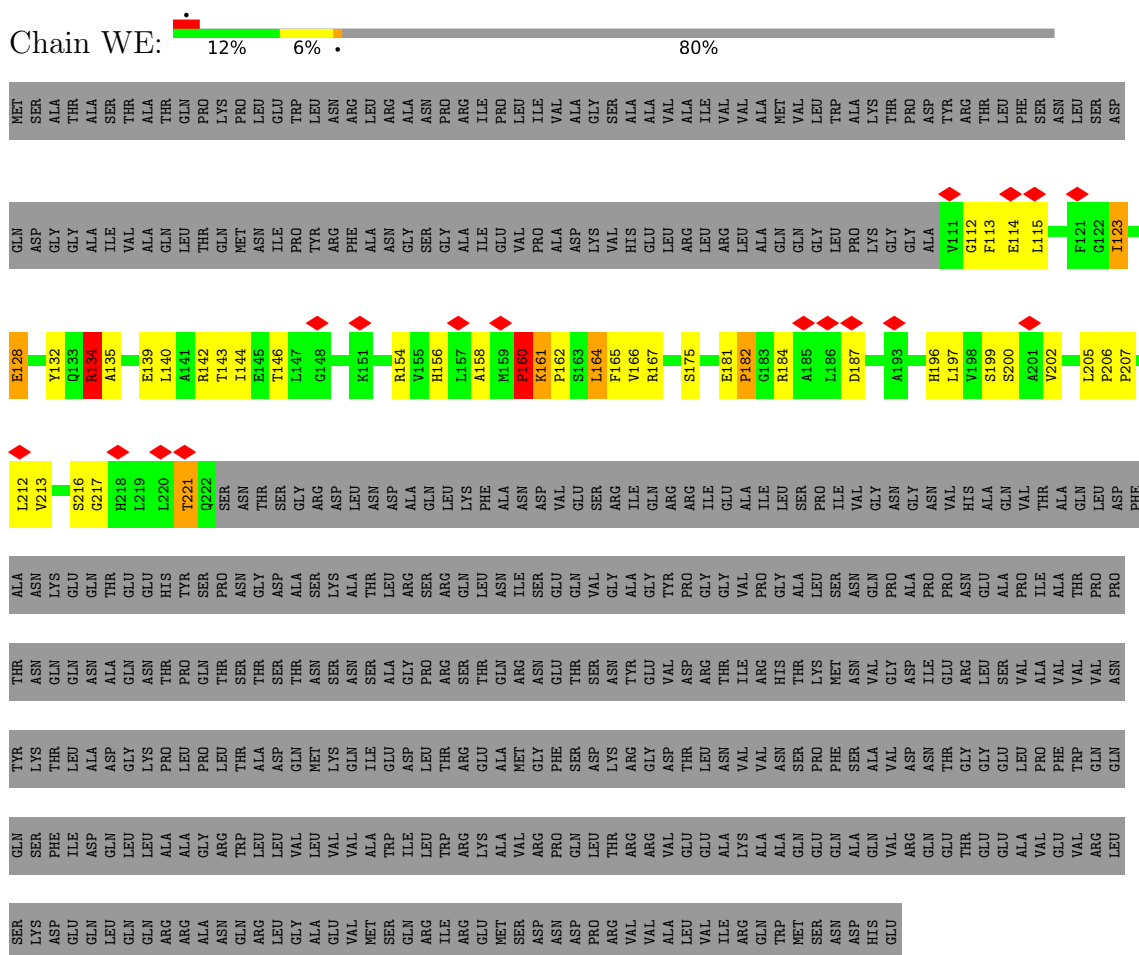
- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein







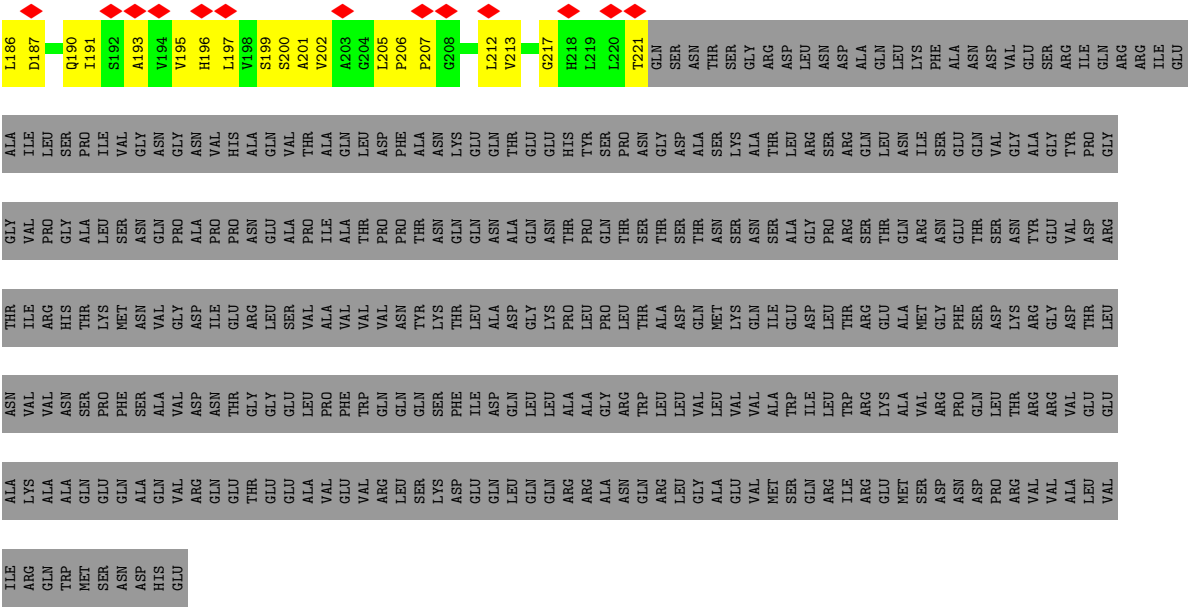
- Molecule 6: Flagellar M-ring protein

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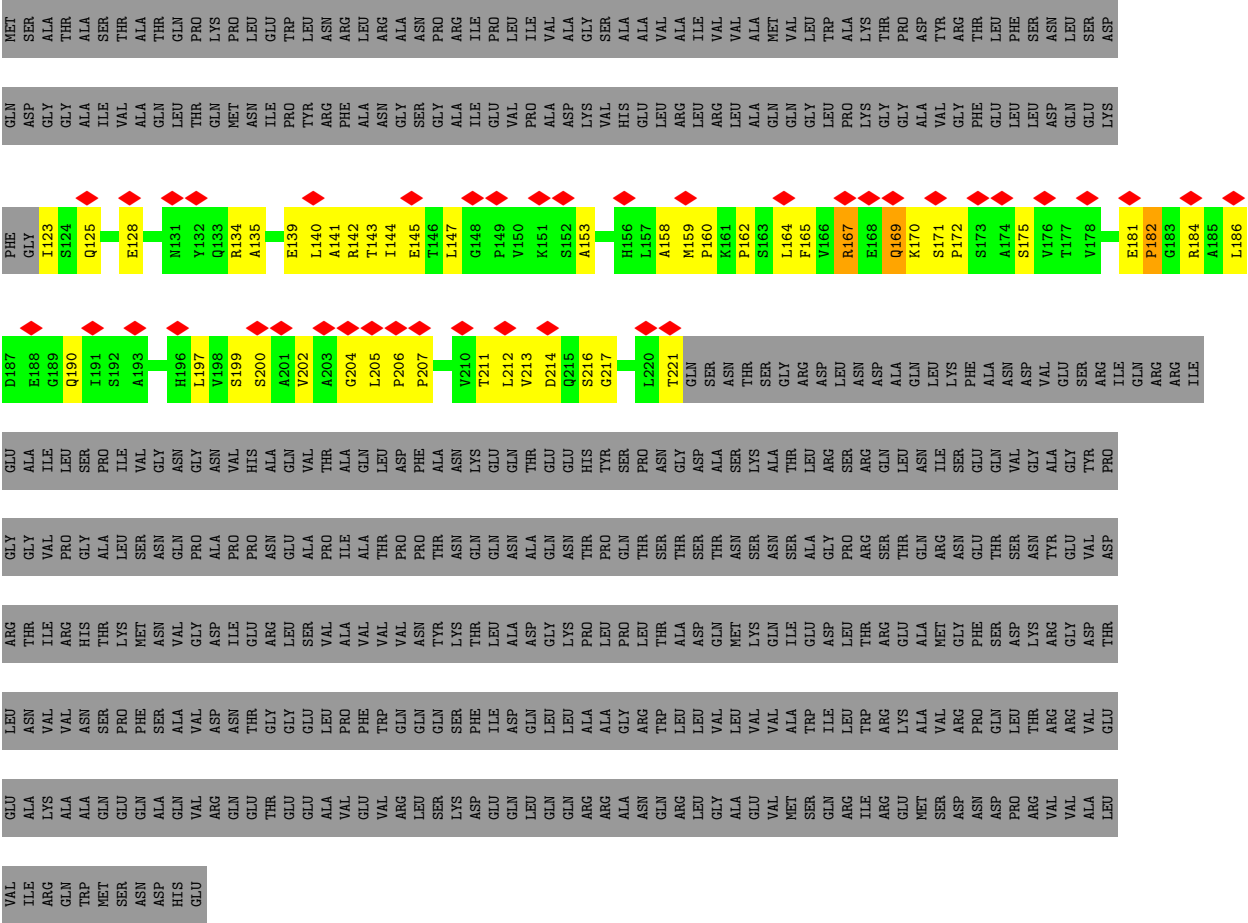
- Molecule 6: Flagellar M-ring protein



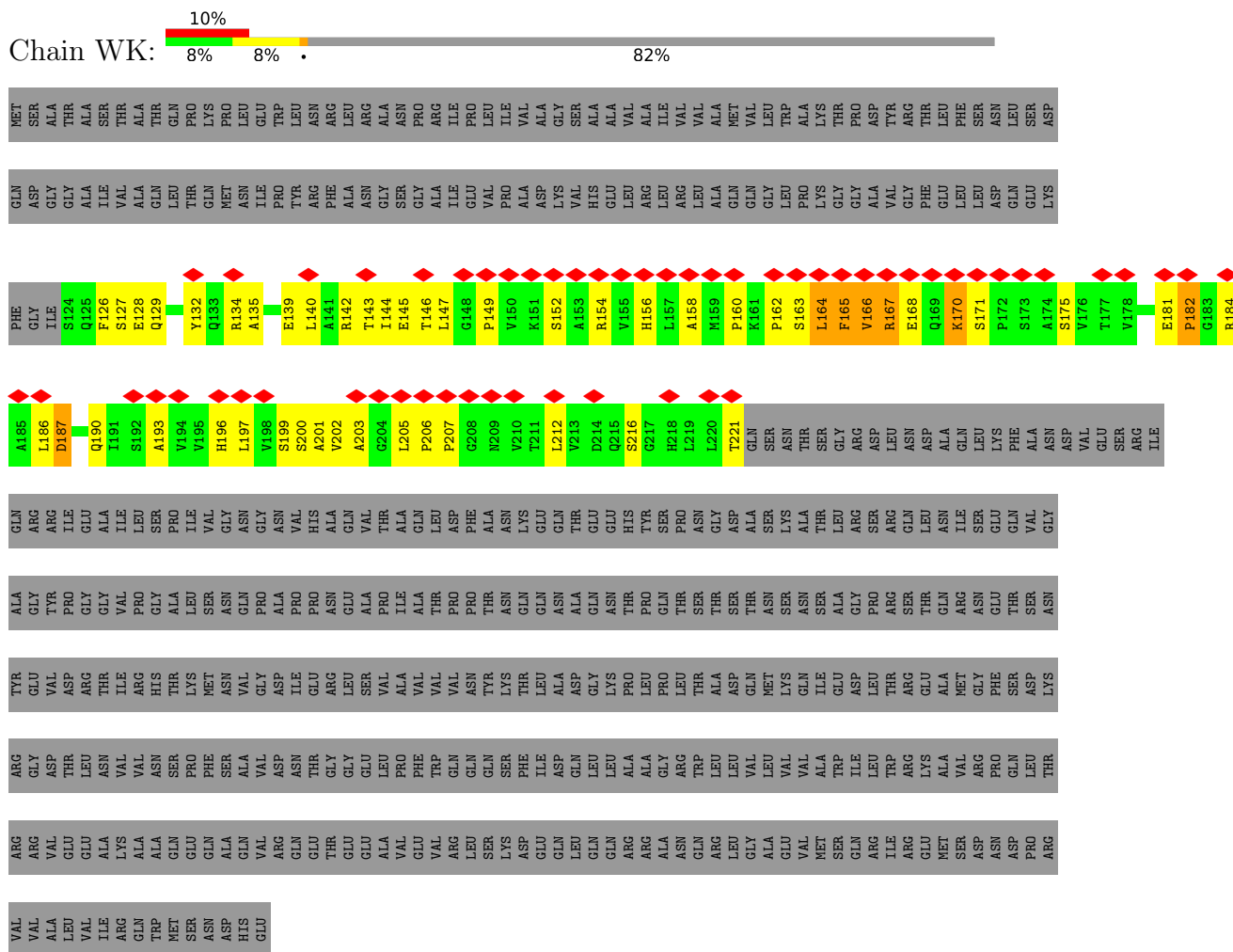
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|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|
| PHE | GLY | ILE | SER | GLN | PHE | S127 | E128 | Q129 | Y132 | Q133 | R134 | A135 | L136 | E137 | G138 | E139 | L140 | A141 | T142 | I144 | E145 | T146 | L147 | G148 | K151 | S152 | A153 | R154 | V155 | H156 | L157 | A158 | M159 | P160 | K161 | P162 | S163 | L164 | P165 | V166 | R167 | E168 | Q169 | S171 | P172 | T173 | A174 | S175 | V176 | E181 | P182 | G183 | R184 | A185 |     |     |     |     |     |
| NET | SER | THR | ALA | GLY | SER | THR  | ALA  | GLN  | THR  | LYS  | PRO  | PRO  | LEU  | TRP  | LEU  | ASN  | ARG  | LEU  | ASN  | ARG  | ALA  | ASN  | GLY  | ILE  | PRO  | LEU  | VAL  | GLY  | ALA  | VAL  | VAL  | VAL  | ILE  | VAL  | VAL  | ALA  | ALA  | VAL  | VAL  | GLN  | GLY  | LEU  | TRP  | ALA  | LYS  | THR  | PRO  | ASP  | TYR  | ARG  | THR  | THR  | LEU  | PHE  | SER | ASN | LEU | SER | ASP |



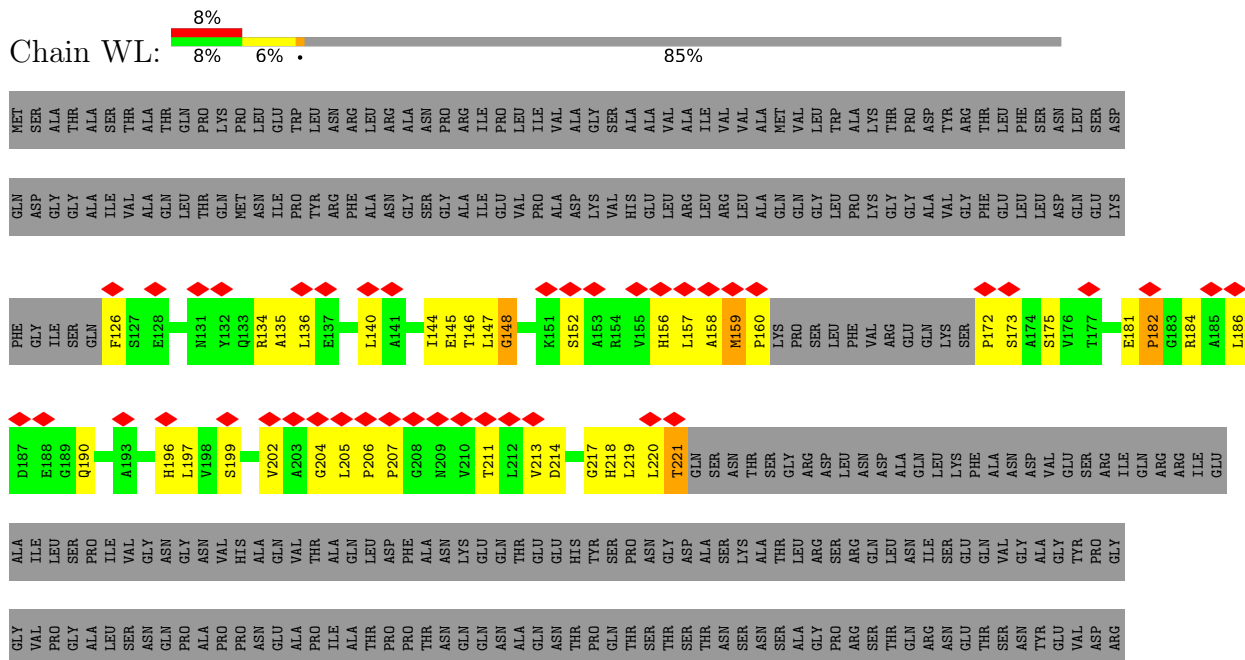
• Molecule 6: Flagellar M-ring protein



• Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



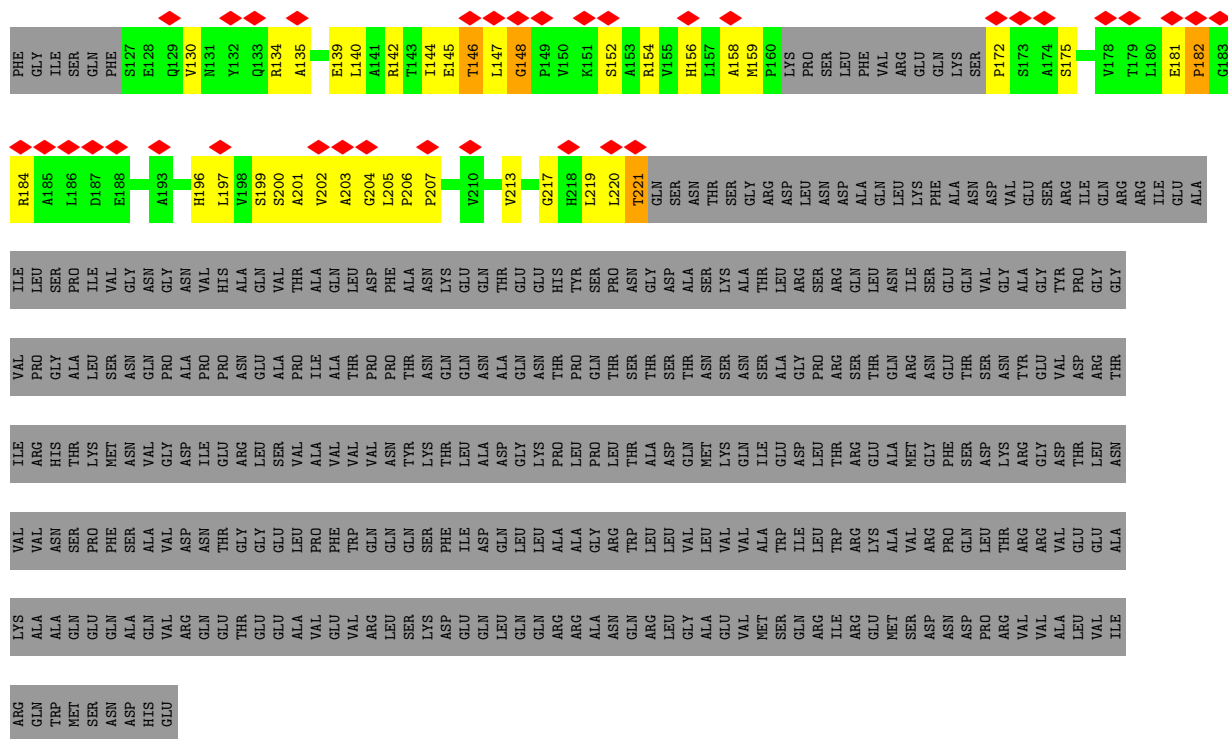
[illegible]

- Molecule 6: Flagellar M-ring protein

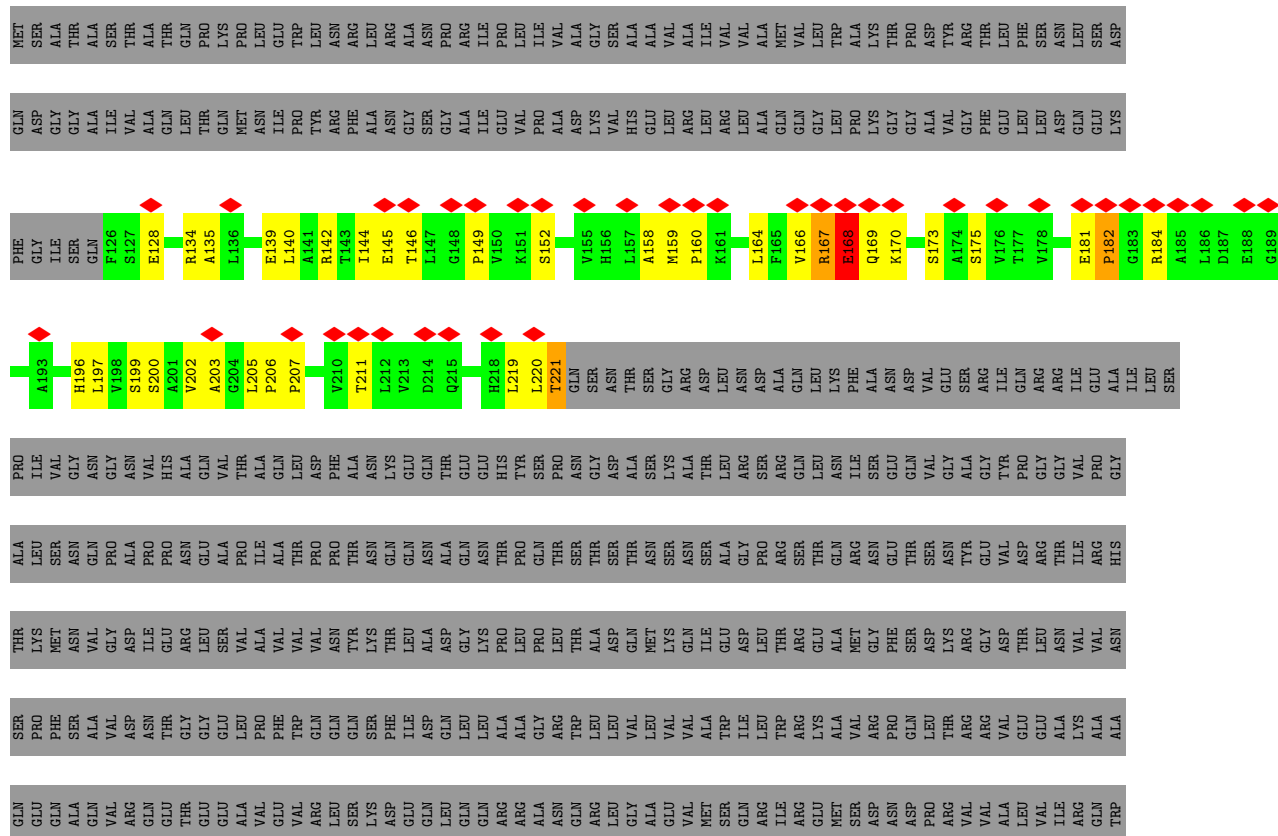
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- Molecule 6: Flagellar M-ring protein

[illegible]



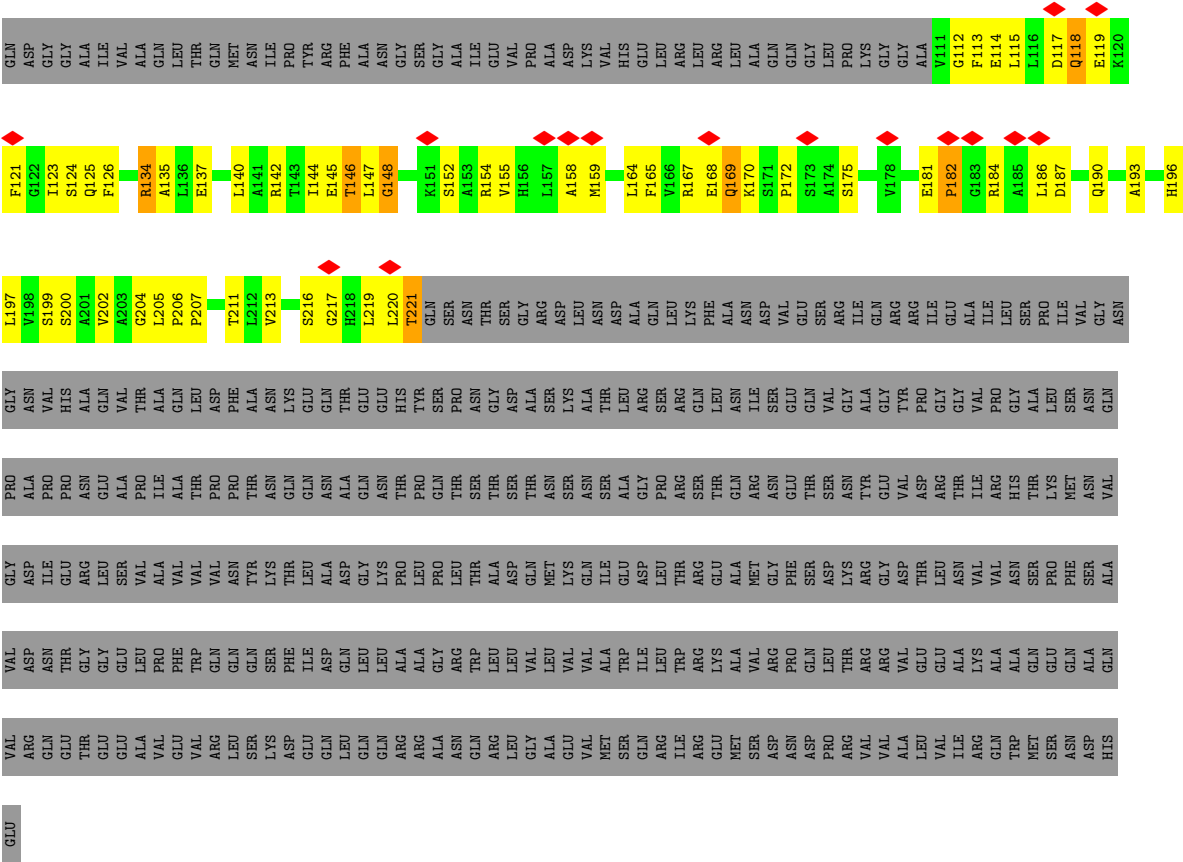
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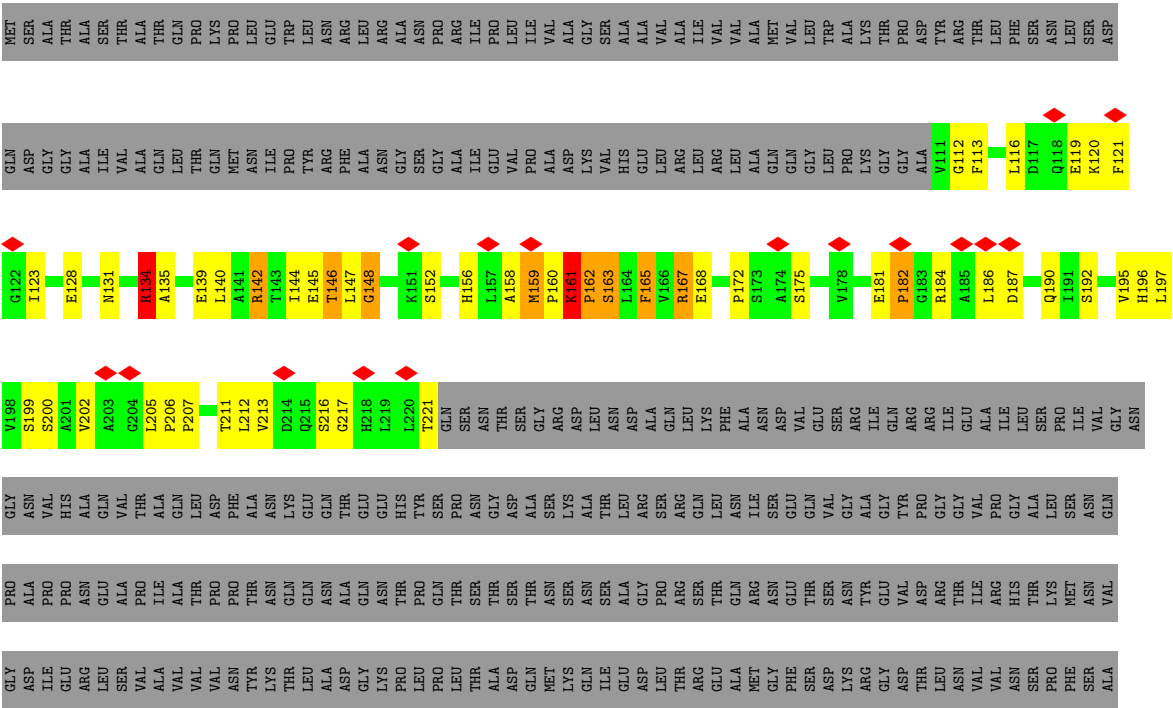








• Molecule 6: Flagellar M-ring protein



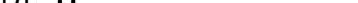






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- Molecule 6: Flagellar M-ring protein

Chain BI:  96%

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

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

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

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

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

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| SER | GLU | GLN | VAL | GLY | ALA | GLY | TYR | PRO | GLY | S311 | A315 | L316 | S317 | N318 | Q319 | P320 | N324 | E325 | A326 | P327 | L328 | A329 | T330 | PRO | PRO | THR | THR | ASN | GLN | GLN | ASN | ALA | GLN | ASN | THR | PRO | THR | GLN | THR | SER | THR | SER | THR | THR | ASN | SER | SER | ALA | GLY | PRO | ARG | SER | THR | GLN | ARG | ASN | GLU | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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

LYS ARG GLY ASP THR LEU ASN VAL VAL ASN ASP SER PRO PHE SER ALA VAL ASP ASN THR GLY GLU LEU PRO PHE TRP TRP LEU LEU VAL VAL VAL ALA ALA GLY ARG TRP LEU LEU VAL VAL VAL ALA ALA LYS ARG ARG PRO GLN LEU

[illegible]

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

- Molecule 6: Flagellar M-ring protein

Chain BJ:  97%

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

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

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

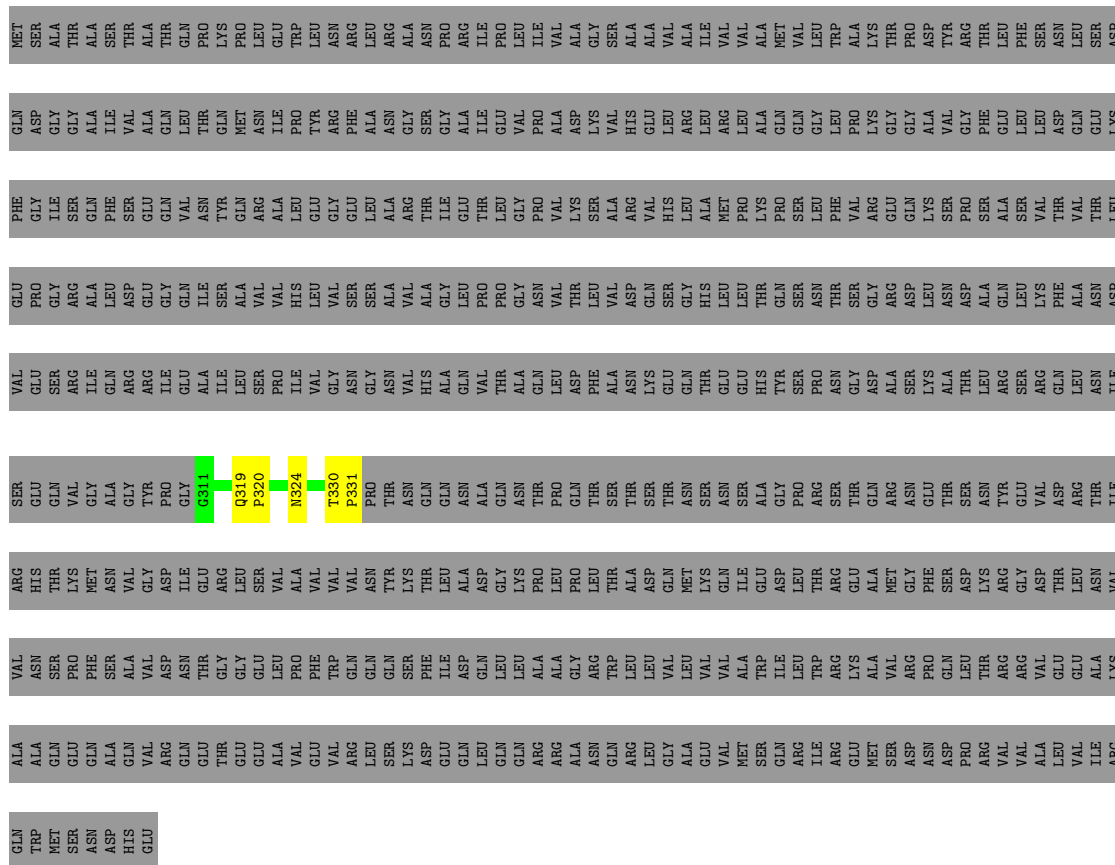
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |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

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

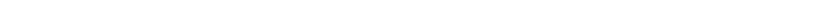


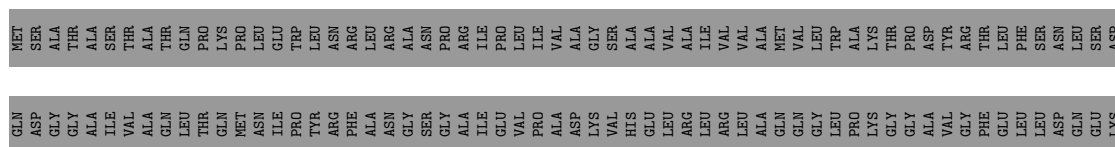
- Molecule 6: Flagellar M-ring protein

Chain BK:  96%



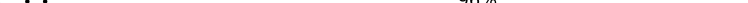
- Molecule 6: Flagellar M-ring protein

Chain BL:  97%



[illegible]

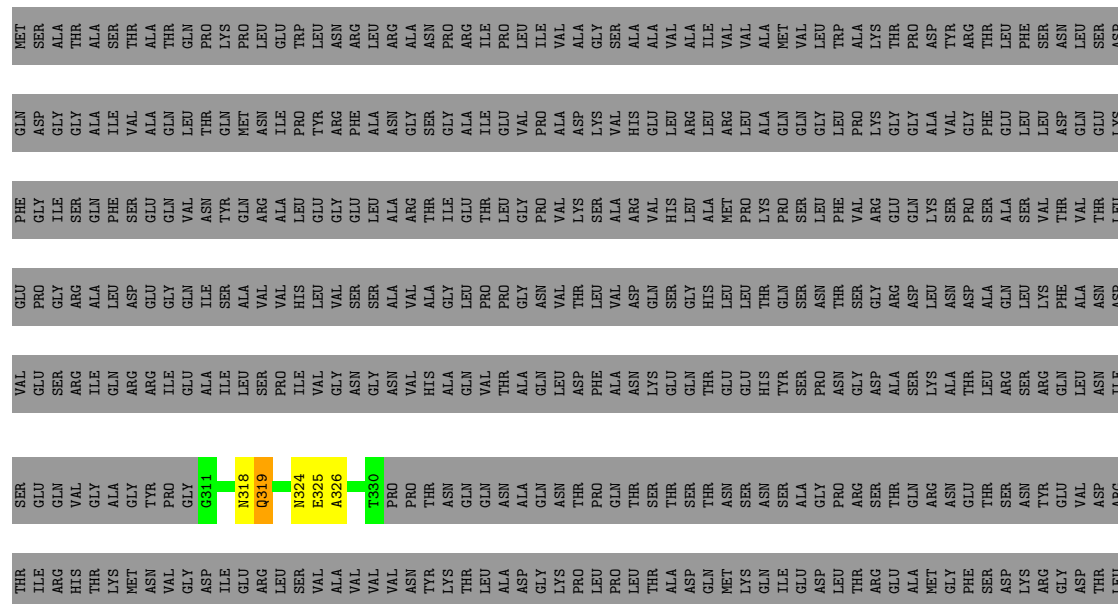
- Molecule 6: Flagellar M-ring protein

Chain BM:  96%

[illegible]

97%

96%



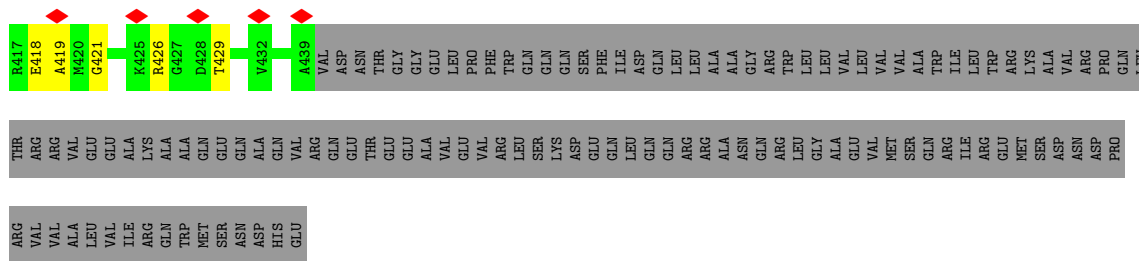
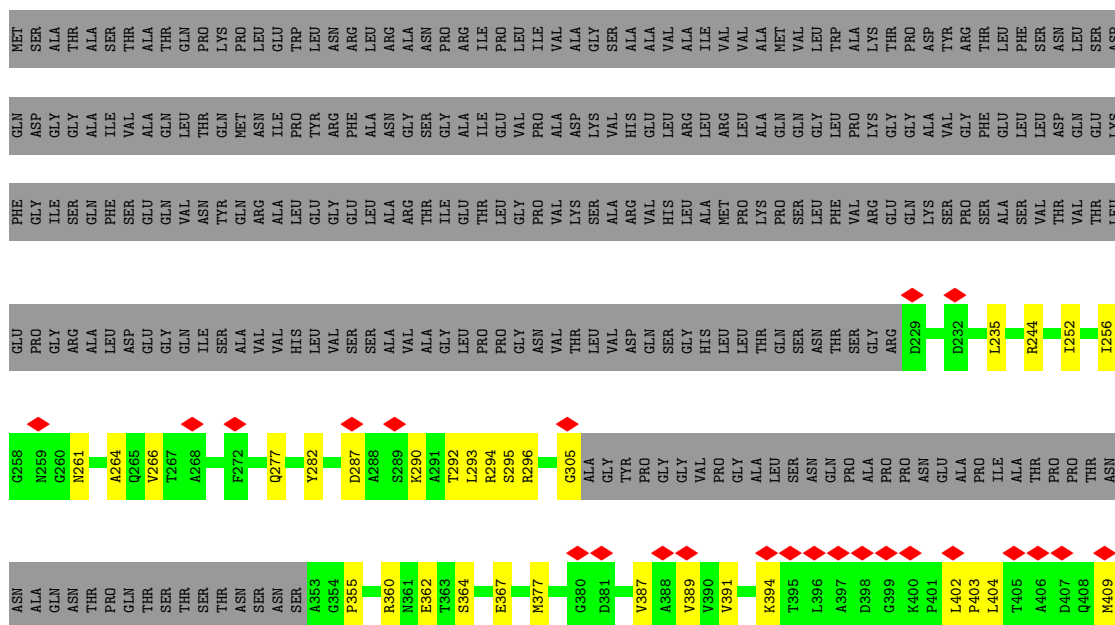




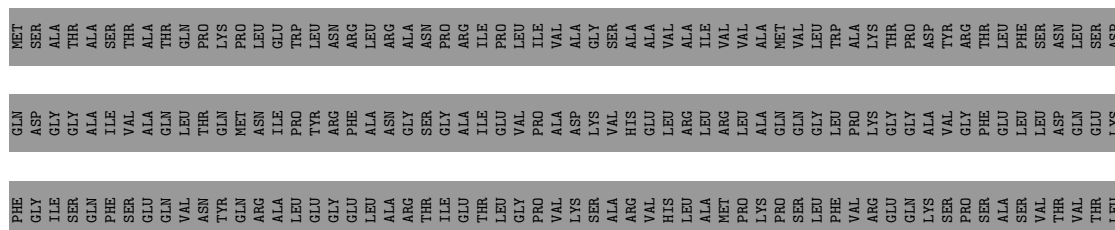


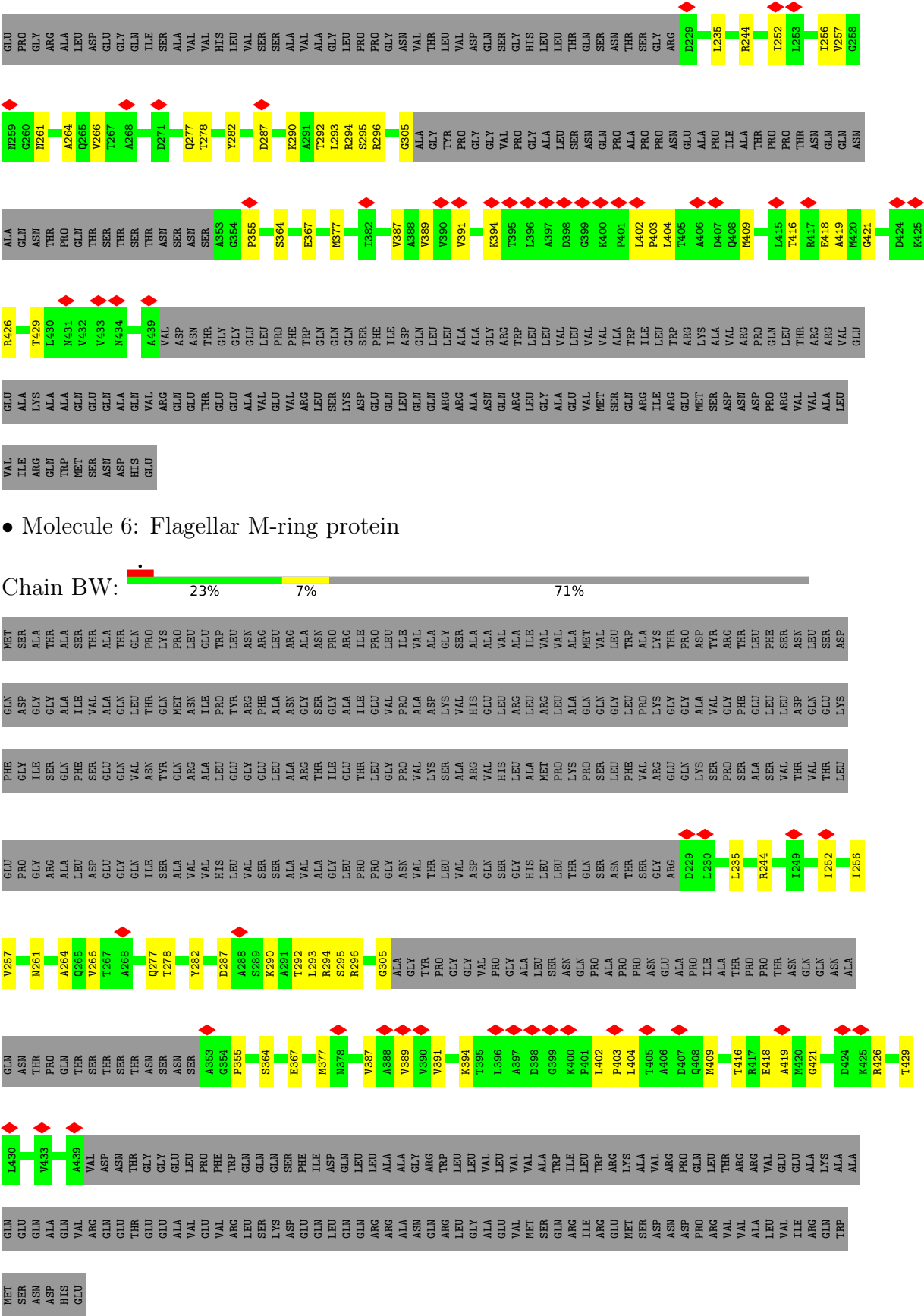


- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein

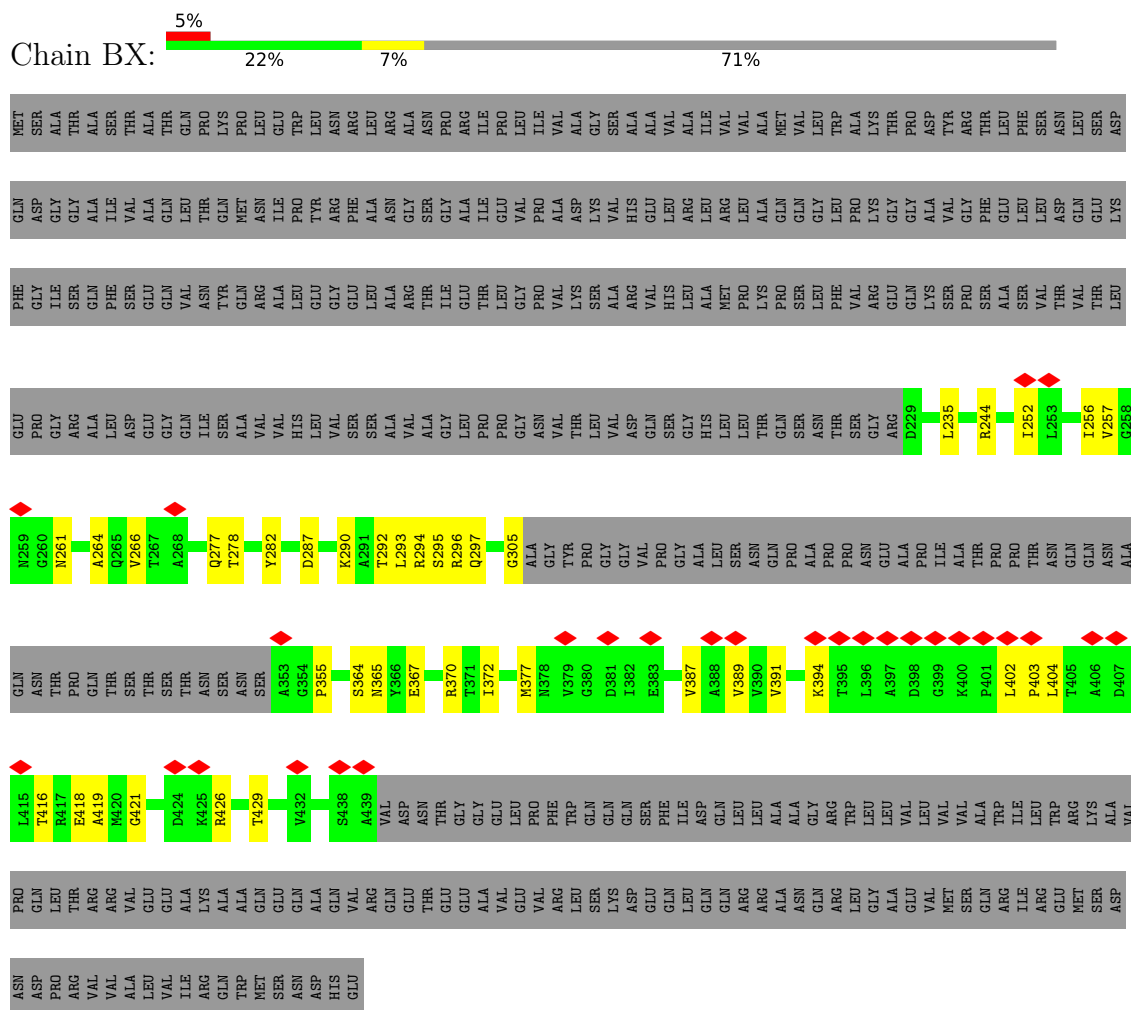




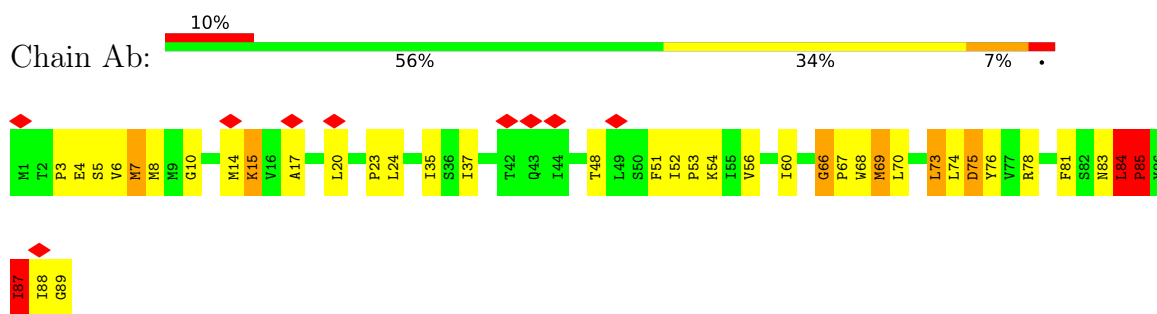
● Molecule 6: Flagellar M-ring protein



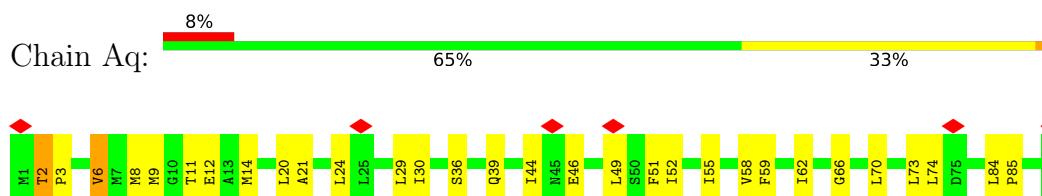
- Molecule 6: Flagellar M-ring protein



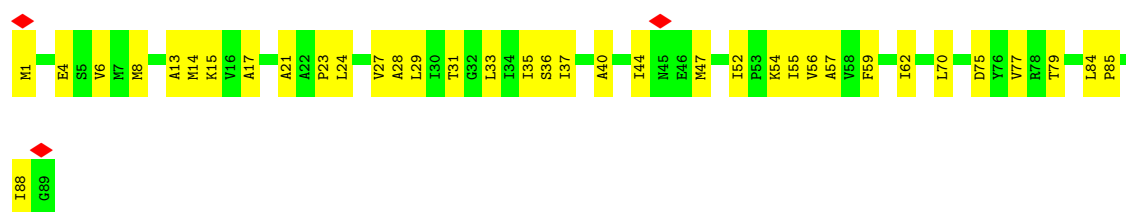
- Molecule 7: Flagellar biosynthetic protein FliQ



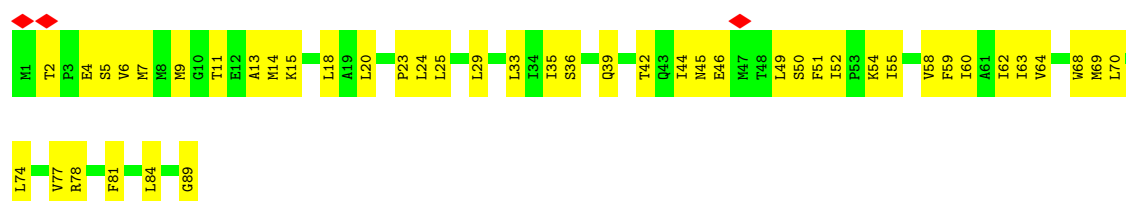
- Molecule 7: Flagellar biosynthetic protein FliQ



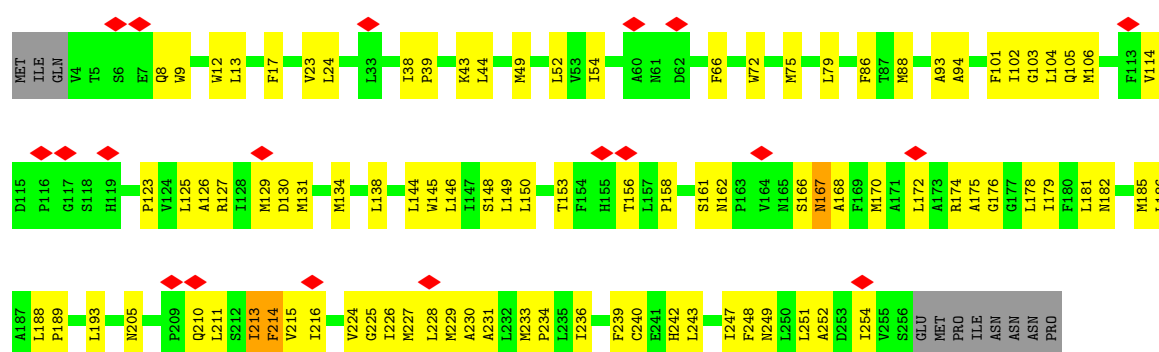
- Molecule 7: Flagellar biosynthetic protein FliQ



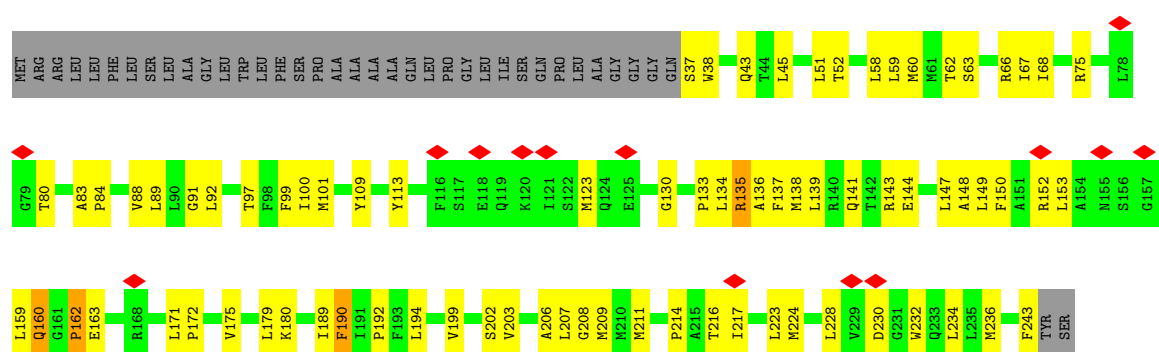
• Molecule 7: Flagellar biosynthetic protein FliQ



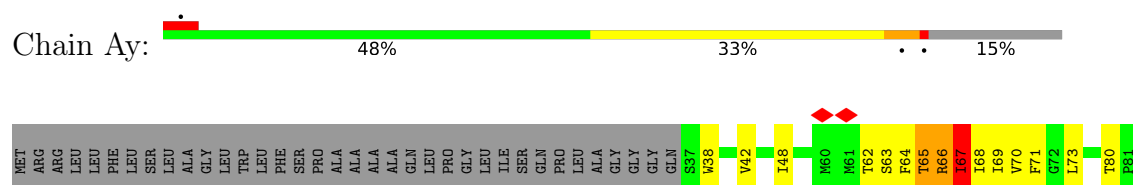
• Molecule 8: Flagellar biosynthetic protein FliR



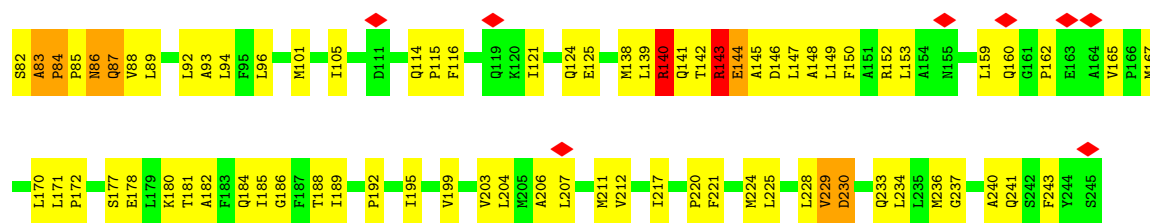
• Molecule 9: Flagellar biosynthetic protein FliP



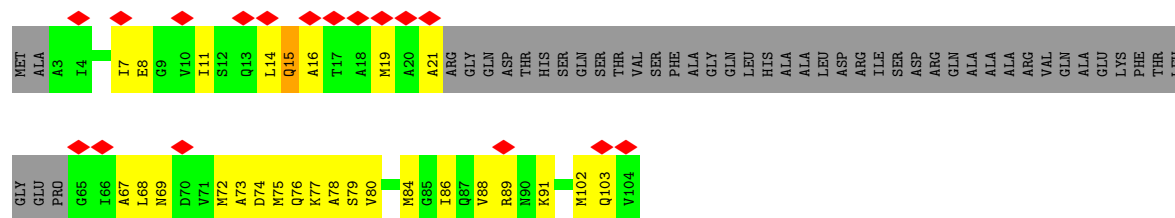
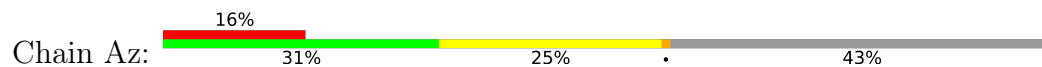
• Molecule 9: Flagellar biosynthetic protein FliP







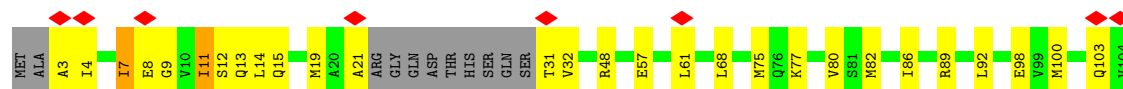
• Molecule 10: Flagellar hook-basal body complex protein FliE



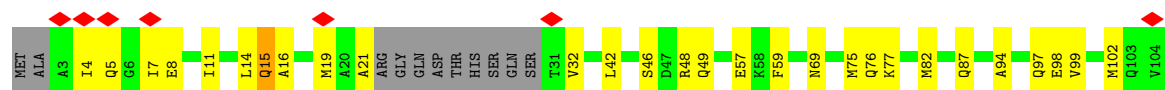
• Molecule 10: Flagellar hook-basal body complex protein FliE



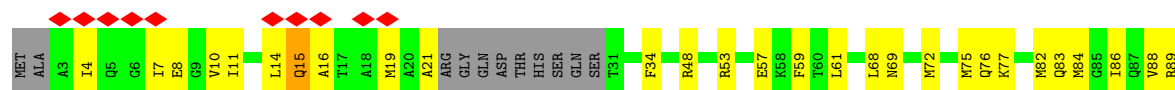
• Molecule 10: Flagellar hook-basal body complex protein FliE



• Molecule 10: Flagellar hook-basal body complex protein FliE

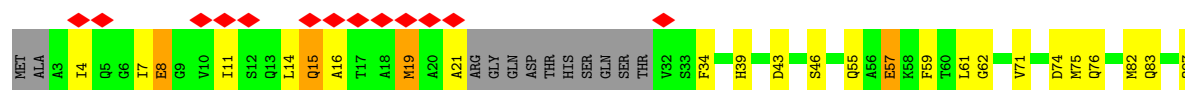


• Molecule 10: Flagellar hook-basal body complex protein FliE

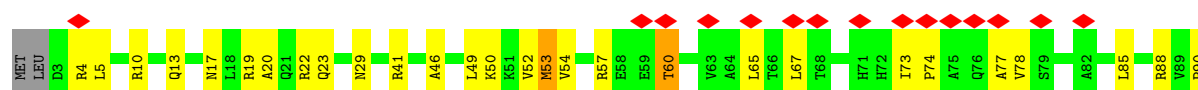




- Molecule 10: Flagellar hook-basal body complex protein FliE

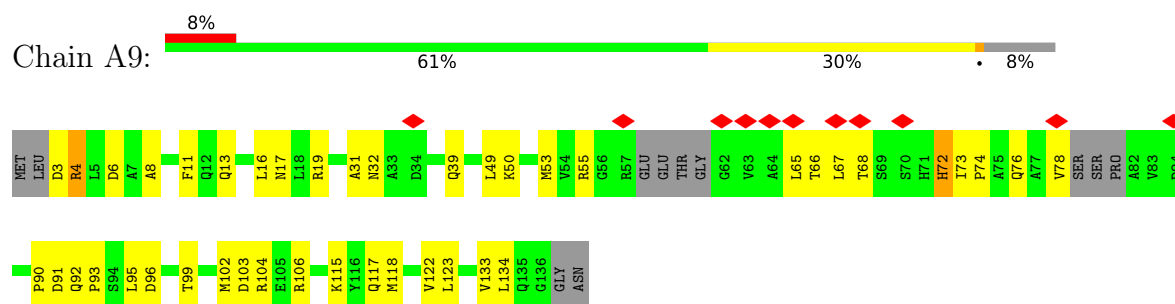


- Molecule 11: Flagellar basal body rod protein FlgB

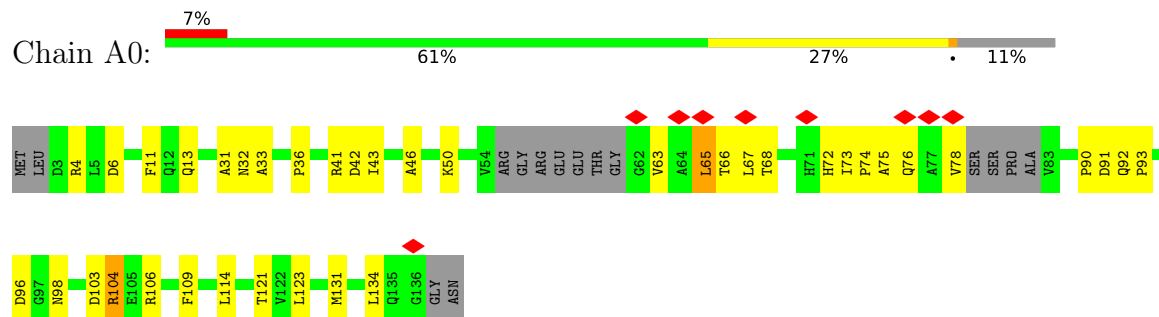


- Molecule 11: Flagellar basal body rod protein FlgB

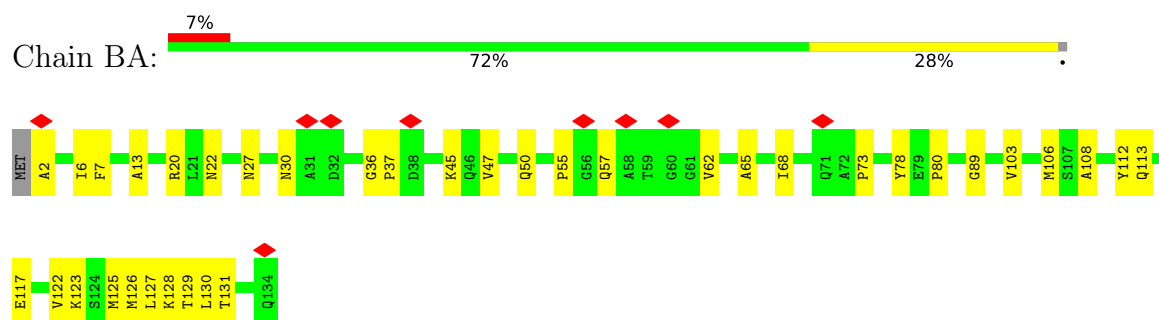




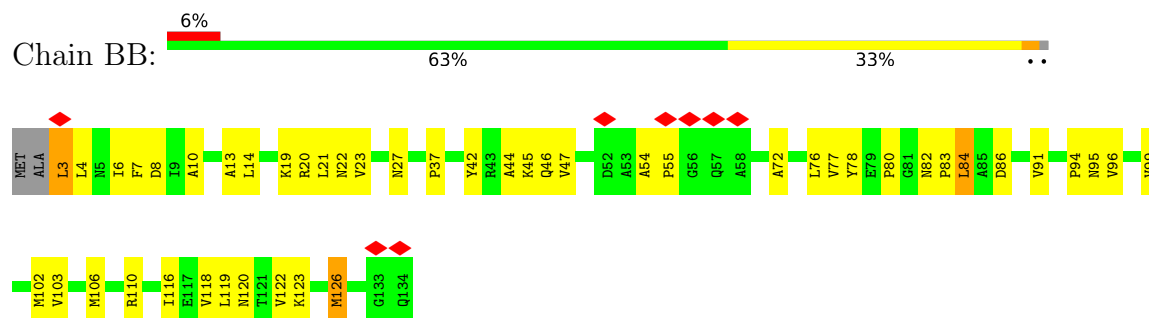
- Molecule 11: Flagellar basal body rod protein FlgB



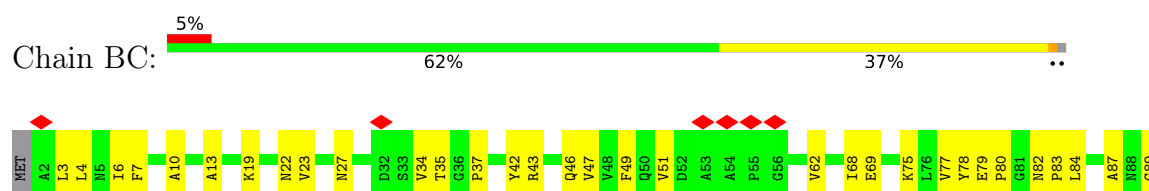
- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC

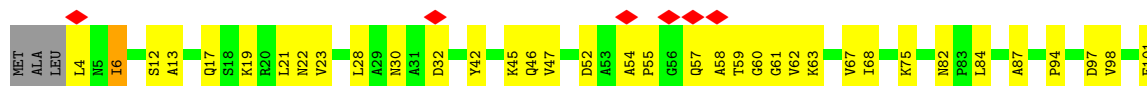




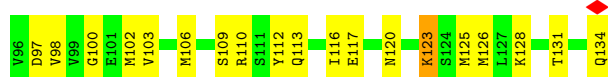
- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: 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             | 11858                                   | 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 ( $e^-/\text{\AA}^2$ ) | 45                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 1.637                                   | Depositor |
| Minimum map value                    | -0.797                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.092                                   | Depositor |
| Recommended contour level            | 0.4                                     | Depositor |
| Map size (Å)                         | 681.984, 681.984, 681.984               | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.332, 1.332, 1.332                     | 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   | A     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | B     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | C     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | D     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | E     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | F     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | G     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | H     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | I     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | J     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | K     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | L     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | M     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | N     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | O     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | P     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | Q     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | R     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | S     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | T     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | U     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | V     | 0.20         | 0/1613      | 0.31        | 0/2194        |
| 1   | W     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | X     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | Y     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 1   | Z     | 0.20         | 0/1613      | 0.32        | 0/2194        |
| 2   | a     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | b     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | c     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | d     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | e     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | f     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | g     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |
| 2   | h     | 0.27         | 0/2243      | 0.45        | 1/3041 (0.0%) |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 2   | i     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | j     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | k     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | l     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | m     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | n     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | o     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | p     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | q     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | r     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | s     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | t     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | u     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | v     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | w     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | x     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | y     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 2   | z     | 0.27         | 0/2243  | 0.45        | 1/3041 (0.0%) |
| 3   | 0     | 0.34         | 0/1888  | 0.61        | 3/2564 (0.1%) |
| 3   | 1     | 0.29         | 0/1917  | 0.54        | 0/2605        |
| 3   | 2     | 0.25         | 0/1973  | 0.53        | 1/2682 (0.0%) |
| 3   | 3     | 0.22         | 0/1973  | 0.50        | 0/2682        |
| 3   | 4     | 0.22         | 0/1973  | 0.47        | 0/2682        |
| 3   | 5     | 0.36         | 0/1973  | 0.59        | 0/2682        |
| 3   | 6     | 0.34         | 0/1973  | 0.65        | 0/2682        |
| 3   | 7     | 0.34         | 0/1973  | 0.59        | 2/2682 (0.1%) |
| 3   | 8     | 0.35         | 0/1973  | 0.68        | 3/2682 (0.1%) |
| 3   | 9     | 0.29         | 0/1973  | 0.54        | 0/2682        |
| 3   | AF    | 0.39         | 0/1926  | 0.64        | 0/2618        |
| 3   | AG    | 0.47         | 0/1934  | 0.77        | 3/2629 (0.1%) |
| 3   | AH    | 0.48         | 0/1942  | 0.73        | 3/2639 (0.1%) |
| 3   | AI    | 0.38         | 0/1926  | 0.67        | 3/2618 (0.1%) |
| 3   | AJ    | 0.41         | 0/1934  | 0.65        | 1/2629 (0.0%) |
| 3   | AK    | 0.36         | 0/1844  | 0.63        | 0/2505        |
| 3   | AL    | 0.36         | 0/1888  | 0.59        | 0/2564        |
| 3   | AM    | 0.36         | 0/1888  | 0.66        | 2/2564 (0.1%) |
| 3   | AN    | 0.30         | 0/1888  | 0.55        | 1/2564 (0.0%) |
| 3   | ZA    | 0.32         | 0/1973  | 0.57        | 0/2682        |
| 3   | ZB    | 0.26         | 0/1973  | 0.49        | 0/2682        |
| 3   | ZC    | 0.40         | 0/1973  | 0.67        | 0/2682        |
| 3   | ZD    | 0.33         | 0/1973  | 0.61        | 0/2682        |
| 3   | ZE    | 0.29         | 0/1973  | 0.54        | 0/2682        |
| 4   | ZF    | 0.23         | 0/2991  | 0.46        | 1/4076 (0.0%) |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 4   | ZG    | 0.35         | 1/2991 (0.0%) | 0.59        | 4/4076 (0.1%) |
| 4   | ZH    | 0.26         | 0/2991        | 0.49        | 1/4076 (0.0%) |
| 4   | ZI    | 0.29         | 0/2991        | 0.51        | 1/4076 (0.0%) |
| 4   | ZJ    | 0.27         | 0/2991        | 0.48        | 0/4076        |
| 4   | ZK    | 0.27         | 0/2991        | 0.51        | 0/4076        |
| 4   | ZL    | 0.25         | 0/2991        | 0.46        | 0/4076        |
| 4   | ZM    | 0.22         | 0/2991        | 0.49        | 1/4076 (0.0%) |
| 4   | ZN    | 0.21         | 0/2991        | 0.46        | 1/4076 (0.0%) |
| 4   | ZO    | 0.27         | 0/2991        | 0.50        | 1/4076 (0.0%) |
| 4   | ZP    | 0.21         | 0/2991        | 0.43        | 1/4076 (0.0%) |
| 4   | ZQ    | 0.23         | 0/2991        | 0.48        | 0/4076        |
| 4   | ZR    | 0.22         | 1/2991 (0.0%) | 0.47        | 2/4076 (0.0%) |
| 4   | ZS    | 0.22         | 0/2991        | 0.44        | 0/4076        |
| 4   | ZT    | 0.24         | 0/2991        | 0.46        | 1/4076 (0.0%) |
| 4   | ZU    | 0.23         | 0/2991        | 0.45        | 0/4076        |
| 4   | ZV    | 0.48         | 4/2991 (0.1%) | 0.65        | 7/4076 (0.2%) |
| 4   | ZW    | 0.19         | 0/2991        | 0.43        | 0/4076        |
| 4   | ZX    | 0.19         | 0/2991        | 0.41        | 0/4076        |
| 4   | ZY    | 0.24         | 1/2991 (0.0%) | 0.47        | 2/4076 (0.0%) |
| 4   | ZZ    | 0.15         | 0/2991        | 0.37        | 0/4076        |
| 4   | Za    | 0.21         | 0/2991        | 0.43        | 1/4076 (0.0%) |
| 4   | Zb    | 0.28         | 0/2991        | 0.49        | 1/4076 (0.0%) |
| 4   | Zc    | 0.24         | 0/2991        | 0.49        | 3/4076 (0.1%) |
| 4   | Zd    | 0.27         | 0/2991        | 0.51        | 1/4076 (0.0%) |
| 4   | Ze    | 0.25         | 0/2991        | 0.48        | 0/4076        |
| 4   | Zf    | 0.21         | 0/2991        | 0.45        | 0/4076        |
| 4   | Zg    | 0.23         | 0/2991        | 0.46        | 0/4076        |
| 4   | Zh    | 0.21         | 0/2991        | 0.42        | 1/4076 (0.0%) |
| 5   | AA    | 0.33         | 0/1828        | 0.57        | 1/2492 (0.0%) |
| 5   | AB    | 0.36         | 0/1836        | 0.62        | 1/2502 (0.0%) |
| 5   | AC    | 0.42         | 0/1844        | 0.62        | 0/2512        |
| 5   | AD    | 0.36         | 0/1844        | 0.63        | 0/2512        |
| 5   | AE    | 0.35         | 0/1836        | 0.57        | 0/2502        |
| 6   | AO    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AP    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AQ    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AR    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AS    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AT    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AU    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AV    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AW    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |
| 6   | AX    | 0.23         | 0/1289        | 0.44        | 1/1741 (0.1%) |



| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 6   | AY    | 0.24         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | AZ    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Aa    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ac    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ad    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ae    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Af    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ag    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ah    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ai    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Aj    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ak    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Al    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Am    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | An    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ao    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | Ap    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BG    | 0.58         | 0/83           | 1.24        | 2/114 (1.8%)   |
| 6   | BH    | 0.16         | 0/107          | 0.37        | 0/148          |
| 6   | BI    | 0.27         | 0/137          | 0.51        | 0/191          |
| 6   | BJ    | 0.21         | 0/107          | 0.45        | 0/148          |
| 6   | BK    | 0.48         | 0/145          | 0.69        | 0/203          |
| 6   | BL    | 0.23         | 0/107          | 0.57        | 0/148          |
| 6   | BM    | 0.14         | 0/145          | 0.29        | 0/203          |
| 6   | BN    | 0.17         | 0/107          | 0.42        | 0/148          |
| 6   | BO    | 0.35         | 0/137          | 0.93        | 0/191          |
| 6   | BP    | 0.17         | 0/107          | 0.30        | 0/148          |
| 6   | BQ    | 0.26         | 0/145          | 0.44        | 0/203          |
| 6   | BR    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BS    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BT    | 0.22         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BU    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BV    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BW    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | BX    | 0.23         | 0/1289         | 0.44        | 1/1741 (0.1%)  |
| 6   | UI    | 1.26         | 19/1191 (1.6%) | 1.29        | 19/1618 (1.2%) |
| 6   | UJ    | 1.27         | 20/1191 (1.7%) | 1.29        | 18/1618 (1.1%) |
| 6   | UK    | 1.26         | 19/1191 (1.6%) | 1.29        | 19/1618 (1.2%) |
| 6   | UL    | 1.24         | 18/1191 (1.5%) | 1.30        | 19/1618 (1.2%) |
| 6   | UM    | 1.27         | 20/1191 (1.7%) | 1.29        | 19/1618 (1.2%) |
| 6   | UN    | 1.27         | 20/1191 (1.7%) | 1.28        | 18/1618 (1.1%) |
| 6   | UO    | 1.26         | 19/1191 (1.6%) | 1.28        | 19/1618 (1.2%) |
| 6   | UP    | 1.27         | 20/1191 (1.7%) | 1.28        | 19/1618 (1.2%) |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 6   | WA    | 0.89         | 0/863   | 1.20        | 2/1172 (0.2%) |
| 6   | WB    | 0.91         | 0/850   | 1.21        | 1/1154 (0.1%) |
| 6   | WC    | 0.88         | 0/825   | 1.15        | 0/1121        |
| 6   | WD    | 0.91         | 0/841   | 1.16        | 0/1142        |
| 6   | WE    | 0.88         | 0/857   | 1.17        | 1/1164 (0.1%) |
| 6   | WF    | 0.89         | 0/848   | 1.17        | 0/1152        |
| 6   | WG    | 0.89         | 0/857   | 1.16        | 0/1164        |
| 6   | WH    | 0.90         | 0/714   | 1.15        | 1/973 (0.1%)  |
| 6   | WI    | 0.87         | 0/714   | 1.20        | 2/973 (0.2%)  |
| 6   | WJ    | 0.90         | 0/749   | 1.19        | 1/1020 (0.1%) |
| 6   | WK    | 0.90         | 0/741   | 1.16        | 0/1009        |
| 6   | WL    | 0.89         | 0/631   | 1.16        | 1/860 (0.1%)  |
| 6   | WM    | 0.88         | 0/604   | 1.15        | 1/824 (0.1%)  |
| 6   | WN    | 0.89         | 0/619   | 1.17        | 1/844 (0.1%)  |
| 6   | WO    | 0.89         | 0/726   | 1.19        | 3/989 (0.3%)  |
| 6   | WP    | 0.89         | 0/753   | 1.15        | 0/1025        |
| 6   | WQ    | 0.90         | 0/848   | 1.19        | 0/1152        |
| 6   | WR    | 0.89         | 0/848   | 1.14        | 0/1152        |
| 6   | WS    | 0.92         | 0/848   | 1.19        | 1/1152 (0.1%) |
| 6   | WT    | 0.89         | 0/848   | 1.18        | 0/1152        |
| 6   | WU    | 0.89         | 0/857   | 1.16        | 1/1164 (0.1%) |
| 6   | WV    | 0.91         | 0/841   | 1.17        | 0/1142        |
| 6   | WW    | 0.90         | 0/848   | 1.19        | 2/1152 (0.2%) |
| 7   | Ab    | 0.63         | 0/681   | 1.02        | 4/930 (0.4%)  |
| 7   | Aq    | 0.33         | 0/681   | 0.60        | 0/930         |
| 7   | Ar    | 0.24         | 0/681   | 0.53        | 1/930 (0.1%)  |
| 7   | As    | 0.19         | 0/681   | 0.45        | 0/930         |
| 8   | At    | 0.29         | 0/1994  | 0.52        | 0/2724        |
| 9   | Au    | 0.32         | 0/1643  | 0.64        | 5/2237 (0.2%) |
| 9   | Av    | 0.27         | 0/1665  | 0.46        | 2/2267 (0.1%) |
| 9   | Aw    | 0.24         | 0/1652  | 0.48        | 3/2249 (0.1%) |
| 9   | Ax    | 0.24         | 0/1652  | 0.45        | 0/2249        |
| 9   | Ay    | 0.36         | 0/1662  | 0.62        | 4/2263 (0.2%) |
| 10  | A1    | 0.42         | 0/675   | 0.64        | 0/905         |
| 10  | A2    | 0.43         | 0/689   | 0.70        | 0/925         |
| 10  | A3    | 0.42         | 0/689   | 0.64        | 0/925         |
| 10  | A4    | 0.42         | 0/689   | 0.66        | 0/925         |
| 10  | A5    | 0.48         | 0/682   | 0.71        | 0/915         |
| 10  | Az    | 0.54         | 0/428   | 0.89        | 0/572         |
| 11  | A0    | 0.40         | 0/959   | 0.53        | 0/1293        |
| 11  | A6    | 0.45         | 0/1042  | 0.67        | 2/1408 (0.1%) |
| 11  | A7    | 0.37         | 0/951   | 0.51        | 0/1282        |
| 11  | A8    | 0.41         | 0/976   | 0.60        | 0/1316        |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 11  | A9    | 0.41         | 0/991             | 0.65        | 3/1335 (0.2%)     |
| 12  | BA    | 0.22         | 0/981             | 0.41        | 0/1334            |
| 12  | BB    | 0.24         | 0/976             | 0.48        | 0/1327            |
| 12  | BC    | 0.35         | 0/981             | 0.55        | 0/1334            |
| 12  | BD    | 0.32         | 0/981             | 0.65        | 1/1334 (0.1%)     |
| 12  | BE    | 0.24         | 0/968             | 0.43        | 0/1316            |
| 12  | BF    | 0.40         | 0/981             | 0.55        | 1/1334 (0.1%)     |
| All | All   | 0.40         | 162/343249 (0.0%) | 0.58        | 310/466323 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 3   | 0     | 0                   | 2                   |
| 3   | 1     | 0                   | 1                   |
| 3   | 5     | 0                   | 2                   |
| 3   | 7     | 0                   | 1                   |
| 3   | 8     | 0                   | 2                   |
| 3   | AF    | 0                   | 1                   |
| 3   | AI    | 0                   | 1                   |
| 3   | AK    | 0                   | 1                   |
| 3   | AL    | 0                   | 1                   |
| 3   | AM    | 0                   | 2                   |
| 3   | AN    | 0                   | 3                   |
| 3   | ZA    | 0                   | 2                   |
| 3   | ZD    | 0                   | 1                   |
| 3   | ZE    | 0                   | 3                   |
| 4   | ZI    | 0                   | 1                   |
| 4   | ZK    | 0                   | 1                   |
| 4   | ZO    | 0                   | 1                   |
| 4   | ZT    | 0                   | 1                   |
| 4   | ZU    | 0                   | 1                   |
| 4   | ZW    | 0                   | 1                   |
| 4   | ZZ    | 0                   | 1                   |
| 4   | Zd    | 0                   | 1                   |
| 4   | Ze    | 0                   | 1                   |
| 5   | AA    | 0                   | 1                   |
| 5   | AB    | 0                   | 2                   |
| 5   | AD    | 0                   | 1                   |
| 6   | UI    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | UJ    | 0                   | 2                   |
| 6   | UK    | 0                   | 3                   |
| 6   | UL    | 0                   | 3                   |
| 6   | UM    | 0                   | 2                   |
| 6   | UN    | 0                   | 2                   |
| 6   | UO    | 0                   | 2                   |
| 6   | UP    | 0                   | 3                   |
| 6   | WA    | 0                   | 3                   |
| 6   | WB    | 0                   | 4                   |
| 6   | WC    | 0                   | 3                   |
| 6   | WD    | 0                   | 1                   |
| 6   | WE    | 0                   | 2                   |
| 6   | WF    | 0                   | 3                   |
| 6   | WG    | 0                   | 3                   |
| 6   | WI    | 0                   | 1                   |
| 6   | WJ    | 0                   | 3                   |
| 6   | WK    | 0                   | 2                   |
| 6   | WL    | 0                   | 2                   |
| 6   | WM    | 0                   | 1                   |
| 6   | WN    | 0                   | 1                   |
| 6   | WO    | 0                   | 1                   |
| 6   | WP    | 0                   | 3                   |
| 6   | WQ    | 0                   | 2                   |
| 6   | WR    | 0                   | 3                   |
| 6   | WS    | 0                   | 1                   |
| 6   | WT    | 0                   | 2                   |
| 6   | WU    | 0                   | 2                   |
| 6   | WV    | 0                   | 3                   |
| 6   | WW    | 0                   | 2                   |
| 9   | Aw    | 0                   | 2                   |
| 9   | Ay    | 0                   | 2                   |
| 11  | A0    | 0                   | 1                   |
| 11  | A6    | 0                   | 1                   |
| 11  | A7    | 0                   | 1                   |
| 11  | A9    | 0                   | 1                   |
| 12  | BD    | 0                   | 1                   |
| 12  | BF    | 0                   | 1                   |
| All | All   | 0                   | 113                 |

All (162) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
|-----|-------|-----|------|-------|---|-------------|----------|

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4   | ZV    | 140 | PRO  | CG-CD | -15.66 | 0.97        | 1.50     |
| 6   | UJ    | 125 | GLN  | C-N   | 13.71  | 1.51        | 1.33     |
| 6   | UK    | 125 | GLN  | C-N   | 13.59  | 1.51        | 1.33     |
| 6   | UO    | 125 | GLN  | C-N   | 13.55  | 1.51        | 1.33     |
| 6   | UP    | 125 | GLN  | C-N   | 13.54  | 1.51        | 1.33     |
| 6   | UI    | 125 | GLN  | C-N   | 13.54  | 1.51        | 1.33     |
| 6   | UL    | 125 | GLN  | C-N   | 13.48  | 1.51        | 1.33     |
| 6   | UM    | 125 | GLN  | C-N   | 13.44  | 1.51        | 1.33     |
| 6   | UN    | 125 | GLN  | C-N   | 13.44  | 1.51        | 1.33     |
| 4   | ZV    | 125 | PRO  | CG-CD | -12.77 | 1.17        | 1.51     |
| 6   | UM    | 172 | PRO  | N-CD  | -9.48  | 1.34        | 1.47     |
| 6   | UL    | 172 | PRO  | N-CD  | -9.47  | 1.34        | 1.47     |
| 6   | UI    | 172 | PRO  | N-CD  | -9.43  | 1.34        | 1.47     |
| 6   | UO    | 172 | PRO  | N-CD  | -9.43  | 1.34        | 1.47     |
| 6   | UN    | 172 | PRO  | N-CD  | -9.42  | 1.34        | 1.47     |
| 6   | UJ    | 172 | PRO  | N-CD  | -9.36  | 1.34        | 1.47     |
| 6   | UP    | 172 | PRO  | N-CD  | -9.36  | 1.34        | 1.47     |
| 6   | UK    | 172 | PRO  | N-CD  | -9.34  | 1.34        | 1.47     |
| 4   | ZV    | 140 | PRO  | N-CD  | 8.35   | 1.59        | 1.47     |
| 6   | UM    | 93  | VAL  | C-N   | -7.43  | 1.24        | 1.33     |
| 6   | UN    | 93  | VAL  | C-N   | -7.28  | 1.24        | 1.33     |
| 6   | UI    | 93  | VAL  | C-N   | -7.24  | 1.24        | 1.33     |
| 6   | UL    | 93  | VAL  | C-N   | -7.23  | 1.24        | 1.33     |
| 6   | UP    | 93  | VAL  | C-N   | -7.21  | 1.24        | 1.33     |
| 6   | UK    | 93  | VAL  | C-N   | -7.20  | 1.24        | 1.33     |
| 6   | UJ    | 93  | VAL  | C-N   | -7.18  | 1.24        | 1.33     |
| 6   | UO    | 93  | VAL  | C-N   | -7.12  | 1.24        | 1.33     |
| 4   | ZY    | 125 | PRO  | CG-CD | -7.04  | 1.32        | 1.51     |
| 6   | UI    | 172 | PRO  | C-N   | -6.98  | 1.23        | 1.33     |
| 6   | UP    | 172 | PRO  | C-N   | -6.94  | 1.23        | 1.33     |
| 6   | UO    | 172 | PRO  | C-N   | -6.92  | 1.23        | 1.33     |
| 6   | UL    | 172 | PRO  | C-N   | -6.92  | 1.23        | 1.33     |
| 6   | UK    | 172 | PRO  | C-N   | -6.91  | 1.23        | 1.33     |
| 6   | UJ    | 172 | PRO  | C-N   | -6.89  | 1.23        | 1.33     |
| 6   | UO    | 141 | ALA  | C-N   | -6.89  | 1.25        | 1.33     |
| 6   | UM    | 172 | PRO  | C-N   | -6.88  | 1.23        | 1.33     |
| 6   | UN    | 172 | PRO  | C-N   | -6.87  | 1.23        | 1.33     |
| 6   | UP    | 141 | ALA  | C-N   | -6.85  | 1.25        | 1.33     |
| 6   | UN    | 138 | GLY  | C-N   | -6.83  | 1.25        | 1.33     |
| 6   | UI    | 138 | GLY  | C-N   | -6.83  | 1.25        | 1.33     |
| 6   | UJ    | 141 | ALA  | C-N   | -6.82  | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | UM    | 138 | GLY  | C-N   | -6.81 | 1.25        | 1.33     |
| 6   | UJ    | 138 | GLY  | C-N   | -6.80 | 1.25        | 1.33     |
| 6   | UP    | 138 | GLY  | C-N   | -6.77 | 1.25        | 1.33     |
| 6   | UK    | 141 | ALA  | C-N   | -6.77 | 1.25        | 1.33     |
| 6   | UI    | 141 | ALA  | C-N   | -6.77 | 1.25        | 1.33     |
| 6   | UK    | 138 | GLY  | C-N   | -6.76 | 1.25        | 1.33     |
| 6   | UO    | 138 | GLY  | C-N   | -6.75 | 1.25        | 1.33     |
| 6   | UL    | 141 | ALA  | C-N   | -6.74 | 1.25        | 1.33     |
| 6   | UL    | 138 | GLY  | C-N   | -6.70 | 1.25        | 1.33     |
| 6   | UM    | 141 | ALA  | C-N   | -6.70 | 1.25        | 1.33     |
| 4   | ZV    | 125 | PRO  | N-CD  | 6.62  | 1.57        | 1.47     |
| 4   | ZR    | 125 | PRO  | CG-CD | -6.62 | 1.33        | 1.51     |
| 6   | UN    | 141 | ALA  | C-N   | -6.61 | 1.25        | 1.33     |
| 6   | UK    | 92  | LYS  | C-N   | -6.44 | 1.25        | 1.33     |
| 6   | UO    | 92  | LYS  | C-N   | -6.44 | 1.25        | 1.33     |
| 6   | UP    | 92  | LYS  | C-N   | -6.42 | 1.25        | 1.33     |
| 6   | UJ    | 92  | LYS  | C-N   | -6.38 | 1.25        | 1.33     |
| 6   | UL    | 92  | LYS  | C-N   | -6.38 | 1.25        | 1.33     |
| 6   | UI    | 92  | LYS  | C-N   | -6.37 | 1.25        | 1.33     |
| 6   | UM    | 92  | LYS  | C-N   | -6.29 | 1.26        | 1.33     |
| 6   | UN    | 92  | LYS  | C-N   | -6.28 | 1.26        | 1.33     |
| 6   | UL    | 201 | ALA  | C-N   | -6.25 | 1.25        | 1.33     |
| 6   | UJ    | 195 | VAL  | C-N   | -6.21 | 1.25        | 1.33     |
| 6   | UP    | 195 | VAL  | C-N   | -6.20 | 1.25        | 1.33     |
| 6   | UI    | 201 | ALA  | C-N   | -6.17 | 1.25        | 1.33     |
| 6   | UK    | 195 | VAL  | C-N   | -6.16 | 1.25        | 1.33     |
| 6   | UL    | 195 | VAL  | C-N   | -6.15 | 1.25        | 1.33     |
| 6   | UM    | 201 | ALA  | C-N   | -6.13 | 1.25        | 1.33     |
| 6   | UN    | 201 | ALA  | C-N   | -6.11 | 1.25        | 1.33     |
| 6   | UP    | 201 | ALA  | C-N   | -6.11 | 1.25        | 1.33     |
| 6   | UO    | 201 | ALA  | C-N   | -6.10 | 1.25        | 1.33     |
| 6   | UJ    | 105 | LEU  | C-N   | -6.09 | 1.24        | 1.34     |
| 6   | UI    | 195 | VAL  | C-N   | -6.08 | 1.25        | 1.33     |
| 6   | UM    | 195 | VAL  | C-N   | -6.07 | 1.25        | 1.33     |
| 6   | UJ    | 250 | ALA  | C-N   | -6.06 | 1.25        | 1.33     |
| 6   | UK    | 201 | ALA  | C-N   | -6.06 | 1.25        | 1.33     |
| 6   | UM    | 182 | PRO  | C-N   | -6.06 | 1.24        | 1.33     |
| 6   | UM    | 105 | LEU  | C-N   | -6.05 | 1.24        | 1.34     |
| 6   | UK    | 105 | LEU  | C-N   | -6.04 | 1.24        | 1.34     |
| 6   | UI    | 182 | PRO  | C-N   | -6.03 | 1.24        | 1.33     |
| 6   | UP    | 105 | LEU  | C-N   | -6.01 | 1.25        | 1.34     |
| 6   | UJ    | 182 | PRO  | C-N   | -6.00 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | UN    | 105 | LEU  | C-N   | -6.00 | 1.25        | 1.34     |
| 6   | UN    | 195 | VAL  | C-N   | -5.99 | 1.25        | 1.33     |
| 6   | UL    | 105 | LEU  | C-N   | -5.99 | 1.25        | 1.34     |
| 6   | UO    | 182 | PRO  | C-N   | -5.98 | 1.24        | 1.33     |
| 6   | UO    | 195 | VAL  | C-N   | -5.98 | 1.25        | 1.33     |
| 6   | UO    | 105 | LEU  | C-N   | -5.96 | 1.25        | 1.34     |
| 6   | UN    | 182 | PRO  | C-N   | -5.95 | 1.25        | 1.33     |
| 6   | UP    | 182 | PRO  | C-N   | -5.94 | 1.25        | 1.33     |
| 6   | UL    | 182 | PRO  | C-N   | -5.94 | 1.25        | 1.33     |
| 6   | UI    | 105 | LEU  | C-N   | -5.91 | 1.25        | 1.34     |
| 6   | UK    | 182 | PRO  | C-N   | -5.90 | 1.25        | 1.33     |
| 6   | UP    | 199 | SER  | C-N   | -5.88 | 1.25        | 1.33     |
| 6   | UK    | 199 | SER  | C-N   | -5.88 | 1.25        | 1.33     |
| 6   | UP    | 62  | ASP  | C-N   | -5.87 | 1.26        | 1.33     |
| 6   | UK    | 142 | ARG  | C-N   | -5.87 | 1.26        | 1.33     |
| 6   | UI    | 199 | SER  | C-N   | -5.86 | 1.25        | 1.33     |
| 6   | UI    | 97  | ARG  | C-N   | -5.85 | 1.26        | 1.33     |
| 6   | UJ    | 248 | SER  | C-N   | -5.85 | 1.25        | 1.33     |
| 6   | UM    | 97  | ARG  | C-N   | -5.85 | 1.26        | 1.33     |
| 6   | UM    | 199 | SER  | C-N   | -5.84 | 1.25        | 1.33     |
| 6   | UL    | 199 | SER  | C-N   | -5.83 | 1.25        | 1.33     |
| 6   | UN    | 199 | SER  | C-N   | -5.83 | 1.25        | 1.33     |
| 6   | UL    | 142 | ARG  | C-N   | -5.79 | 1.26        | 1.33     |
| 6   | UM    | 62  | ASP  | C-N   | -5.79 | 1.26        | 1.33     |
| 6   | UJ    | 97  | ARG  | C-N   | -5.78 | 1.26        | 1.33     |
| 6   | UK    | 97  | ARG  | C-N   | -5.77 | 1.26        | 1.33     |
| 6   | UP    | 97  | ARG  | C-N   | -5.77 | 1.26        | 1.33     |
| 6   | UJ    | 62  | ASP  | C-N   | -5.75 | 1.26        | 1.33     |
| 6   | UL    | 97  | ARG  | C-N   | -5.75 | 1.26        | 1.33     |
| 6   | UO    | 199 | SER  | C-N   | -5.75 | 1.25        | 1.33     |
| 6   | UP    | 142 | ARG  | C-N   | -5.75 | 1.26        | 1.33     |
| 6   | UI    | 142 | ARG  | C-N   | -5.73 | 1.26        | 1.33     |
| 4   | ZG    | 4   | SER  | CA-CB | -5.73 | 1.46        | 1.54     |
| 6   | UN    | 62  | ASP  | C-N   | -5.72 | 1.26        | 1.33     |
| 6   | UN    | 97  | ARG  | C-N   | -5.71 | 1.26        | 1.33     |
| 6   | UK    | 131 | ASN  | C-N   | -5.70 | 1.26        | 1.33     |
| 6   | UI    | 131 | ASN  | C-N   | -5.70 | 1.26        | 1.33     |
| 6   | UL    | 131 | ASN  | C-N   | -5.69 | 1.26        | 1.33     |
| 6   | UM    | 142 | ARG  | C-N   | -5.68 | 1.26        | 1.33     |
| 6   | UO    | 131 | ASN  | C-N   | -5.68 | 1.26        | 1.33     |
| 6   | UJ    | 142 | ARG  | C-N   | -5.65 | 1.26        | 1.33     |
| 6   | UN    | 185 | ALA  | C-N   | -5.65 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | UI    | 185 | ALA  | C-N   | -5.64 | 1.25        | 1.33     |
| 6   | UN    | 142 | ARG  | C-N   | -5.62 | 1.26        | 1.33     |
| 6   | UO    | 185 | ALA  | C-N   | -5.62 | 1.25        | 1.33     |
| 6   | UM    | 131 | ASN  | C-N   | -5.60 | 1.26        | 1.33     |
| 6   | UN    | 131 | ASN  | C-N   | -5.59 | 1.26        | 1.33     |
| 6   | UJ    | 131 | ASN  | C-N   | -5.59 | 1.26        | 1.33     |
| 6   | UK    | 215 | GLN  | C-N   | -5.59 | 1.25        | 1.33     |
| 6   | UI    | 215 | GLN  | C-N   | -5.59 | 1.25        | 1.33     |
| 6   | UM    | 208 | GLY  | C-N   | -5.59 | 1.26        | 1.33     |
| 6   | UL    | 185 | ALA  | C-N   | -5.59 | 1.25        | 1.33     |
| 6   | UP    | 185 | ALA  | C-N   | -5.57 | 1.25        | 1.33     |
| 6   | UJ    | 185 | ALA  | C-N   | -5.57 | 1.25        | 1.33     |
| 6   | UP    | 131 | ASN  | C-N   | -5.57 | 1.26        | 1.33     |
| 6   | UM    | 185 | ALA  | C-N   | -5.57 | 1.25        | 1.33     |
| 6   | UK    | 185 | ALA  | C-N   | -5.56 | 1.25        | 1.33     |
| 6   | UJ    | 264 | GLN  | C-N   | -5.55 | 1.25        | 1.33     |
| 6   | UO    | 70  | LEU  | C-N   | -5.54 | 1.26        | 1.33     |
| 6   | UO    | 97  | ARG  | C-N   | -5.53 | 1.26        | 1.33     |
| 6   | UO    | 215 | GLN  | C-N   | -5.53 | 1.25        | 1.33     |
| 6   | UI    | 208 | GLY  | C-N   | -5.53 | 1.26        | 1.33     |
| 6   | UJ    | 257 | GLY  | C-N   | -5.53 | 1.26        | 1.33     |
| 6   | UL    | 208 | GLY  | C-N   | -5.51 | 1.26        | 1.33     |
| 6   | UN    | 215 | GLN  | C-N   | -5.51 | 1.25        | 1.33     |
| 6   | UP    | 208 | GLY  | C-N   | -5.50 | 1.26        | 1.33     |
| 6   | UO    | 142 | ARG  | C-N   | -5.48 | 1.26        | 1.33     |
| 6   | UN    | 70  | LEU  | C-N   | -5.48 | 1.26        | 1.33     |
| 6   | UK    | 208 | GLY  | C-N   | -5.47 | 1.26        | 1.33     |
| 6   | UP    | 215 | GLN  | C-N   | -5.47 | 1.25        | 1.33     |
| 6   | UM    | 215 | GLN  | C-N   | -5.45 | 1.25        | 1.33     |
| 6   | UN    | 208 | GLY  | C-N   | -5.45 | 1.26        | 1.33     |
| 6   | UK    | 70  | LEU  | C-N   | -5.45 | 1.26        | 1.33     |
| 6   | UL    | 70  | LEU  | C-N   | -5.41 | 1.26        | 1.33     |
| 6   | UO    | 208 | GLY  | C-N   | -5.41 | 1.26        | 1.33     |
| 6   | UM    | 70  | LEU  | C-N   | -5.40 | 1.26        | 1.33     |
| 6   | UJ    | 70  | LEU  | C-N   | -5.39 | 1.26        | 1.33     |
| 6   | UP    | 70  | LEU  | C-N   | -5.34 | 1.26        | 1.33     |
| 6   | UI    | 70  | LEU  | C-N   | -5.33 | 1.26        | 1.33     |

All (310) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4   | ZV    | 140 | PRO  | N-CD-CG | -17.33 | 77.21       | 103.20   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4   | ZV    | 125 | PRO  | N-CD-CG  | -14.57 | 86.32       | 103.80   |
| 4   | ZR    | 125 | PRO  | CA-N-CD  | -13.96 | 91.96       | 111.50   |
| 6   | UL    | 126 | PHE  | O-C-N    | 13.88  | 136.83      | 122.12   |
| 6   | UO    | 126 | PHE  | O-C-N    | 13.87  | 136.82      | 122.12   |
| 6   | UI    | 126 | PHE  | O-C-N    | 13.83  | 136.78      | 122.12   |
| 6   | UK    | 126 | PHE  | O-C-N    | 13.82  | 136.76      | 122.12   |
| 6   | UN    | 126 | PHE  | O-C-N    | 13.80  | 136.75      | 122.12   |
| 6   | UJ    | 126 | PHE  | O-C-N    | 13.79  | 136.74      | 122.12   |
| 6   | UP    | 126 | PHE  | O-C-N    | 13.79  | 136.74      | 122.12   |
| 6   | UM    | 126 | PHE  | O-C-N    | 13.78  | 136.73      | 122.12   |
| 4   | ZY    | 125 | PRO  | CA-N-CD  | -13.33 | 92.84       | 111.50   |
| 4   | ZV    | 125 | PRO  | CA-N-CD  | -13.27 | 92.93       | 111.50   |
| 9   | Au    | 162 | PRO  | CA-N-CD  | -12.32 | 94.75       | 112.00   |
| 4   | Zc    | 125 | PRO  | CA-N-CD  | -11.26 | 95.73       | 111.50   |
| 4   | ZV    | 140 | PRO  | CA-N-CD  | -10.58 | 97.19       | 112.00   |
| 6   | UP    | 129 | GLN  | O-C-N    | 10.56  | 132.95      | 122.07   |
| 6   | UK    | 129 | GLN  | O-C-N    | 10.55  | 132.93      | 122.07   |
| 6   | UO    | 129 | GLN  | O-C-N    | 10.50  | 132.89      | 122.07   |
| 6   | UJ    | 129 | GLN  | O-C-N    | 10.42  | 132.80      | 122.07   |
| 6   | UN    | 129 | GLN  | O-C-N    | 10.39  | 132.77      | 122.07   |
| 6   | UM    | 129 | GLN  | O-C-N    | 10.39  | 132.77      | 122.07   |
| 6   | UI    | 129 | GLN  | O-C-N    | 10.38  | 132.76      | 122.07   |
| 6   | UL    | 129 | GLN  | O-C-N    | 10.37  | 132.75      | 122.07   |
| 4   | ZR    | 125 | PRO  | N-CD-CG  | -9.98  | 91.82       | 103.80   |
| 4   | ZY    | 125 | PRO  | N-CD-CG  | -9.80  | 92.05       | 103.80   |
| 4   | ZV    | 140 | PRO  | CA-CB-CG | -9.56  | 86.34       | 104.50   |
| 6   | BG    | 320 | PRO  | N-CA-C   | -9.26  | 101.15      | 113.65   |
| 6   | UL    | 126 | PHE  | CA-C-N   | -9.15  | 107.30      | 120.29   |
| 6   | UL    | 126 | PHE  | C-N-CA   | -9.15  | 107.30      | 120.29   |
| 6   | UM    | 126 | PHE  | CA-C-N   | -9.12  | 107.35      | 120.29   |
| 6   | UM    | 126 | PHE  | C-N-CA   | -9.12  | 107.35      | 120.29   |
| 6   | UO    | 126 | PHE  | CA-C-N   | -9.09  | 107.38      | 120.29   |
| 6   | UO    | 126 | PHE  | C-N-CA   | -9.09  | 107.38      | 120.29   |
| 6   | UP    | 126 | PHE  | CA-C-N   | -9.09  | 107.39      | 120.29   |
| 6   | UP    | 126 | PHE  | C-N-CA   | -9.09  | 107.39      | 120.29   |
| 6   | UJ    | 126 | PHE  | CA-C-N   | -9.08  | 107.39      | 120.29   |
| 6   | UJ    | 126 | PHE  | C-N-CA   | -9.08  | 107.39      | 120.29   |
| 6   | UN    | 126 | PHE  | CA-C-N   | -9.08  | 107.40      | 120.29   |
| 6   | UN    | 126 | PHE  | C-N-CA   | -9.08  | 107.40      | 120.29   |
| 6   | UK    | 126 | PHE  | CA-C-N   | -9.08  | 107.40      | 120.29   |
| 6   | UK    | 126 | PHE  | C-N-CA   | -9.08  | 107.40      | 120.29   |
| 6   | UI    | 126 | PHE  | CA-C-N   | -9.06  | 107.42      | 120.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | UI    | 126 | PHE  | C-N-CA   | -9.06 | 107.42      | 120.29   |
| 3   | AH    | 2   | ILE  | N-CA-C   | -8.94 | 103.67      | 112.17   |
| 4   | ZM    | 223 | PRO  | CA-N-CD  | -8.74 | 99.77       | 112.00   |
| 6   | UN    | 130 | VAL  | O-C-N    | 8.68  | 130.29      | 121.87   |
| 6   | UI    | 130 | VAL  | O-C-N    | 8.65  | 130.26      | 121.87   |
| 6   | UJ    | 130 | VAL  | O-C-N    | 8.64  | 130.26      | 121.87   |
| 6   | UK    | 130 | VAL  | O-C-N    | 8.63  | 130.25      | 121.87   |
| 6   | UL    | 130 | VAL  | O-C-N    | 8.58  | 130.19      | 121.87   |
| 6   | UO    | 130 | VAL  | O-C-N    | 8.55  | 130.16      | 121.87   |
| 6   | UM    | 130 | VAL  | O-C-N    | 8.52  | 130.13      | 121.87   |
| 6   | UP    | 130 | VAL  | O-C-N    | 8.52  | 130.13      | 121.87   |
| 5   | AB    | 53  | THR  | CB-CA-C  | -8.30 | 96.43       | 109.80   |
| 4   | Zc    | 125 | PRO  | N-CD-CG  | -7.78 | 94.46       | 103.80   |
| 7   | Ab    | 66  | GLY  | O-C-N    | -7.76 | 118.27      | 121.07   |
| 6   | WA    | 162 | PRO  | N-CA-C   | 7.75  | 128.44      | 112.47   |
| 11  | A9    | 72  | HIS  | CA-C-N   | -7.44 | 116.19      | 123.04   |
| 11  | A9    | 72  | HIS  | C-N-CA   | -7.44 | 116.19      | 123.04   |
| 7   | Ar    | 15  | LYS  | N-CA-C   | -7.33 | 102.89      | 111.03   |
| 11  | A9    | 72  | HIS  | CA-CB-CG | -7.33 | 106.47      | 113.80   |
| 4   | ZG    | 235 | ASN  | N-CA-C   | -7.30 | 104.89      | 114.31   |
| 7   | Ab    | 84  | LEU  | O-C-N    | -7.07 | 113.19      | 121.32   |
| 12  | BD    | 5   | ASN  | CB-CA-C  | -7.04 | 108.45      | 116.54   |
| 9   | Au    | 135 | ARG  | N-CA-C   | -6.83 | 103.45      | 111.03   |
| 6   | UI    | 129 | GLN  | CA-C-N   | -6.73 | 111.24      | 120.46   |
| 6   | UI    | 129 | GLN  | C-N-CA   | -6.73 | 111.24      | 120.46   |
| 6   | UP    | 129 | GLN  | CA-C-N   | -6.72 | 111.26      | 120.46   |
| 6   | UP    | 129 | GLN  | C-N-CA   | -6.72 | 111.26      | 120.46   |
| 6   | UO    | 129 | GLN  | CA-C-N   | -6.71 | 111.27      | 120.46   |
| 6   | UO    | 129 | GLN  | C-N-CA   | -6.71 | 111.27      | 120.46   |
| 6   | UK    | 129 | GLN  | CA-C-N   | -6.69 | 111.29      | 120.46   |
| 6   | UK    | 129 | GLN  | C-N-CA   | -6.69 | 111.29      | 120.46   |
| 6   | UJ    | 129 | GLN  | CA-C-N   | -6.69 | 111.30      | 120.46   |
| 6   | UJ    | 129 | GLN  | C-N-CA   | -6.69 | 111.30      | 120.46   |
| 6   | UM    | 129 | GLN  | CA-C-N   | -6.68 | 111.31      | 120.46   |
| 6   | UM    | 129 | GLN  | C-N-CA   | -6.68 | 111.31      | 120.46   |
| 6   | WA    | 162 | PRO  | CB-CA-C  | -6.65 | 100.58      | 111.56   |
| 6   | UL    | 129 | GLN  | CA-C-N   | -6.64 | 111.36      | 120.46   |
| 6   | UL    | 129 | GLN  | C-N-CA   | -6.64 | 111.36      | 120.46   |
| 6   | UN    | 129 | GLN  | CA-C-N   | -6.64 | 111.36      | 120.46   |
| 6   | UN    | 129 | GLN  | C-N-CA   | -6.64 | 111.36      | 120.46   |
| 9   | Au    | 162 | PRO  | N-CD-CG  | -6.59 | 93.31       | 103.20   |
| 6   | UN    | 181 | GLU  | O-C-N    | 6.42  | 127.91      | 121.30   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | UK    | 181 | GLU  | O-C-N   | 6.39  | 127.88      | 121.30   |
| 9   | Au    | 134 | LEU  | CA-C-N  | -6.37 | 111.96      | 120.63   |
| 9   | Au    | 134 | LEU  | C-N-CA  | -6.37 | 111.96      | 120.63   |
| 3   | AM    | 140 | ILE  | CA-C-N  | -6.37 | 113.93      | 122.72   |
| 3   | AM    | 140 | ILE  | C-N-CA  | -6.37 | 113.93      | 122.72   |
| 6   | UI    | 181 | GLU  | O-C-N   | 6.37  | 127.86      | 121.30   |
| 6   | UL    | 131 | ASN  | O-C-N   | 6.35  | 129.39      | 122.15   |
| 6   | UJ    | 181 | GLU  | O-C-N   | 6.33  | 127.82      | 121.30   |
| 6   | UN    | 131 | ASN  | O-C-N   | 6.32  | 129.36      | 122.15   |
| 6   | UK    | 131 | ASN  | O-C-N   | 6.30  | 129.33      | 122.15   |
| 6   | UL    | 221 | THR  | O-C-N   | -6.29 | 115.68      | 123.04   |
| 6   | UL    | 181 | GLU  | O-C-N   | 6.28  | 127.77      | 121.30   |
| 12  | BF    | 37  | PRO  | N-CA-C  | -6.28 | 104.48      | 113.47   |
| 6   | UK    | 221 | THR  | O-C-N   | -6.28 | 115.69      | 123.04   |
| 6   | UM    | 181 | GLU  | O-C-N   | 6.28  | 127.77      | 121.30   |
| 6   | UJ    | 270 | THR  | O-C-N   | -6.27 | 115.70      | 123.04   |
| 6   | UP    | 131 | ASN  | O-C-N   | 6.27  | 129.29      | 122.15   |
| 6   | UJ    | 131 | ASN  | O-C-N   | 6.27  | 129.29      | 122.15   |
| 6   | UP    | 181 | GLU  | O-C-N   | 6.26  | 127.75      | 121.30   |
| 6   | UN    | 221 | THR  | O-C-N   | -6.25 | 115.73      | 123.04   |
| 6   | UO    | 131 | ASN  | O-C-N   | 6.24  | 129.26      | 122.15   |
| 4   | Zb    | 397 | ASN  | N-CA-C  | -6.24 | 104.40      | 111.14   |
| 7   | Ab    | 85  | PRO  | CA-N-CD | -6.23 | 103.28      | 112.00   |
| 6   | UP    | 221 | THR  | O-C-N   | -6.23 | 115.75      | 123.04   |
| 6   | UO    | 181 | GLU  | O-C-N   | 6.22  | 127.71      | 121.30   |
| 6   | UM    | 131 | ASN  | O-C-N   | 6.21  | 129.23      | 122.15   |
| 6   | UM    | 221 | THR  | O-C-N   | -6.20 | 115.78      | 123.04   |
| 6   | UO    | 221 | THR  | O-C-N   | -6.20 | 115.78      | 123.04   |
| 9   | Av    | 162 | PRO  | N-CA-CB | -6.18 | 96.76       | 103.25   |
| 6   | UI    | 221 | THR  | O-C-N   | -6.18 | 115.81      | 123.04   |
| 6   | UI    | 131 | ASN  | O-C-N   | 6.17  | 129.19      | 122.15   |
| 6   | UN    | 127 | SER  | O-C-N   | 6.14  | 129.16      | 122.15   |
| 7   | Ab    | 87  | ILE  | N-CA-C  | -6.13 | 107.31      | 113.20   |
| 6   | UO    | 127 | SER  | O-C-N   | 6.13  | 129.14      | 122.15   |
| 6   | UJ    | 127 | SER  | O-C-N   | 6.13  | 129.14      | 122.15   |
| 6   | UL    | 127 | SER  | O-C-N   | 6.12  | 129.13      | 122.15   |
| 6   | UK    | 127 | SER  | O-C-N   | 6.11  | 129.12      | 122.15   |
| 3   | 0     | 52  | PRO  | N-CA-CB | -6.09 | 96.30       | 103.00   |
| 6   | UM    | 127 | SER  | O-C-N   | 6.09  | 129.10      | 122.15   |
| 6   | UI    | 127 | SER  | O-C-N   | 6.08  | 129.09      | 122.15   |
| 9   | Ay    | 84  | PRO  | N-CA-C  | -6.04 | 103.33      | 110.70   |
| 11  | A6    | 52  | VAL  | CA-C-N  | -6.00 | 110.69      | 120.71   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | A6    | 52  | VAL  | C-N-CA   | -6.00 | 110.69      | 120.71   |
| 6   | UP    | 127 | SER  | O-C-N    | 5.95  | 128.93      | 122.15   |
| 3   | AG    | 140 | ILE  | CA-C-N   | -5.89 | 114.59      | 122.72   |
| 3   | AG    | 140 | ILE  | C-N-CA   | -5.89 | 114.59      | 122.72   |
| 3   | AG    | 196 | GLN  | N-CA-C   | -5.89 | 104.86      | 111.28   |
| 6   | UK    | 132 | TYR  | O-C-N    | 5.84  | 128.08      | 122.07   |
| 3   | 7     | 19  | MET  | CA-C-N   | -5.80 | 112.44      | 120.38   |
| 3   | 7     | 19  | MET  | C-N-CA   | -5.80 | 112.44      | 120.38   |
| 6   | UJ    | 132 | TYR  | O-C-N    | 5.76  | 128.00      | 122.07   |
| 6   | UP    | 132 | TYR  | O-C-N    | 5.76  | 128.00      | 122.07   |
| 3   | 8     | 19  | MET  | CA-C-N   | -5.75 | 112.57      | 120.28   |
| 3   | 8     | 19  | MET  | C-N-CA   | -5.75 | 112.57      | 120.28   |
| 3   | AH    | 5   | LEU  | N-CA-C   | -5.75 | 106.10      | 113.23   |
| 4   | ZI    | 322 | ASN  | CB-CA-C  | -5.75 | 103.03      | 111.77   |
| 6   | UI    | 132 | TYR  | O-C-N    | 5.73  | 127.97      | 122.07   |
| 4   | ZV    | 125 | PRO  | CA-CB-CG | -5.68 | 93.20       | 104.00   |
| 6   | UM    | 132 | TYR  | O-C-N    | 5.68  | 127.92      | 122.07   |
| 6   | UO    | 132 | TYR  | O-C-N    | 5.68  | 127.92      | 122.07   |
| 6   | UL    | 132 | TYR  | O-C-N    | 5.68  | 127.92      | 122.07   |
| 3   | AH    | 4   | SER  | N-CA-C   | -5.67 | 107.36      | 114.56   |
| 6   | UN    | 132 | TYR  | O-C-N    | 5.66  | 127.90      | 122.07   |
| 6   | WI    | 167 | ARG  | CB-CA-C  | -5.63 | 109.58      | 117.23   |
| 6   | WB    | 221 | THR  | CB-CA-C  | -5.62 | 108.98      | 117.07   |
| 4   | ZF    | 134 | PRO  | N-CA-CB  | -5.61 | 98.32       | 103.25   |
| 4   | ZH    | 397 | ASN  | N-CA-C   | -5.61 | 105.07      | 111.07   |
| 9   | Av    | 120 | LYS  | N-CA-C   | -5.61 | 104.25      | 113.50   |
| 6   | BG    | 322 | PRO  | N-CA-CB  | -5.61 | 96.83       | 103.00   |
| 4   | Zc    | 125 | PRO  | CB-CG-CD | -5.60 | 92.52       | 105.40   |
| 4   | ZG    | 4   | SER  | N-CA-C   | -5.57 | 107.13      | 114.31   |
| 4   | ZP    | 125 | PRO  | CA-N-CD  | -5.56 | 103.71      | 111.50   |
| 4   | ZV    | 140 | PRO  | N-CA-CB  | -5.55 | 98.37       | 103.31   |
| 6   | WJ    | 214 | ASP  | CB-CA-C  | -5.53 | 99.98       | 113.15   |
| 6   | AV    | 261 | ASN  | N-CA-C   | -5.49 | 106.44      | 113.02   |
| 6   | UN    | 125 | GLN  | CA-C-N   | -5.49 | 112.86      | 120.38   |
| 6   | UN    | 125 | GLN  | C-N-CA   | -5.49 | 112.86      | 120.38   |
| 6   | UJ    | 125 | GLN  | CA-C-N   | -5.48 | 112.87      | 120.38   |
| 6   | UJ    | 125 | GLN  | C-N-CA   | -5.48 | 112.87      | 120.38   |
| 4   | ZT    | 3   | PHE  | N-CA-C   | -5.47 | 106.58      | 113.20   |
| 6   | UK    | 125 | GLN  | CA-C-N   | -5.46 | 112.90      | 120.38   |
| 6   | UK    | 125 | GLN  | C-N-CA   | -5.46 | 112.90      | 120.38   |
| 6   | UO    | 125 | GLN  | CA-C-N   | -5.45 | 112.91      | 120.38   |
| 6   | UO    | 125 | GLN  | C-N-CA   | -5.45 | 112.91      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | UI    | 125 | GLN  | CA-C-N | -5.45 | 112.92      | 120.38   |
| 6   | UI    | 125 | GLN  | C-N-CA | -5.45 | 112.92      | 120.38   |
| 6   | UP    | 125 | GLN  | CA-C-N | -5.45 | 112.92      | 120.38   |
| 6   | UP    | 125 | GLN  | C-N-CA | -5.45 | 112.92      | 120.38   |
| 3   | AJ    | 65  | GLY  | CA-C-O | -5.43 | 117.89      | 122.29   |
| 6   | AR    | 261 | ASN  | N-CA-C | -5.43 | 106.51      | 113.02   |
| 6   | WM    | 220 | LEU  | N-CA-C | -5.43 | 106.63      | 113.20   |
| 6   | UL    | 125 | GLN  | CA-C-N | -5.42 | 112.96      | 120.38   |
| 6   | UL    | 125 | GLN  | C-N-CA | -5.42 | 112.96      | 120.38   |
| 6   | WO    | 220 | LEU  | N-CA-C | -5.41 | 106.65      | 113.20   |
| 6   | Ak    | 261 | ASN  | N-CA-C | -5.41 | 106.53      | 113.02   |
| 6   | Ao    | 261 | ASN  | N-CA-C | -5.41 | 106.53      | 113.02   |
| 3   | AI    | 63  | PRO  | O-C-N  | -5.40 | 115.35      | 122.64   |
| 6   | Aj    | 261 | ASN  | N-CA-C | -5.40 | 106.54      | 113.02   |
| 4   | ZO    | 141 | ASN  | N-CA-C | -5.40 | 106.69      | 113.28   |
| 6   | AT    | 261 | ASN  | N-CA-C | -5.40 | 106.54      | 113.02   |
| 4   | ZG    | 47  | LYS  | N-CA-C | -5.40 | 106.62      | 114.12   |
| 6   | AY    | 261 | ASN  | N-CA-C | -5.40 | 106.54      | 113.02   |
| 6   | BW    | 261 | ASN  | N-CA-C | -5.39 | 106.55      | 113.02   |
| 6   | UM    | 125 | GLN  | CA-C-N | -5.39 | 112.99      | 120.38   |
| 6   | UM    | 125 | GLN  | C-N-CA | -5.39 | 112.99      | 120.38   |
| 6   | AP    | 261 | ASN  | N-CA-C | -5.39 | 106.55      | 113.02   |
| 6   | AQ    | 261 | ASN  | N-CA-C | -5.38 | 106.56      | 113.02   |
| 6   | Ad    | 261 | ASN  | N-CA-C | -5.38 | 106.56      | 113.02   |
| 6   | Am    | 261 | ASN  | N-CA-C | -5.38 | 106.56      | 113.02   |
| 6   | WS    | 220 | LEU  | N-CA-C | -5.37 | 106.70      | 113.20   |
| 6   | BS    | 261 | ASN  | N-CA-C | -5.37 | 106.57      | 113.02   |
| 6   | BV    | 261 | ASN  | N-CA-C | -5.37 | 106.58      | 113.02   |
| 6   | Ae    | 261 | ASN  | N-CA-C | -5.36 | 106.58      | 113.02   |
| 6   | BX    | 261 | ASN  | N-CA-C | -5.36 | 106.58      | 113.02   |
| 6   | WW    | 220 | LEU  | N-CA-C | -5.36 | 106.72      | 113.20   |
| 6   | AZ    | 261 | ASN  | N-CA-C | -5.35 | 106.60      | 113.02   |
| 9   | Aw    | 134 | LEU  | CA-C-N | -5.35 | 113.17      | 120.44   |
| 9   | Aw    | 134 | LEU  | C-N-CA | -5.35 | 113.17      | 120.44   |
| 6   | Ah    | 261 | ASN  | N-CA-C | -5.35 | 106.60      | 113.02   |
| 6   | BU    | 261 | ASN  | N-CA-C | -5.35 | 106.61      | 113.02   |
| 6   | Af    | 261 | ASN  | N-CA-C | -5.34 | 106.61      | 113.02   |
| 6   | AO    | 261 | ASN  | N-CA-C | -5.34 | 106.61      | 113.02   |
| 9   | Ay    | 66  | ARG  | N-CA-C | -5.34 | 106.61      | 113.02   |
| 6   | UN    | 130 | VAL  | CA-C-N | -5.34 | 112.71      | 120.29   |
| 6   | UN    | 130 | VAL  | C-N-CA | -5.34 | 112.71      | 120.29   |
| 6   | An    | 261 | ASN  | N-CA-C | -5.33 | 106.62      | 113.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | WH    | 220 | LEU  | N-CA-C  | -5.33 | 106.75      | 113.20   |
| 6   | WL    | 220 | LEU  | N-CA-C  | -5.33 | 106.75      | 113.20   |
| 6   | Ac    | 261 | ASN  | N-CA-C  | -5.32 | 106.63      | 113.02   |
| 6   | AW    | 261 | ASN  | N-CA-C  | -5.32 | 106.64      | 113.02   |
| 6   | Ap    | 261 | ASN  | N-CA-C  | -5.32 | 106.64      | 113.02   |
| 6   | Al    | 261 | ASN  | N-CA-C  | -5.32 | 106.64      | 113.02   |
| 6   | AS    | 261 | ASN  | N-CA-C  | -5.31 | 106.65      | 113.02   |
| 6   | AU    | 261 | ASN  | N-CA-C  | -5.31 | 106.65      | 113.02   |
| 6   | UI    | 130 | VAL  | CA-C-N  | -5.31 | 112.75      | 120.29   |
| 6   | UI    | 130 | VAL  | C-N-CA  | -5.31 | 112.75      | 120.29   |
| 6   | BT    | 261 | ASN  | N-CA-C  | -5.31 | 106.65      | 113.02   |
| 6   | AX    | 261 | ASN  | N-CA-C  | -5.31 | 106.65      | 113.02   |
| 6   | Aa    | 261 | ASN  | N-CA-C  | -5.30 | 106.66      | 113.02   |
| 6   | UK    | 130 | VAL  | CA-C-N  | -5.30 | 112.77      | 120.29   |
| 6   | UK    | 130 | VAL  | C-N-CA  | -5.30 | 112.77      | 120.29   |
| 3   | 8     | 153 | ARG  | N-CA-C  | -5.29 | 106.85      | 113.15   |
| 6   | WE    | 160 | PRO  | N-CA-CB | -5.29 | 97.70       | 103.25   |
| 6   | Ai    | 261 | ASN  | N-CA-C  | -5.29 | 106.68      | 113.02   |
| 6   | UO    | 130 | VAL  | CA-C-N  | -5.29 | 112.79      | 120.29   |
| 6   | UO    | 130 | VAL  | C-N-CA  | -5.29 | 112.79      | 120.29   |
| 6   | BR    | 261 | ASN  | N-CA-C  | -5.29 | 106.68      | 113.02   |
| 3   | AI    | 257 | LEU  | CA-C-N  | -5.28 | 112.29      | 120.31   |
| 3   | AI    | 257 | LEU  | C-N-CA  | -5.28 | 112.29      | 120.31   |
| 6   | UJ    | 130 | VAL  | CA-C-N  | -5.27 | 112.81      | 120.29   |
| 6   | UJ    | 130 | VAL  | C-N-CA  | -5.27 | 112.81      | 120.29   |
| 6   | UP    | 130 | VAL  | CA-C-N  | -5.26 | 112.82      | 120.29   |
| 6   | UP    | 130 | VAL  | C-N-CA  | -5.26 | 112.82      | 120.29   |
| 3   | 0     | 4   | SER  | CA-C-N  | -5.25 | 113.24      | 120.28   |
| 3   | 0     | 4   | SER  | C-N-CA  | -5.25 | 113.24      | 120.28   |
| 6   | UM    | 130 | VAL  | CA-C-N  | -5.25 | 112.83      | 120.29   |
| 6   | UM    | 130 | VAL  | C-N-CA  | -5.25 | 112.83      | 120.29   |
| 6   | WN    | 220 | LEU  | N-CA-C  | -5.25 | 106.84      | 113.20   |
| 2   | h     | 248 | PRO  | N-CA-CB | -5.24 | 97.75       | 103.25   |
| 2   | y     | 248 | PRO  | N-CA-CB | -5.24 | 97.74       | 103.25   |
| 2   | p     | 248 | PRO  | N-CA-CB | -5.24 | 97.75       | 103.25   |
| 6   | UL    | 130 | VAL  | CA-C-N  | -5.24 | 112.85      | 120.29   |
| 6   | UL    | 130 | VAL  | C-N-CA  | -5.24 | 112.85      | 120.29   |
| 2   | n     | 248 | PRO  | N-CA-CB | -5.23 | 97.76       | 103.25   |
| 2   | u     | 248 | PRO  | N-CA-CB | -5.23 | 97.76       | 103.25   |
| 6   | Ag    | 261 | ASN  | N-CA-C  | -5.23 | 106.75      | 113.02   |
| 2   | j     | 248 | PRO  | N-CA-CB | -5.23 | 97.76       | 103.25   |
| 2   | w     | 248 | PRO  | N-CA-CB | -5.23 | 97.76       | 103.25   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | Ay    | 143 | ARG  | CB-CG-CD | -5.23 | 99.28       | 111.30   |
| 2   | e     | 248 | PRO  | N-CA-CB  | -5.22 | 97.77       | 103.25   |
| 2   | i     | 248 | PRO  | N-CA-CB  | -5.22 | 97.76       | 103.25   |
| 2   | d     | 248 | PRO  | N-CA-CB  | -5.22 | 97.77       | 103.25   |
| 2   | k     | 248 | PRO  | N-CA-CB  | -5.22 | 97.77       | 103.25   |
| 2   | r     | 248 | PRO  | N-CA-CB  | -5.21 | 97.78       | 103.25   |
| 2   | o     | 248 | PRO  | N-CA-CB  | -5.21 | 97.78       | 103.25   |
| 2   | g     | 248 | PRO  | N-CA-CB  | -5.21 | 97.78       | 103.25   |
| 2   | f     | 248 | PRO  | N-CA-CB  | -5.21 | 97.78       | 103.25   |
| 2   | m     | 248 | PRO  | N-CA-CB  | -5.20 | 97.79       | 103.25   |
| 2   | q     | 248 | PRO  | N-CA-CB  | -5.20 | 97.80       | 103.25   |
| 2   | z     | 248 | PRO  | N-CA-CB  | -5.19 | 97.81       | 103.25   |
| 3   | AN    | 116 | ARG  | N-CA-C   | -5.19 | 107.62      | 114.31   |
| 2   | c     | 248 | PRO  | N-CA-CB  | -5.18 | 97.81       | 103.25   |
| 6   | WI    | 165 | PHE  | CB-CA-C  | 5.18  | 119.70      | 111.51   |
| 4   | ZN    | 218 | PRO  | CA-N-CD  | -5.18 | 104.75      | 112.00   |
| 2   | t     | 248 | PRO  | N-CA-CB  | -5.18 | 97.81       | 103.25   |
| 6   | UL    | 128 | GLU  | O-C-N    | 5.18  | 127.68      | 122.09   |
| 9   | Aw    | 135 | ARG  | N-CA-C   | -5.17 | 105.55      | 111.14   |
| 2   | x     | 248 | PRO  | N-CA-CB  | -5.17 | 97.82       | 103.25   |
| 2   | b     | 248 | PRO  | N-CA-CB  | -5.17 | 97.82       | 103.25   |
| 2   | l     | 248 | PRO  | N-CA-CB  | -5.17 | 97.82       | 103.25   |
| 6   | UI    | 128 | GLU  | CA-C-N   | -5.17 | 113.72      | 120.44   |
| 6   | UI    | 128 | GLU  | C-N-CA   | -5.17 | 113.72      | 120.44   |
| 6   | UL    | 128 | GLU  | CA-C-N   | -5.16 | 113.73      | 120.44   |
| 6   | UL    | 128 | GLU  | C-N-CA   | -5.16 | 113.73      | 120.44   |
| 2   | v     | 248 | PRO  | N-CA-CB  | -5.16 | 97.84       | 103.25   |
| 2   | s     | 248 | PRO  | N-CA-CB  | -5.15 | 97.84       | 103.25   |
| 2   | a     | 248 | PRO  | N-CA-CB  | -5.15 | 97.84       | 103.25   |
| 6   | UP    | 128 | GLU  | CA-C-N   | -5.14 | 113.75      | 120.44   |
| 6   | UP    | 128 | GLU  | C-N-CA   | -5.14 | 113.75      | 120.44   |
| 6   | WO    | 167 | ARG  | CA-C-O   | -5.13 | 114.91      | 120.09   |
| 6   | UM    | 128 | GLU  | CA-C-N   | -5.13 | 113.77      | 120.44   |
| 6   | UM    | 128 | GLU  | C-N-CA   | -5.13 | 113.77      | 120.44   |
| 6   | WU    | 164 | LEU  | N-CA-C   | -5.13 | 106.97      | 113.18   |
| 6   | UK    | 128 | GLU  | CA-C-N   | -5.13 | 113.77      | 120.44   |
| 6   | UK    | 128 | GLU  | C-N-CA   | -5.13 | 113.77      | 120.44   |
| 3   | 2     | 237 | GLN  | N-CA-C   | -5.12 | 105.14      | 111.33   |
| 6   | UM    | 128 | GLU  | O-C-N    | 5.12  | 127.61      | 122.09   |
| 4   | Zh    | 3   | PHE  | N-CA-C   | -5.11 | 105.14      | 111.33   |
| 4   | Za    | 126 | PRO  | CA-N-CD  | -5.10 | 104.86      | 112.00   |
| 4   | ZG    | 3   | PHE  | N-CA-C   | -5.09 | 106.47      | 113.30   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | UJ    | 128 | GLU  | CA-C-N  | -5.09 | 113.82      | 120.44   |
| 6   | UJ    | 128 | GLU  | C-N-CA  | -5.09 | 113.82      | 120.44   |
| 6   | UN    | 128 | GLU  | CA-C-N  | -5.09 | 113.82      | 120.44   |
| 6   | UN    | 128 | GLU  | C-N-CA  | -5.09 | 113.82      | 120.44   |
| 9   | Ay    | 67  | ILE  | N-CA-C  | -5.09 | 105.91      | 113.39   |
| 5   | AA    | 48  | GLY  | CA-C-O  | -5.08 | 116.72      | 121.90   |
| 6   | UK    | 128 | GLU  | O-C-N   | 5.07  | 127.57      | 122.09   |
| 6   | WO    | 168 | GLU  | CB-CA-C | -5.07 | 100.33      | 110.42   |
| 6   | UP    | 128 | GLU  | O-C-N   | 5.06  | 127.56      | 122.09   |
| 4   | Zd    | 323 | ASN  | N-CA-C  | -5.06 | 105.95      | 111.82   |
| 6   | UO    | 128 | GLU  | CA-C-N  | -5.06 | 113.87      | 120.44   |
| 6   | UO    | 128 | GLU  | C-N-CA  | -5.06 | 113.87      | 120.44   |
| 6   | UI    | 128 | GLU  | O-C-N   | 5.05  | 127.54      | 122.09   |
| 6   | UO    | 128 | GLU  | O-C-N   | 5.00  | 127.49      | 122.09   |
| 6   | WW    | 164 | LEU  | N-CA-C  | -5.00 | 106.43      | 112.88   |

There are no chirality outliers.

All (113) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 0     | 36  | ARG  | Sidechain |
| 3   | 0     | 50  | ARG  | Sidechain |
| 3   | 1     | 36  | ARG  | Sidechain |
| 3   | 5     | 50  | ARG  | Sidechain |
| 3   | 5     | 73  | ARG  | Sidechain |
| 3   | 7     | 73  | ARG  | Sidechain |
| 3   | 8     | 238 | ARG  | Sidechain |
| 3   | 8     | 38  | ARG  | Sidechain |
| 11  | A0    | 104 | ARG  | Sidechain |
| 11  | A6    | 106 | ARG  | Sidechain |
| 11  | A7    | 55  | ARG  | Sidechain |
| 11  | A9    | 4   | ARG  | Sidechain |
| 5   | AA    | 243 | ARG  | Sidechain |
| 5   | AB    | 225 | ARG  | Sidechain |
| 5   | AB    | 54  | ARG  | Sidechain |
| 5   | AD    | 200 | ARG  | Sidechain |
| 3   | AF    | 36  | ARG  | Sidechain |
| 3   | AI    | 116 | ARG  | Sidechain |
| 3   | AK    | 79  | ARG  | Sidechain |
| 3   | AL    | 73  | ARG  | Sidechain |
| 3   | AM    | 36  | ARG  | Sidechain |
| 3   | AM    | 50  | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | AN    | 116 | ARG  | Sidechain |
| 3   | AN    | 153 | ARG  | Sidechain |
| 3   | AN    | 238 | ARG  | Sidechain |
| 9   | Aw    | 135 | ARG  | Sidechain |
| 9   | Aw    | 143 | ARG  | Sidechain |
| 9   | Ay    | 140 | ARG  | Sidechain |
| 9   | Ay    | 143 | ARG  | Sidechain |
| 12  | BD    | 110 | ARG  | Sidechain |
| 12  | BF    | 110 | ARG  | Sidechain |
| 6   | UI    | 221 | THR  | Mainchain |
| 6   | UI    | 50  | ASP  | Mainchain |
| 6   | UJ    | 270 | THR  | Mainchain |
| 6   | UJ    | 50  | ASP  | Mainchain |
| 6   | UK    | 167 | ARG  | Sidechain |
| 6   | UK    | 221 | THR  | Mainchain |
| 6   | UK    | 50  | ASP  | Mainchain |
| 6   | UL    | 167 | ARG  | Sidechain |
| 6   | UL    | 221 | THR  | Mainchain |
| 6   | UL    | 50  | ASP  | Mainchain |
| 6   | UM    | 221 | THR  | Mainchain |
| 6   | UM    | 50  | ASP  | Mainchain |
| 6   | UN    | 221 | THR  | Mainchain |
| 6   | UN    | 50  | ASP  | Mainchain |
| 6   | UO    | 221 | THR  | Mainchain |
| 6   | UO    | 50  | ASP  | Mainchain |
| 6   | UP    | 167 | ARG  | Sidechain |
| 6   | UP    | 221 | THR  | Mainchain |
| 6   | UP    | 50  | ASP  | Mainchain |
| 6   | WA    | 134 | ARG  | Sidechain |
| 6   | WA    | 142 | ARG  | Sidechain |
| 6   | WA    | 167 | ARG  | Sidechain |
| 6   | WB    | 134 | ARG  | Sidechain |
| 6   | WB    | 142 | ARG  | Sidechain |
| 6   | WB    | 154 | ARG  | Sidechain |
| 6   | WB    | 167 | ARG  | Sidechain |
| 6   | WC    | 134 | ARG  | Sidechain |
| 6   | WC    | 142 | ARG  | Sidechain |
| 6   | WC    | 167 | ARG  | Sidechain |
| 6   | WD    | 134 | ARG  | Sidechain |
| 6   | WE    | 134 | ARG  | Sidechain |
| 6   | WE    | 142 | ARG  | Sidechain |
| 6   | WF    | 134 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 6   | WF    | 142 | ARG  | Sidechain |
| 6   | WF    | 167 | ARG  | Sidechain |
| 6   | WG    | 134 | ARG  | Sidechain |
| 6   | WG    | 142 | ARG  | Sidechain |
| 6   | WG    | 167 | ARG  | Sidechain |
| 6   | WI    | 142 | ARG  | Sidechain |
| 6   | WJ    | 134 | ARG  | Sidechain |
| 6   | WJ    | 142 | ARG  | Sidechain |
| 6   | WJ    | 167 | ARG  | Sidechain |
| 6   | WK    | 134 | ARG  | Sidechain |
| 6   | WK    | 142 | ARG  | Sidechain |
| 6   | WL    | 134 | ARG  | Sidechain |
| 6   | WL    | 157 | LEU  | Mainchain |
| 6   | WM    | 134 | ARG  | Sidechain |
| 6   | WN    | 134 | ARG  | Sidechain |
| 6   | WO    | 134 | ARG  | Sidechain |
| 6   | WP    | 134 | ARG  | Sidechain |
| 6   | WP    | 142 | ARG  | Sidechain |
| 6   | WP    | 154 | ARG  | Sidechain |
| 6   | WQ    | 134 | ARG  | Sidechain |
| 6   | WQ    | 142 | ARG  | Sidechain |
| 6   | WR    | 134 | ARG  | Sidechain |
| 6   | WR    | 142 | ARG  | Sidechain |
| 6   | WR    | 167 | ARG  | Sidechain |
| 6   | WS    | 167 | ARG  | Sidechain |
| 6   | WT    | 134 | ARG  | Sidechain |
| 6   | WT    | 142 | ARG  | Sidechain |
| 6   | WU    | 134 | ARG  | Sidechain |
| 6   | WU    | 142 | ARG  | Sidechain |
| 6   | WV    | 134 | ARG  | Sidechain |
| 6   | WV    | 142 | ARG  | Sidechain |
| 6   | WV    | 167 | ARG  | Sidechain |
| 6   | WW    | 134 | ARG  | Sidechain |
| 6   | WW    | 167 | ARG  | Sidechain |
| 3   | ZA    | 50  | ARG  | Sidechain |
| 3   | ZA    | 79  | ARG  | Sidechain |
| 3   | ZD    | 238 | ARG  | Sidechain |
| 3   | ZE    | 238 | ARG  | Sidechain |
| 3   | ZE    | 50  | ARG  | Sidechain |
| 3   | ZE    | 79  | ARG  | Sidechain |
| 4   | ZI    | 380 | ARG  | Sidechain |
| 4   | ZK    | 71  | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | ZO    | 71  | ARG  | Sidechain |
| 4   | ZT    | 106 | ARG  | Sidechain |
| 4   | ZU    | 96  | ARG  | Sidechain |
| 4   | ZW    | 71  | ARG  | Sidechain |
| 4   | ZZ    | 380 | ARG  | Sidechain |
| 4   | Zd    | 380 | ARG  | Sidechain |
| 4   | Ze    | 380 | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1580  | 0        | 1534     | 99      | 0            |
| 1   | B     | 1580  | 0        | 1534     | 100     | 0            |
| 1   | C     | 1580  | 0        | 1534     | 104     | 0            |
| 1   | D     | 1580  | 0        | 1534     | 101     | 0            |
| 1   | E     | 1580  | 0        | 1534     | 105     | 0            |
| 1   | F     | 1580  | 0        | 1534     | 104     | 0            |
| 1   | G     | 1580  | 0        | 1534     | 100     | 0            |
| 1   | H     | 1580  | 0        | 1534     | 102     | 0            |
| 1   | I     | 1580  | 0        | 1534     | 102     | 0            |
| 1   | J     | 1580  | 0        | 1534     | 102     | 0            |
| 1   | K     | 1580  | 0        | 1534     | 104     | 0            |
| 1   | L     | 1580  | 0        | 1534     | 110     | 0            |
| 1   | M     | 1580  | 0        | 1534     | 105     | 0            |
| 1   | N     | 1580  | 0        | 1534     | 106     | 0            |
| 1   | O     | 1580  | 0        | 1534     | 103     | 0            |
| 1   | P     | 1580  | 0        | 1534     | 102     | 0            |
| 1   | Q     | 1580  | 0        | 1534     | 105     | 0            |
| 1   | R     | 1580  | 0        | 1534     | 106     | 0            |
| 1   | S     | 1580  | 0        | 1534     | 102     | 0            |
| 1   | T     | 1580  | 0        | 1534     | 104     | 0            |
| 1   | U     | 1580  | 0        | 1534     | 102     | 0            |
| 1   | V     | 1580  | 0        | 1534     | 101     | 0            |
| 1   | W     | 1580  | 0        | 1534     | 103     | 0            |
| 1   | X     | 1580  | 0        | 1534     | 101     | 0            |
| 1   | Y     | 1580  | 0        | 1534     | 100     | 0            |
| 1   | Z     | 1580  | 0        | 1534     | 101     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | a     | 2228  | 0        | 2265     | 137     | 0            |
| 2   | b     | 2228  | 0        | 2265     | 138     | 0            |
| 2   | c     | 2228  | 0        | 2265     | 140     | 0            |
| 2   | d     | 2228  | 0        | 2265     | 134     | 0            |
| 2   | e     | 2228  | 0        | 2265     | 137     | 0            |
| 2   | f     | 2228  | 0        | 2265     | 136     | 0            |
| 2   | g     | 2228  | 0        | 2265     | 133     | 0            |
| 2   | h     | 2228  | 0        | 2265     | 130     | 0            |
| 2   | i     | 2228  | 0        | 2265     | 129     | 0            |
| 2   | j     | 2228  | 0        | 2265     | 133     | 0            |
| 2   | k     | 2228  | 0        | 2265     | 132     | 0            |
| 2   | l     | 2228  | 0        | 2265     | 131     | 0            |
| 2   | m     | 2228  | 0        | 2265     | 134     | 0            |
| 2   | n     | 2228  | 0        | 2265     | 132     | 0            |
| 2   | o     | 2228  | 0        | 2265     | 133     | 0            |
| 2   | p     | 2228  | 0        | 2265     | 138     | 0            |
| 2   | q     | 2228  | 0        | 2265     | 135     | 0            |
| 2   | r     | 2228  | 0        | 2265     | 141     | 0            |
| 2   | s     | 2228  | 0        | 2265     | 135     | 0            |
| 2   | t     | 2228  | 0        | 2265     | 130     | 0            |
| 2   | u     | 2228  | 0        | 2265     | 131     | 0            |
| 2   | v     | 2228  | 0        | 2265     | 133     | 0            |
| 2   | w     | 2228  | 0        | 2265     | 133     | 0            |
| 2   | x     | 2228  | 0        | 2265     | 135     | 0            |
| 2   | y     | 2228  | 0        | 2265     | 136     | 0            |
| 2   | z     | 2228  | 0        | 2265     | 129     | 0            |
| 3   | 0     | 1866  | 0        | 1848     | 134     | 0            |
| 3   | 1     | 1894  | 0        | 1878     | 129     | 0            |
| 3   | 2     | 1949  | 0        | 1926     | 104     | 0            |
| 3   | 3     | 1949  | 0        | 1926     | 91      | 0            |
| 3   | 4     | 1949  | 0        | 1926     | 114     | 0            |
| 3   | 5     | 1949  | 0        | 1926     | 117     | 0            |
| 3   | 6     | 1949  | 0        | 1926     | 112     | 0            |
| 3   | 7     | 1949  | 0        | 1926     | 89      | 0            |
| 3   | 8     | 1949  | 0        | 1926     | 114     | 0            |
| 3   | 9     | 1949  | 0        | 1926     | 92      | 0            |
| 3   | AF    | 1903  | 0        | 1878     | 145     | 0            |
| 3   | AG    | 1911  | 0        | 1889     | 189     | 0            |
| 3   | AH    | 1919  | 0        | 1901     | 151     | 0            |
| 3   | AI    | 1903  | 0        | 1878     | 177     | 0            |
| 3   | AJ    | 1911  | 0        | 1889     | 193     | 0            |
| 3   | AK    | 1823  | 0        | 1797     | 131     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | AL    | 1866  | 0        | 1848     | 156     | 0            |
| 3   | AM    | 1866  | 0        | 1848     | 161     | 0            |
| 3   | AN    | 1866  | 0        | 1848     | 106     | 0            |
| 3   | ZA    | 1949  | 0        | 1926     | 148     | 0            |
| 3   | ZB    | 1949  | 0        | 1926     | 117     | 0            |
| 3   | ZC    | 1949  | 0        | 1926     | 101     | 0            |
| 3   | ZD    | 1949  | 0        | 1926     | 124     | 0            |
| 3   | ZE    | 1949  | 0        | 1926     | 103     | 0            |
| 4   | ZF    | 2947  | 0        | 2839     | 103     | 0            |
| 4   | ZG    | 2947  | 0        | 2839     | 103     | 0            |
| 4   | ZH    | 2947  | 0        | 2839     | 131     | 0            |
| 4   | ZI    | 2947  | 0        | 2839     | 122     | 0            |
| 4   | ZJ    | 2947  | 0        | 2839     | 101     | 0            |
| 4   | ZK    | 2947  | 0        | 2839     | 80      | 0            |
| 4   | ZL    | 2947  | 0        | 2839     | 96      | 0            |
| 4   | ZM    | 2947  | 0        | 2839     | 90      | 0            |
| 4   | ZN    | 2947  | 0        | 2839     | 101     | 0            |
| 4   | ZO    | 2947  | 0        | 2839     | 88      | 0            |
| 4   | ZP    | 2947  | 0        | 2839     | 118     | 0            |
| 4   | ZQ    | 2947  | 0        | 2839     | 135     | 0            |
| 4   | ZR    | 2947  | 0        | 2839     | 100     | 0            |
| 4   | ZS    | 2947  | 0        | 2839     | 116     | 0            |
| 4   | ZT    | 2947  | 0        | 2839     | 108     | 0            |
| 4   | ZU    | 2947  | 0        | 2839     | 149     | 0            |
| 4   | ZV    | 2947  | 0        | 2839     | 118     | 0            |
| 4   | ZW    | 2947  | 0        | 2839     | 111     | 0            |
| 4   | ZX    | 2947  | 0        | 2839     | 94      | 0            |
| 4   | ZY    | 2947  | 0        | 2839     | 109     | 0            |
| 4   | ZZ    | 2947  | 0        | 2839     | 90      | 0            |
| 4   | Za    | 2947  | 0        | 2839     | 104     | 0            |
| 4   | Zb    | 2947  | 0        | 2839     | 97      | 0            |
| 4   | Zc    | 2947  | 0        | 2839     | 98      | 0            |
| 4   | Zd    | 2947  | 0        | 2839     | 84      | 0            |
| 4   | Ze    | 2947  | 0        | 2839     | 55      | 0            |
| 4   | Zf    | 2947  | 0        | 2839     | 111     | 0            |
| 4   | Zg    | 2947  | 0        | 2839     | 69      | 0            |
| 4   | Zh    | 2947  | 0        | 2839     | 68      | 0            |
| 5   | AA    | 1804  | 0        | 1791     | 187     | 0            |
| 5   | AB    | 1812  | 0        | 1800     | 226     | 0            |
| 5   | AC    | 1820  | 0        | 1812     | 167     | 0            |
| 5   | AD    | 1820  | 0        | 1812     | 213     | 0            |
| 5   | AE    | 1812  | 0        | 1800     | 239     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | AO    | 1275  | 0        | 1254     | 31      | 0            |
| 6   | AP    | 1275  | 0        | 1254     | 39      | 0            |
| 6   | AQ    | 1275  | 0        | 1254     | 34      | 0            |
| 6   | AR    | 1275  | 0        | 1254     | 33      | 0            |
| 6   | AS    | 1275  | 0        | 1254     | 60      | 0            |
| 6   | AT    | 1275  | 0        | 1254     | 42      | 0            |
| 6   | AU    | 1275  | 0        | 1254     | 29      | 0            |
| 6   | AV    | 1275  | 0        | 1254     | 43      | 0            |
| 6   | AW    | 1275  | 0        | 1254     | 40      | 0            |
| 6   | AX    | 1275  | 0        | 1254     | 50      | 0            |
| 6   | AY    | 1275  | 0        | 1254     | 54      | 0            |
| 6   | AZ    | 1275  | 0        | 1254     | 33      | 0            |
| 6   | Aa    | 1275  | 0        | 1254     | 29      | 0            |
| 6   | Ac    | 1275  | 0        | 1254     | 31      | 0            |
| 6   | Ad    | 1275  | 0        | 1254     | 44      | 0            |
| 6   | Ae    | 1275  | 0        | 1254     | 46      | 0            |
| 6   | Af    | 1275  | 0        | 1254     | 47      | 0            |
| 6   | Ag    | 1275  | 0        | 1254     | 45      | 0            |
| 6   | Ah    | 1275  | 0        | 1254     | 31      | 0            |
| 6   | Ai    | 1275  | 0        | 1254     | 36      | 0            |
| 6   | Aj    | 1275  | 0        | 1254     | 55      | 0            |
| 6   | Ak    | 1275  | 0        | 1254     | 49      | 0            |
| 6   | Al    | 1275  | 0        | 1254     | 43      | 0            |
| 6   | Am    | 1275  | 0        | 1254     | 40      | 0            |
| 6   | An    | 1275  | 0        | 1254     | 40      | 0            |
| 6   | Ao    | 1275  | 0        | 1254     | 40      | 0            |
| 6   | Ap    | 1275  | 0        | 1254     | 29      | 0            |
| 6   | BG    | 81    | 0        | 78       | 11      | 0            |
| 6   | BH    | 103   | 0        | 99       | 5       | 0            |
| 6   | BI    | 133   | 0        | 129      | 11      | 0            |
| 6   | BJ    | 103   | 0        | 99       | 3       | 0            |
| 6   | BK    | 140   | 0        | 136      | 10      | 0            |
| 6   | BL    | 103   | 0        | 99       | 11      | 0            |
| 6   | BM    | 140   | 0        | 136      | 11      | 0            |
| 6   | BN    | 103   | 0        | 99       | 15      | 0            |
| 6   | BO    | 133   | 0        | 129      | 11      | 0            |
| 6   | BP    | 103   | 0        | 99       | 9       | 0            |
| 6   | BQ    | 140   | 0        | 136      | 6       | 0            |
| 6   | BR    | 1275  | 0        | 1254     | 46      | 0            |
| 6   | BS    | 1275  | 0        | 1254     | 34      | 0            |
| 6   | BT    | 1275  | 0        | 1254     | 29      | 0            |
| 6   | BU    | 1275  | 0        | 1254     | 30      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | BV    | 1275  | 0        | 1254     | 35      | 0            |
| 6   | BW    | 1275  | 0        | 1254     | 36      | 0            |
| 6   | BX    | 1275  | 0        | 1254     | 52      | 0            |
| 6   | UI    | 1172  | 0        | 1181     | 67      | 0            |
| 6   | UJ    | 1172  | 0        | 1181     | 81      | 0            |
| 6   | UK    | 1172  | 0        | 1181     | 78      | 0            |
| 6   | UL    | 1172  | 0        | 1181     | 72      | 0            |
| 6   | UM    | 1172  | 0        | 1181     | 69      | 0            |
| 6   | UN    | 1172  | 0        | 1181     | 73      | 0            |
| 6   | UO    | 1172  | 0        | 1181     | 68      | 0            |
| 6   | UP    | 1172  | 0        | 1181     | 68      | 0            |
| 6   | WA    | 849   | 0        | 860      | 80      | 0            |
| 6   | WB    | 836   | 0        | 846      | 83      | 0            |
| 6   | WC    | 812   | 0        | 826      | 61      | 0            |
| 6   | WD    | 827   | 0        | 840      | 105     | 0            |
| 6   | WE    | 843   | 0        | 855      | 96      | 0            |
| 6   | WF    | 834   | 0        | 847      | 64      | 0            |
| 6   | WG    | 843   | 0        | 855      | 76      | 0            |
| 6   | WH    | 703   | 0        | 722      | 67      | 0            |
| 6   | WI    | 703   | 0        | 722      | 77      | 0            |
| 6   | WJ    | 737   | 0        | 755      | 91      | 0            |
| 6   | WK    | 729   | 0        | 744      | 85      | 0            |
| 6   | WL    | 622   | 0        | 632      | 61      | 0            |
| 6   | WM    | 596   | 0        | 612      | 47      | 0            |
| 6   | WN    | 611   | 0        | 623      | 59      | 0            |
| 6   | WO    | 714   | 0        | 731      | 48      | 0            |
| 6   | WP    | 741   | 0        | 758      | 70      | 0            |
| 6   | WQ    | 834   | 0        | 847      | 70      | 0            |
| 6   | WR    | 834   | 0        | 847      | 64      | 0            |
| 6   | WS    | 834   | 0        | 847      | 86      | 0            |
| 6   | WT    | 834   | 0        | 847      | 71      | 0            |
| 6   | WU    | 843   | 0        | 855      | 67      | 0            |
| 6   | WV    | 827   | 0        | 838      | 66      | 0            |
| 6   | WW    | 834   | 0        | 847      | 96      | 0            |
| 7   | Ab    | 670   | 0        | 739      | 73      | 0            |
| 7   | Aq    | 670   | 0        | 739      | 53      | 0            |
| 7   | Ar    | 670   | 0        | 739      | 51      | 0            |
| 7   | As    | 670   | 0        | 739      | 88      | 0            |
| 8   | At    | 1945  | 0        | 2063     | 136     | 0            |
| 9   | Au    | 1605  | 0        | 1701     | 88      | 0            |
| 9   | Av    | 1626  | 0        | 1718     | 90      | 0            |
| 9   | Aw    | 1614  | 0        | 1709     | 87      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 9   | Ax    | 1614   | 0        | 1709     | 117     | 0            |
| 9   | Ay    | 1623   | 0        | 1715     | 149     | 0            |
| 10  | A1    | 672    | 0        | 684      | 62      | 0            |
| 10  | A2    | 686    | 0        | 700      | 73      | 0            |
| 10  | A3    | 686    | 0        | 700      | 54      | 0            |
| 10  | A4    | 686    | 0        | 700      | 66      | 0            |
| 10  | A5    | 679    | 0        | 693      | 66      | 0            |
| 10  | Az    | 429    | 0        | 445      | 57      | 0            |
| 11  | A0    | 950    | 0        | 946      | 79      | 0            |
| 11  | A6    | 1030   | 0        | 1025     | 50      | 0            |
| 11  | A7    | 942    | 0        | 943      | 92      | 0            |
| 11  | A8    | 967    | 0        | 968      | 94      | 0            |
| 11  | A9    | 982    | 0        | 984      | 80      | 0            |
| 12  | BA    | 969    | 0        | 981      | 53      | 0            |
| 12  | BB    | 964    | 0        | 976      | 98      | 0            |
| 12  | BC    | 969    | 0        | 981      | 77      | 0            |
| 12  | BD    | 969    | 0        | 981      | 81      | 0            |
| 12  | BE    | 956    | 0        | 965      | 85      | 0            |
| 12  | BF    | 969    | 0        | 981      | 106     | 0            |
| All | All   | 338664 | 0        | 335363   | 12325   | 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 (12325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:AE:228:GLU:CB  | 3:AK:258:THR:HG21 | 1.27                     | 1.63              |
| 5:AB:202:MET:HE1 | 3:AM:73:ARG:CD    | 1.40                     | 1.49              |
| 5:AD:74:THR:HG21 | 3:AI:38:ARG:NH1   | 1.18                     | 1.48              |
| 3:6:56:SER:HA    | 5:AE:138:ALA:CB   | 1.40                     | 1.48              |
| 5:AE:231:MET:HE3 | 3:AJ:257:LEU:CA   | 1.40                     | 1.48              |
| 3:AG:73:ARG:HD3  | 12:BB:78:TYR:CE2  | 1.48                     | 1.47              |
| 5:AA:70:GLN:CG   | 3:AL:3:SER:HA     | 1.44                     | 1.45              |
| 11:A7:51:LYS:HB3 | 11:A7:55:ARG:NH2  | 1.13                     | 1.43              |
| 5:AD:16:LEU:HD23 | 3:AI:253:MET:CE   | 1.49                     | 1.42              |
| 8:At:145:TRP:CD1 | 6:WJ:164:LEU:HD22 | 1.54                     | 1.41              |
| 6:WD:168:GLU:CD  | 6:WD:170:LYS:HE3  | 1.40                     | 1.41              |
| 1:L:101:LYS:NZ   | 3:6:168:VAL:HG11  | 1.36                     | 1.39              |
| 7:Aq:89:GLY:HA2  | 6:WW:165:PHE:CE1  | 1.57                     | 1.38              |
| 3:9:85:ASN:ND2   | 4:ZK:4:SER:HB2    | 1.40                     | 1.35              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:ZD:85:ASN:OD1   | 4:ZO:50:LEU:HD13  | 1.24                     | 1.35              |
| 3:1:193:ILE:CG2   | 5:AE:152:PRO:HG3  | 1.53                     | 1.34              |
| 5:AA:70:GLN:HG3   | 3:AL:3:SER:CA     | 1.56                     | 1.34              |
| 3:AG:73:ARG:HD3   | 12:BB:78:TYR:CZ   | 1.59                     | 1.34              |
| 5:AE:131:GLU:HB3  | 3:AJ:179:MET:SD   | 1.66                     | 1.34              |
| 3:1:258:THR:HA    | 5:AE:217:MET:CE   | 1.56                     | 1.34              |
| 3:1:193:ILE:CG2   | 5:AE:152:PRO:CG   | 2.06                     | 1.33              |
| 6:AS:365:ASN:HB3  | 11:A0:72:HIS:CD2  | 1.64                     | 1.33              |
| 6:Aj:372:ILE:CD1  | 10:A1:11:ILE:HG22 | 1.58                     | 1.33              |
| 10:A4:7:ILE:HG21  | 6:BX:278:THR:CG2  | 1.56                     | 1.32              |
| 6:UP:103:GLN:CG   | 6:WW:182:PRO:HB3  | 1.56                     | 1.32              |
| 3:ZA:20:ASP:OD1   | 4:ZF:2:SER:HB2    | 1.16                     | 1.32              |
| 6:UP:103:GLN:HG2  | 6:WW:182:PRO:CB   | 1.58                     | 1.32              |
| 5:AA:72:ASP:HB3   | 3:AL:9:LYS:NZ     | 1.42                     | 1.32              |
| 3:0:2:ILE:HG22    | 5:AD:211:VAL:O    | 1.18                     | 1.32              |
| 3:1:193:ILE:HG21  | 5:AE:152:PRO:CG   | 1.59                     | 1.31              |
| 5:AB:202:MET:HE3  | 3:AM:73:ARG:NH1   | 1.41                     | 1.31              |
| 3:AH:44:LEU:HB3   | 12:BC:90:TYR:OH   | 1.19                     | 1.31              |
| 3:6:86:LEU:HD12   | 4:ZH:42:MET:CE    | 1.60                     | 1.31              |
| 3:6:56:SER:CA     | 5:AE:138:ALA:HB1  | 1.61                     | 1.30              |
| 5:AE:231:MET:CE   | 3:AJ:257:LEU:HA   | 1.59                     | 1.30              |
| 6:Ag:297:GLN:HB2  | 11:A8:73:ILE:CD1  | 1.61                     | 1.30              |
| 3:9:85:ASN:HD22   | 4:ZK:4:SER:CB     | 1.43                     | 1.29              |
| 9:Ax:143:ARG:HA   | 6:WD:165:PHE:CB   | 1.63                     | 1.28              |
| 6:WF:197:LEU:HD12 | 6:WG:175:SER:OG   | 1.34                     | 1.28              |
| 6:Al:365:ASN:HB3  | 11:A7:72:HIS:ND1  | 1.47                     | 1.28              |
| 8:At:145:TRP:HD1  | 6:WJ:164:LEU:CD2  | 1.47                     | 1.27              |
| 3:2:56:SER:O      | 5:AA:138:ALA:HB1  | 1.10                     | 1.26              |
| 10:A4:7:ILE:CG2   | 6:BX:278:THR:HG21 | 1.65                     | 1.26              |
| 11:A6:111:ASP:OD1 | 12:BB:3:LEU:HB2   | 1.19                     | 1.26              |
| 6:WR:197:LEU:HD12 | 6:WS:175:SER:OG   | 1.36                     | 1.26              |
| 6:WD:168:GLU:CG   | 6:WD:170:LYS:HE3  | 1.64                     | 1.25              |
| 3:ZE:248:SER:HB2  | 4:ZJ:402:LEU:CD2  | 1.66                     | 1.25              |
| 5:AB:70:GLN:HE21  | 3:AM:1:MET:N      | 1.31                     | 1.25              |
| 3:ZD:27:ALA:O     | 4:ZI:52:VAL:HG21  | 1.31                     | 1.24              |
| 7:Ab:75:ASP:OD1   | 6:WQ:124:SER:HA   | 1.23                     | 1.24              |
| 3:4:56:SER:O      | 5:AC:138:ALA:HB1  | 1.38                     | 1.24              |
| 5:AE:228:GLU:HB3  | 3:AK:258:THR:CG2  | 1.67                     | 1.24              |
| 5:AD:26:LEU:CD1   | 3:AI:242:ILE:HG21 | 1.65                     | 1.23              |
| 3:AG:73:ARG:CD    | 12:BB:78:TYR:CE2  | 2.21                     | 1.23              |
| 5:AB:70:GLN:HB3   | 3:AM:6:TRP:CD1    | 1.73                     | 1.22              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:p:80:GLN:OE1    | 5:AD:154:THR:HA   | 1.31                     | 1.22              |
| 6:Ak:370:ARG:NH2  | 10:A1:7:ILE:HD11  | 1.54                     | 1.22              |
| 6:Aj:372:ILE:HG21 | 10:A1:11:ILE:CG2  | 1.68                     | 1.22              |
| 6:WA:128:GLU:HG2  | 6:WB:126:PHE:CD2  | 1.73                     | 1.22              |
| 6:Ao:278:THR:CG2  | 10:Az:7:ILE:HG21  | 1.69                     | 1.22              |
| 3:ZB:233:MET:HE1  | 4:ZG:388:THR:OG1  | 1.40                     | 1.21              |
| 6:WA:128:GLU:CG   | 6:WB:126:PHE:CD2  | 2.23                     | 1.21              |
| 3:4:55:GLN:O      | 5:AC:138:ALA:HB2  | 1.37                     | 1.21              |
| 3:AL:52:PRO:CG    | 12:BB:80:PRO:HB3  | 1.71                     | 1.21              |
| 7:As:55:ILE:HD11  | 9:Ax:205:MET:CE   | 1.70                     | 1.21              |
| 3:2:56:SER:C      | 5:AA:138:ALA:HB1  | 1.64                     | 1.21              |
| 3:ZC:28:ASN:OD1   | 4:ZH:52:VAL:HG23  | 1.37                     | 1.21              |
| 9:Ay:241:GLN:HG2  | 6:WG:164:LEU:O    | 1.38                     | 1.21              |
| 3:ZA:240:TYR:CE2  | 4:ZF:395:ILE:HG23 | 1.77                     | 1.20              |
| 9:Ax:161:GLY:HA2  | 6:WE:167:ARG:CD   | 1.71                     | 1.20              |
| 10:A5:7:ILE:CG2   | 6:BR:278:THR:HG21 | 1.70                     | 1.20              |
| 5:AB:202:MET:CE   | 3:AM:73:ARG:CD    | 2.18                     | 1.19              |
| 9:Ax:142:THR:O    | 6:WD:165:PHE:HB2  | 1.39                     | 1.19              |
| 5:AA:26:LEU:HD13  | 3:AF:242:ILE:CG2  | 1.72                     | 1.19              |
| 5:AC:70:GLN:HB2   | 3:AN:6:TRP:CE3    | 1.77                     | 1.18              |
| 5:AD:16:LEU:HD23  | 3:AI:253:MET:HE1  | 1.22                     | 1.18              |
| 6:Aj:370:ARG:HH21 | 10:A1:14:LEU:HD21 | 1.07                     | 1.18              |
| 5:AB:71:LEU:CD2   | 3:AM:44:LEU:HD13  | 1.72                     | 1.18              |
| 6:WQ:197:LEU:HD12 | 6:WR:175:SER:OG   | 1.39                     | 1.18              |
| 9:Au:160:GLN:HB3  | 6:WP:166:VAL:CG2  | 1.72                     | 1.18              |
| 6:WI:197:LEU:HD12 | 6:WJ:175:SER:CB   | 1.74                     | 1.18              |
| 3:AH:44:LEU:CD2   | 12:BC:78:TYR:HB2  | 1.74                     | 1.17              |
| 9:Au:160:GLN:CB   | 6:WP:166:VAL:HG22 | 1.72                     | 1.17              |
| 1:I:62:TYR:HD1    | 2:g:129:VAL:CG1   | 1.58                     | 1.17              |
| 1:N:62:TYR:HD1    | 2:l:129:VAL:CG1   | 1.58                     | 1.17              |
| 3:3:55:GLN:O      | 5:AB:138:ALA:HB2  | 1.43                     | 1.17              |
| 5:AD:16:LEU:CD2   | 3:AI:253:MET:CE   | 2.21                     | 1.17              |
| 6:AS:299:ASN:HD22 | 11:A0:78:VAL:CG1  | 1.58                     | 1.17              |
| 1:J:62:TYR:HD1    | 2:h:129:VAL:CG1   | 1.58                     | 1.17              |
| 1:R:62:TYR:HD1    | 2:p:129:VAL:CG1   | 1.58                     | 1.17              |
| 1:S:62:TYR:HD1    | 2:q:129:VAL:CG1   | 1.58                     | 1.17              |
| 6:AY:365:ASN:HB3  | 11:A9:72:HIS:CD2  | 1.78                     | 1.17              |
| 6:WJ:197:LEU:HD12 | 6:WK:175:SER:OG   | 1.41                     | 1.17              |
| 1:M:62:TYR:HD1    | 2:k:129:VAL:CG1   | 1.58                     | 1.17              |
| 1:O:62:TYR:HD1    | 2:m:129:VAL:CG1   | 1.58                     | 1.17              |
| 6:Ai:303:GLN:NE2  | 6:BK:319:GLN:HB3  | 1.60                     | 1.17              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:62:TYR:HD1    | 2:b:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:T:62:TYR:HD1    | 2:r:129:VAL:CG1   | 1.58                     | 1.16              |
| 5:AA:247:LEU:HB3  | 12:BB:120:ASN:ND2 | 1.59                     | 1.16              |
| 1:E:62:TYR:HD1    | 2:c:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:H:62:TYR:HD1    | 2:f:129:VAL:CG1   | 1.58                     | 1.16              |
| 5:AE:228:GLU:CB   | 3:AK:258:THR:CG2  | 2.21                     | 1.16              |
| 6:Aj:372:ILE:CG2  | 10:A1:11:ILE:HG21 | 1.74                     | 1.16              |
| 1:K:62:TYR:HD1    | 2:i:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:W:62:TYR:HD1    | 2:u:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:X:62:TYR:HD1    | 2:v:129:VAL:CG1   | 1.58                     | 1.16              |
| 7:As:55:ILE:CD1   | 9:Ax:205:MET:HE1  | 1.74                     | 1.16              |
| 1:C:62:TYR:HD1    | 2:a:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:Q:62:TYR:HD1    | 2:o:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:Y:62:TYR:HD1    | 2:w:129:VAL:CG1   | 1.58                     | 1.16              |
| 1:F:62:TYR:HD1    | 2:d:129:VAL:CG1   | 1.58                     | 1.16              |
| 11:A7:51:LYS:CB   | 11:A7:55:ARG:NH2  | 2.09                     | 1.16              |
| 1:P:62:TYR:HD1    | 2:n:129:VAL:CG1   | 1.58                     | 1.15              |
| 3:0:193:ILE:HD12  | 5:AD:152:PRO:CD   | 1.76                     | 1.15              |
| 6:WS:200:SER:O    | 6:WT:158:ALA:HB2  | 1.46                     | 1.15              |
| 1:L:62:TYR:HD1    | 2:j:129:VAL:CG1   | 1.58                     | 1.15              |
| 1:V:62:TYR:HD1    | 2:t:129:VAL:CG1   | 1.58                     | 1.15              |
| 3:5:226:VAL:HG11  | 3:ZA:242:ILE:HD13 | 1.27                     | 1.15              |
| 5:AB:71:LEU:HD23  | 3:AM:44:LEU:CD1   | 1.76                     | 1.15              |
| 5:AD:26:LEU:HD12  | 3:AI:242:ILE:CG2  | 1.74                     | 1.15              |
| 1:Z:62:TYR:HD1    | 2:x:129:VAL:CG1   | 1.58                     | 1.15              |
| 3:AJ:3:SER:HB2    | 12:BE:75:LYS:NZ   | 1.61                     | 1.15              |
| 6:WK:193:ALA:HB1  | 6:WL:213:VAL:HG21 | 1.29                     | 1.15              |
| 1:B:62:TYR:HD1    | 2:z:129:VAL:CG1   | 1.58                     | 1.15              |
| 1:U:62:TYR:HD1    | 2:s:129:VAL:CG1   | 1.58                     | 1.15              |
| 6:AS:299:ASN:ND2  | 11:A0:78:VAL:HG11 | 1.61                     | 1.15              |
| 1:G:62:TYR:HD1    | 2:e:129:VAL:CG1   | 1.58                     | 1.15              |
| 2:r:54:GLN:OE1    | 3:AI:139:ALA:HB3  | 1.45                     | 1.15              |
| 6:WK:197:LEU:HD12 | 6:WL:175:SER:CB   | 1.77                     | 1.15              |
| 3:ZD:76:ALA:CB    | 4:ZI:47:LYS:HE3   | 1.76                     | 1.14              |
| 5:AA:200:ARG:NH2  | 3:AG:189:GLU:HB3  | 1.62                     | 1.14              |
| 6:WA:128:GLU:CG   | 6:WB:126:PHE:HD2  | 1.56                     | 1.14              |
| 6:WR:197:LEU:HD12 | 6:WS:175:SER:CB   | 1.75                     | 1.14              |
| 5:AE:228:GLU:HB2  | 3:AK:258:THR:HG21 | 1.16                     | 1.14              |
| 1:A:62:TYR:HD1    | 2:y:129:VAL:CG1   | 1.58                     | 1.14              |
| 5:AE:231:MET:HE1  | 3:AJ:257:LEU:CD1  | 1.77                     | 1.14              |
| 10:A5:7:ILE:HG21  | 6:BR:278:THR:HG21 | 1.21                     | 1.14              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WT:181:GLU:HB2  | 6:WT:184:ARG:HG3   | 1.14                     | 1.14              |
| 5:AB:16:LEU:HD22  | 3:AG:2:ILE:HD11    | 1.29                     | 1.14              |
| 10:A4:21:ALA:CB   | 6:BV:278:THR:HG21  | 1.78                     | 1.14              |
| 6:WD:168:GLU:CD   | 6:WD:170:LYS:CE    | 2.21                     | 1.14              |
| 6:WR:181:GLU:HB2  | 6:WR:184:ARG:HG3   | 1.14                     | 1.14              |
| 2:m:80:GLN:HE22   | 3:AJ:204:SER:CA    | 1.62                     | 1.13              |
| 5:AD:26:LEU:CD1   | 3:AI:242:ILE:CG2   | 2.26                     | 1.13              |
| 6:An:278:THR:CG2  | 10:Az:14:LEU:HD23  | 1.78                     | 1.13              |
| 6:WA:158:ALA:HB2  | 6:WW:200:SER:O     | 1.44                     | 1.13              |
| 6:WQ:181:GLU:HB2  | 6:WQ:184:ARG:HG3   | 1.13                     | 1.13              |
| 6:WS:181:GLU:HB2  | 6:WS:184:ARG:HG3   | 1.14                     | 1.13              |
| 3:0:1:MET:HG3     | 5:AD:213:PRO:HG3   | 1.16                     | 1.13              |
| 5:AC:71:LEU:HD13  | 3:AN:70:THR:HG21   | 1.17                     | 1.13              |
| 7:Ar:36:SER:OG    | 7:As:44:ILE:HG23   | 1.45                     | 1.13              |
| 6:WI:197:LEU:HD12 | 6:WJ:175:SER:OG    | 1.47                     | 1.13              |
| 6:WR:112:GLY:HA2  | 6:WR:135:ALA:HA    | 1.27                     | 1.13              |
| 5:AA:247:LEU:HB3  | 12:BB:120:ASN:HD21 | 1.01                     | 1.13              |
| 11:A7:51:LYS:HB3  | 11:A7:55:ARG:CZ    | 1.79                     | 1.13              |
| 3:8:54:ALA:HB1    | 3:AG:150:THR:HG21  | 1.25                     | 1.13              |
| 5:AE:16:LEU:HD23  | 3:AJ:253:MET:CE    | 1.78                     | 1.13              |
| 3:ZC:122:VAL:O    | 4:ZH:322:ASN:HB2   | 1.47                     | 1.12              |
| 5:AA:200:ARG:HH22 | 3:AG:189:GLU:CB    | 1.61                     | 1.12              |
| 10:A2:11:ILE:HD12 | 10:A2:12:SER:N     | 1.64                     | 1.12              |
| 6:WA:128:GLU:HG2  | 6:WB:126:PHE:HD2   | 0.96                     | 1.12              |
| 6:WH:181:GLU:HB2  | 6:WH:184:ARG:HG3   | 1.13                     | 1.12              |
| 5:AB:202:MET:HE1  | 3:AM:73:ARG:HD2    | 1.12                     | 1.12              |
| 6:Ak:370:ARG:HH21 | 10:A1:7:ILE:HD11   | 1.00                     | 1.12              |
| 7:As:58:VAL:HG11  | 9:Ay:207:LEU:CD1   | 1.79                     | 1.12              |
| 8:At:156:THR:HG22 | 6:WK:167:ARG:HG2   | 1.31                     | 1.12              |
| 7:Aq:89:GLY:CA    | 6:WW:165:PHE:HE1   | 1.63                     | 1.12              |
| 6:WA:181:GLU:HB2  | 6:WA:184:ARG:HG3   | 1.14                     | 1.12              |
| 6:WE:181:GLU:HB2  | 6:WE:184:ARG:HG3   | 1.14                     | 1.12              |
| 6:WF:181:GLU:HB2  | 6:WF:184:ARG:HG3   | 1.14                     | 1.12              |
| 6:WU:181:GLU:HB2  | 6:WU:184:ARG:HG3   | 1.14                     | 1.12              |
| 6:WV:181:GLU:HB2  | 6:WV:184:ARG:HG3   | 1.14                     | 1.12              |
| 6:AY:367:GLU:OE1  | 11:A9:68:THR:HG21  | 1.49                     | 1.12              |
| 6:Ad:278:THR:HG21 | 10:A2:7:ILE:HB     | 1.16                     | 1.12              |
| 8:At:145:TRP:NE1  | 6:WJ:164:LEU:HB2   | 1.65                     | 1.12              |
| 6:WG:181:GLU:HB2  | 6:WG:184:ARG:HG3   | 1.14                     | 1.12              |
| 4:ZU:182:GLY:HA2  | 4:Zf:131:GLY:HA3   | 1.30                     | 1.12              |
| 4:ZY:24:ILE:HD11  | 4:Zd:384:SER:OG    | 1.50                     | 1.12              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Za:269:GLN:OE1  | 4:Zg:286:PRO:HG3  | 1.49                     | 1.12              |
| 5:AA:26:LEU:HD13  | 3:AF:242:ILE:HG22 | 1.29                     | 1.12              |
| 6:Ai:303:GLN:HE22 | 6:BK:319:GLN:CB   | 1.63                     | 1.12              |
| 6:WW:181:GLU:HB2  | 6:WW:184:ARG:HG3  | 1.14                     | 1.12              |
| 3:AG:73:ARG:CD    | 12:BB:78:TYR:CZ   | 2.33                     | 1.11              |
| 5:AC:21:VAL:CG2   | 3:AH:68:ILE:HG22  | 1.80                     | 1.11              |
| 8:At:145:TRP:CD1  | 6:WJ:164:LEU:HD13 | 1.86                     | 1.11              |
| 3:0:193:ILE:HD12  | 5:AD:152:PRO:HD3  | 1.25                     | 1.11              |
| 6:AP:278:THR:HG21 | 10:A5:21:ALA:HB1  | 1.29                     | 1.11              |
| 11:A8:35:THR:HG22 | 12:BC:49:PHE:HB3  | 1.32                     | 1.11              |
| 6:WE:112:GLY:HA2  | 6:WE:135:ALA:HA   | 1.31                     | 1.11              |
| 5:AB:26:LEU:HD22  | 3:AG:242:ILE:HG21 | 1.28                     | 1.11              |
| 6:WD:181:GLU:HB2  | 6:WD:184:ARG:HG3  | 1.14                     | 1.11              |
| 2:s:80:GLN:HE22   | 3:AI:141:THR:CG2  | 1.62                     | 1.10              |
| 3:1:257:LEU:O     | 5:AE:217:MET:HE3  | 1.49                     | 1.10              |
| 3:6:57:SER:HB3    | 3:AK:108:PRO:CB   | 1.79                     | 1.10              |
| 5:AE:231:MET:CE   | 3:AJ:257:LEU:HB2  | 1.81                     | 1.10              |
| 6:Ak:372:ILE:CG2  | 10:A1:4:ILE:HG12  | 1.81                     | 1.10              |
| 6:AP:278:THR:HG21 | 10:A5:21:ALA:CB   | 1.80                     | 1.10              |
| 6:WL:197:LEU:HD12 | 6:WM:175:SER:OG   | 1.49                     | 1.10              |
| 2:i:273:CYS:HB2   | 2:j:264:MET:O     | 1.51                     | 1.10              |
| 2:k:273:CYS:HB2   | 2:l:264:MET:O     | 1.52                     | 1.10              |
| 2:l:273:CYS:HB2   | 2:m:264:MET:O     | 1.52                     | 1.10              |
| 5:AA:202:MET:HG3  | 3:AL:45:LEU:HD11  | 1.15                     | 1.10              |
| 9:Ax:241:GLN:HG2  | 6:WC:164:LEU:O    | 1.51                     | 1.10              |
| 6:WO:200:SER:OG   | 6:WP:175:SER:HB2  | 1.50                     | 1.10              |
| 6:WP:181:GLU:HB2  | 6:WP:184:ARG:HG3  | 1.14                     | 1.10              |
| 6:WS:112:GLY:HA2  | 6:WS:135:ALA:HA   | 1.12                     | 1.10              |
| 6:WU:197:LEU:HD12 | 6:WV:175:SER:OG   | 1.52                     | 1.10              |
| 2:j:273:CYS:HB2   | 2:k:264:MET:O     | 1.52                     | 1.10              |
| 5:AD:74:THR:CG2   | 3:AI:38:ARG:NH1   | 2.13                     | 1.10              |
| 6:AP:276:GLU:OE2  | 10:A5:19:MET:HA   | 1.51                     | 1.10              |
| 6:WI:181:GLU:HB2  | 6:WI:184:ARG:HG3  | 1.13                     | 1.10              |
| 2:m:273:CYS:HB2   | 2:n:264:MET:O     | 1.52                     | 1.10              |
| 6:AS:367:GLU:OE1  | 11:A0:68:THR:HG21 | 1.49                     | 1.10              |
| 6:WJ:181:GLU:HB2  | 6:WJ:184:ARG:HG3  | 1.14                     | 1.10              |
| 3:2:56:SER:O      | 5:AA:138:ALA:CB   | 1.99                     | 1.10              |
| 6:AS:299:ASN:ND2  | 11:A0:78:VAL:CG1  | 2.14                     | 1.10              |
| 6:UJ:103:GLN:HB3  | 6:WD:182:PRO:HB3  | 1.20                     | 1.10              |
| 2:c:273:CYS:HB2   | 2:d:264:MET:O     | 1.52                     | 1.09              |
| 2:d:273:CYS:HB2   | 2:e:264:MET:O     | 1.52                     | 1.09              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AC:62:PRO:HA    | 3:AH:63:PRO:HG2   | 1.21                     | 1.09              |
| 5:AE:231:MET:CE   | 3:AJ:257:LEU:CB   | 2.29                     | 1.09              |
| 2:b:273:CYS:HB2   | 2:c:264:MET:O     | 1.52                     | 1.09              |
| 2:f:273:CYS:HB2   | 2:g:264:MET:O     | 1.52                     | 1.09              |
| 2:n:273:CYS:HB2   | 2:o:264:MET:O     | 1.52                     | 1.09              |
| 5:AB:202:MET:HE1  | 3:AM:73:ARG:HD3   | 1.33                     | 1.09              |
| 6:WA:197:LEU:HD12 | 6:WB:175:SER:OG   | 1.50                     | 1.09              |
| 1:L:101:LYS:NZ    | 3:6:168:VAL:CG1   | 2.16                     | 1.09              |
| 2:e:273:CYS:HB2   | 2:f:264:MET:O     | 1.52                     | 1.09              |
| 6:WJ:197:LEU:HD12 | 6:WK:175:SER:CB   | 1.82                     | 1.09              |
| 6:WO:181:GLU:HB2  | 6:WO:184:ARG:HG3  | 1.14                     | 1.09              |
| 2:a:273:CYS:HB2   | 2:b:264:MET:O     | 1.51                     | 1.08              |
| 3:5:257:LEU:HG    | 3:AI:230:LEU:HD12 | 1.32                     | 1.08              |
| 6:WB:181:GLU:HB2  | 6:WB:184:ARG:HG3  | 1.13                     | 1.08              |
| 2:h:273:CYS:HB2   | 2:i:264:MET:O     | 1.52                     | 1.08              |
| 2:s:273:CYS:HB2   | 2:t:264:MET:O     | 1.52                     | 1.08              |
| 2:t:273:CYS:HB2   | 2:u:264:MET:O     | 1.52                     | 1.08              |
| 4:ZV:181:LYS:HD3  | 4:Zg:129:GLN:HE21 | 1.18                     | 1.08              |
| 10:A4:7:ILE:CG2   | 6:BX:278:THR:CG2  | 2.25                     | 1.08              |
| 6:WA:158:ALA:CB   | 6:WW:200:SER:O    | 2.00                     | 1.08              |
| 6:WK:181:GLU:HB2  | 6:WK:184:ARG:HG3  | 1.14                     | 1.08              |
| 2:o:273:CYS:HB2   | 2:p:264:MET:O     | 1.52                     | 1.08              |
| 2:r:273:CYS:HB2   | 2:s:264:MET:O     | 1.51                     | 1.08              |
| 2:u:273:CYS:HB2   | 2:v:264:MET:O     | 1.52                     | 1.08              |
| 6:Af:365:ASN:HB3  | 11:A8:72:HIS:ND1  | 1.68                     | 1.08              |
| 6:UN:167:ARG:NH2  | 6:WQ:188:GLU:HB3  | 1.68                     | 1.08              |
| 6:WK:196:HIS:HB3  | 6:WL:211:THR:HG21 | 1.33                     | 1.08              |
| 2:p:273:CYS:HB2   | 2:q:264:MET:O     | 1.52                     | 1.08              |
| 5:AA:229:MET:HG2  | 3:AG:258:THR:HG22 | 1.33                     | 1.08              |
| 6:WN:196:HIS:HB3  | 6:WO:211:THR:HG21 | 1.34                     | 1.08              |
| 3:0:70:THR:HG21   | 5:AD:71:LEU:HD13  | 1.12                     | 1.08              |
| 3:ZD:76:ALA:HB1   | 4:ZI:47:LYS:HE3   | 1.26                     | 1.08              |
| 6:AV:278:THR:HG21 | 10:A3:21:ALA:CB   | 1.84                     | 1.08              |
| 10:A4:77:LYS:HE3  | 11:A0:13:GLN:NE2  | 1.69                     | 1.08              |
| 11:A9:68:THR:OG1  | 11:A9:72:HIS:CE1  | 2.07                     | 1.08              |
| 3:4:86:LEU:HD12   | 4:ZF:42:MET:CE    | 1.84                     | 1.07              |
| 6:Aj:372:ILE:HD13 | 10:A1:11:ILE:HG22 | 1.37                     | 1.07              |
| 2:a:264:MET:O     | 2:z:273:CYS:HB2   | 1.52                     | 1.07              |
| 2:q:273:CYS:HB2   | 2:r:264:MET:O     | 1.52                     | 1.07              |
| 2:v:273:CYS:HB2   | 2:w:264:MET:O     | 1.52                     | 1.07              |
| 6:Af:295:SER:HB2  | 11:A8:65:LEU:HB2  | 1.35                     | 1.07              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WN:181:GLU:HB2  | 6:WN:184:ARG:HG3  | 1.14                     | 1.07              |
| 6:Ao:278:THR:HG21 | 10:Az:7:ILE:HG21  | 1.20                     | 1.07              |
| 2:g:273:CYS:HB2   | 2:h:264:MET:O     | 1.52                     | 1.07              |
| 4:ZU:331:ASP:HA   | 4:ZZ:40:ALA:HB1   | 1.37                     | 1.07              |
| 5:AC:217:MET:HE3  | 3:AN:258:THR:HA   | 1.35                     | 1.07              |
| 6:UK:207:PRO:HD2  | 6:WE:187:ASP:CG   | 1.80                     | 1.07              |
| 2:y:80:GLN:HE22   | 3:AM:200:ALA:HA   | 0.94                     | 1.07              |
| 3:6:86:LEU:CD1    | 4:ZH:42:MET:HE3   | 1.84                     | 1.07              |
| 4:Za:104:GLU:OE2  | 4:Zf:341:GLY:HA2  | 1.53                     | 1.06              |
| 6:WG:200:SER:OG   | 6:WH:175:SER:HB2  | 1.54                     | 1.06              |
| 6:WL:181:GLU:HB2  | 6:WL:184:ARG:HG3  | 1.14                     | 1.06              |
| 2:a:80:GLN:HE22   | 3:8:58:GLU:CG     | 1.68                     | 1.06              |
| 2:w:273:CYS:HB2   | 2:x:264:MET:O     | 1.52                     | 1.06              |
| 3:8:36:ARG:NE     | 3:8:38:ARG:HH22   | 1.53                     | 1.06              |
| 6:Am:278:THR:HG21 | 10:Az:21:ALA:CB   | 1.83                     | 1.06              |
| 6:WN:201:ALA:HA   | 6:WO:158:ALA:HB2  | 1.33                     | 1.06              |
| 2:f:54:GLN:OE1    | 3:AF:168:VAL:HG12 | 1.55                     | 1.06              |
| 3:6:57:SER:HB3    | 3:AK:108:PRO:HB3  | 1.10                     | 1.06              |
| 3:AJ:3:SER:HB2    | 12:BE:75:LYS:HZ2  | 1.02                     | 1.06              |
| 6:An:278:THR:HG21 | 10:Az:14:LEU:HD23 | 1.37                     | 1.06              |
| 6:WM:181:GLU:HB2  | 6:WM:184:ARG:HG3  | 1.13                     | 1.06              |
| 2:y:273:CYS:HB2   | 2:z:264:MET:O     | 1.52                     | 1.06              |
| 6:Ak:370:ARG:HH21 | 10:A1:7:ILE:CD1   | 1.67                     | 1.06              |
| 7:As:58:VAL:HG11  | 9:Ay:207:LEU:HD11 | 1.07                     | 1.06              |
| 3:2:58:GLU:HG2    | 5:AA:160:ARG:NH1  | 1.70                     | 1.06              |
| 5:AA:200:ARG:HH22 | 3:AG:189:GLU:HB3  | 1.17                     | 1.06              |
| 6:WC:186:LEU:HD22 | 6:WC:190:GLN:HG2  | 1.38                     | 1.06              |
| 2:x:273:CYS:HB2   | 2:y:264:MET:O     | 1.52                     | 1.05              |
| 3:ZE:248:SER:HB2  | 4:ZJ:402:LEU:HD22 | 1.37                     | 1.05              |
| 3:ZA:111:THR:HG21 | 3:AN:163:GLY:HA2  | 1.35                     | 1.05              |
| 5:AB:172:GLN:HE22 | 3:AG:52:PRO:HG3   | 1.20                     | 1.05              |
| 6:Aj:372:ILE:HD12 | 10:A1:11:ILE:HG22 | 1.38                     | 1.05              |
| 2:s:80:GLN:HE22   | 3:AI:141:THR:HG23 | 1.18                     | 1.05              |
| 3:1:193:ILE:HG21  | 5:AE:152:PRO:HG3  | 1.08                     | 1.05              |
| 3:1:193:ILE:HG22  | 5:AE:152:PRO:CG   | 1.81                     | 1.05              |
| 6:Ao:278:THR:HG21 | 10:Az:7:ILE:CG2   | 1.85                     | 1.05              |
| 7:As:74:LEU:HD11  | 9:Ay:228:LEU:HD13 | 1.38                     | 1.05              |
| 6:WA:160:PRO:HB3  | 6:WW:203:ALA:HB1  | 1.38                     | 1.05              |
| 5:AD:229:MET:HG3  | 3:AJ:258:THR:HG22 | 1.31                     | 1.05              |
| 5:AE:109:PRO:HG3  | 3:AJ:197:SER:HA   | 1.34                     | 1.05              |
| 6:UJ:103:GLN:HB3  | 6:WD:182:PRO:CB   | 1.85                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UK:207:PRO:CB   | 6:WE:187:ASP:OD1  | 2.04                     | 1.05              |
| 4:ZH:205:ASP:OD1  | 4:ZN:252:ASN:HA   | 1.56                     | 1.05              |
| 4:ZU:66:THR:HB    | 4:Zf:42:MET:HE3   | 1.39                     | 1.05              |
| 4:Za:331:ASP:HA   | 4:Zf:40:ALA:HB1   | 1.06                     | 1.04              |
| 9:Ax:161:GLY:CA   | 6:WE:167:ARG:HD3  | 1.87                     | 1.04              |
| 5:AD:26:LEU:HD11  | 3:AI:242:ILE:HG21 | 1.34                     | 1.04              |
| 2:a:80:GLN:HE22   | 3:8:58:GLU:HG3    | 1.21                     | 1.04              |
| 6:UK:207:PRO:HB2  | 6:WE:187:ASP:OD1  | 1.56                     | 1.04              |
| 2:k:80:GLN:OE1    | 5:AE:157:PRO:CD   | 2.05                     | 1.04              |
| 5:AB:221:ILE:HD13 | 3:AH:251:ASP:OD2  | 1.58                     | 1.04              |
| 6:Ag:295:SER:HB3  | 11:A8:72:HIS:CB   | 1.87                     | 1.04              |
| 10:A5:7:ILE:HG21  | 6:BR:278:THR:CG2  | 1.87                     | 1.04              |
| 6:WM:200:SER:OG   | 6:WN:175:SER:HB2  | 1.58                     | 1.04              |
| 3:4:56:SER:C      | 5:AC:138:ALA:HB1  | 1.81                     | 1.04              |
| 6:Aj:372:ILE:HG21 | 10:A1:11:ILE:HG21 | 1.34                     | 1.04              |
| 3:ZE:54:ALA:HB1   | 3:AM:150:THR:HG21 | 1.39                     | 1.03              |
| 3:AL:52:PRO:HG3   | 12:BB:80:PRO:HB3  | 1.06                     | 1.03              |
| 6:WJ:128:GLU:HG2  | 6:WK:126:PHE:HD2  | 1.22                     | 1.03              |
| 6:WL:197:LEU:HD12 | 6:WM:175:SER:CB   | 1.88                     | 1.03              |
| 6:WM:143:THR:OG1  | 6:WN:154:ARG:HG2  | 1.57                     | 1.03              |
| 2:y:80:GLN:NE2    | 3:AM:200:ALA:HA   | 1.71                     | 1.03              |
| 5:AC:217:MET:CE   | 3:AN:258:THR:HA   | 1.88                     | 1.03              |
| 6:WV:112:GLY:HA2  | 6:WV:135:ALA:HA   | 1.40                     | 1.03              |
| 3:6:86:LEU:HB2    | 4:ZH:42:MET:HE1   | 1.39                     | 1.03              |
| 6:Ad:372:ILE:CG2  | 10:A2:11:ILE:HG22 | 1.87                     | 1.03              |
| 10:A4:7:ILE:HG21  | 6:BX:278:THR:HG22 | 1.36                     | 1.03              |
| 1:O:166:GLU:HB2   | 1:P:35:THR:HG21   | 1.41                     | 1.03              |
| 3:1:70:THR:HG21   | 5:AE:71:LEU:HG    | 1.40                     | 1.03              |
| 4:ZW:349:GLY:O    | 4:Zc:89:ASN:ND2   | 1.92                     | 1.03              |
| 8:At:145:TRP:CD1  | 6:WJ:164:LEU:CD2  | 2.30                     | 1.03              |
| 9:Ax:143:ARG:HA   | 6:WD:165:PHE:HB3  | 1.04                     | 1.03              |
| 6:UJ:103:GLN:OE1  | 6:WD:182:PRO:HB3  | 1.58                     | 1.03              |
| 9:Ay:240:ALA:HB3  | 6:WG:165:PHE:HE1  | 1.21                     | 1.03              |
| 6:WO:197:LEU:HD12 | 6:WP:175:SER:OG   | 1.58                     | 1.03              |
| 1:N:166:GLU:HB2   | 1:O:35:THR:HG21   | 1.41                     | 1.02              |
| 1:P:166:GLU:HB2   | 1:Q:35:THR:HG21   | 1.41                     | 1.02              |
| 3:AF:44:LEU:HD21  | 12:BA:78:TYR:CG   | 1.93                     | 1.02              |
| 6:WD:168:GLU:CG   | 6:WD:170:LYS:CE   | 2.37                     | 1.02              |
| 6:WD:200:SER:O    | 6:WE:158:ALA:HB2  | 1.58                     | 1.02              |
| 1:W:166:GLU:HB2   | 1:X:35:THR:HG21   | 1.41                     | 1.02              |
| 3:6:55:GLN:O      | 5:AE:138:ALA:HB2  | 1.59                     | 1.02              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:ZH:234:GLU:OE2  | 4:ZN:255:THR:HB  | 1.57                     | 1.02              |
| 4:ZU:349:GLY:O    | 4:Za:89:ASN:ND2  | 1.91                     | 1.02              |
| 6:WL:197:LEU:CD1  | 6:WM:175:SER:OG  | 2.06                     | 1.02              |
| 6:WT:197:LEU:HD12 | 6:WU:175:SER:OG  | 1.57                     | 1.02              |
| 1:V:166:GLU:HB2   | 1:W:35:THR:HG21  | 1.41                     | 1.02              |
| 3:ZB:31:THR:HG22  | 4:ZG:39:PHE:HB2  | 1.40                     | 1.02              |
| 5:AA:109:PRO:HG3  | 3:AF:197:SER:C   | 1.84                     | 1.02              |
| 6:WF:197:LEU:HD12 | 6:WG:175:SER:CB  | 1.89                     | 1.02              |
| 2:h:188:GLN:HB3   | 2:i:101:GLN:NE2  | 1.75                     | 1.02              |
| 4:ZW:331:ASP:HA   | 4:Zb:40:ALA:HB1  | 1.37                     | 1.02              |
| 6:AS:297:GLN:HB2  | 11:A0:65:LEU:CD2 | 1.90                     | 1.02              |
| 1:Q:166:GLU:HB2   | 1:R:35:THR:HG21  | 1.41                     | 1.02              |
| 2:g:188:GLN:HB3   | 2:h:101:GLN:NE2  | 1.75                     | 1.02              |
| 2:i:188:GLN:HB3   | 2:j:101:GLN:NE2  | 1.75                     | 1.02              |
| 3:0:70:THR:HG21   | 5:AD:71:LEU:CD1  | 1.90                     | 1.02              |
| 3:ZB:56:SER:O     | 3:AJ:153:ARG:N   | 1.92                     | 1.02              |
| 5:AA:217:MET:CE   | 3:AL:257:LEU:O   | 2.06                     | 1.02              |
| 6:WH:203:ALA:HB1  | 6:WI:160:PRO:HB3 | 1.39                     | 1.02              |
| 6:WN:200:SER:O    | 6:WO:158:ALA:HB3 | 1.59                     | 1.02              |
| 1:K:62:TYR:HD1    | 2:i:129:VAL:HG13 | 1.25                     | 1.01              |
| 1:M:166:GLU:HB2   | 1:N:35:THR:HG21  | 1.41                     | 1.01              |
| 1:X:166:GLU:HB2   | 1:Y:35:THR:HG21  | 1.41                     | 1.01              |
| 1:Y:62:TYR:HD1    | 2:w:129:VAL:HG13 | 1.25                     | 1.01              |
| 6:AY:365:ASN:HB3  | 11:A9:72:HIS:HD2 | 1.15                     | 1.01              |
| 10:A2:11:ILE:HD12 | 10:A2:11:ILE:C   | 1.84                     | 1.01              |
| 6:WG:112:GLY:HA2  | 6:WG:135:ALA:HA  | 1.36                     | 1.01              |
| 1:E:62:TYR:HD1    | 2:c:129:VAL:HG13 | 1.25                     | 1.01              |
| 1:I:166:GLU:HB2   | 1:J:35:THR:HG21  | 1.41                     | 1.01              |
| 1:U:166:GLU:HB2   | 1:V:35:THR:HG21  | 1.41                     | 1.01              |
| 1:Z:62:TYR:HD1    | 2:x:129:VAL:HG13 | 1.25                     | 1.01              |
| 2:f:188:GLN:HB3   | 2:g:101:GLN:NE2  | 1.75                     | 1.01              |
| 2:j:188:GLN:HB3   | 2:k:101:GLN:NE2  | 1.75                     | 1.01              |
| 3:ZC:28:ASN:OD1   | 4:ZH:52:VAL:CG2  | 2.08                     | 1.01              |
| 7:Ab:75:ASP:OD1   | 6:WQ:124:SER:CA  | 2.08                     | 1.01              |
| 9:Ay:240:ALA:HB3  | 6:WG:165:PHE:CE1 | 1.95                     | 1.01              |
| 1:J:62:TYR:HD1    | 2:h:129:VAL:HG13 | 1.25                     | 1.01              |
| 9:Ay:152:ARG:HH22 | 6:WJ:164:LEU:C   | 1.65                     | 1.01              |
| 11:A6:111:ASP:OD1 | 12:BB:3:LEU:CB   | 2.09                     | 1.01              |
| 6:WA:128:GLU:HG3  | 6:WB:126:PHE:CE2 | 1.95                     | 1.01              |
| 6:WK:197:LEU:HD12 | 6:WL:175:SER:HB3 | 1.07                     | 1.01              |
| 6:WR:197:LEU:CD1  | 6:WS:175:SER:OG  | 2.06                     | 1.01              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:62:TYR:HD1   | 2:d:129:VAL:HG13  | 1.25                     | 1.01              |
| 1:T:62:TYR:HD1   | 2:r:129:VAL:HG13  | 1.25                     | 1.01              |
| 5:AD:104:ASN:ND2 | 3:AI:38:ARG:NH2   | 2.09                     | 1.01              |
| 10:A3:76:GLN:NE2 | 12:BD:132:LEU:O   | 1.93                     | 1.01              |
| 1:H:166:GLU:HB2  | 1:I:35:THR:HG21   | 1.41                     | 1.01              |
| 1:R:166:GLU:HB2  | 1:S:35:THR:HG21   | 1.41                     | 1.01              |
| 1:U:62:TYR:HD1   | 2:s:129:VAL:HG13  | 1.26                     | 1.01              |
| 2:c:188:GLN:HB3  | 2:d:101:GLN:NE2   | 1.75                     | 1.01              |
| 2:e:188:GLN:HB3  | 2:f:101:GLN:NE2   | 1.75                     | 1.01              |
| 5:AB:202:MET:CE  | 3:AM:73:ARG:CZ    | 2.39                     | 1.01              |
| 6:WN:200:SER:O   | 6:WO:158:ALA:CB   | 2.07                     | 1.01              |
| 6:WT:196:HIS:HB3 | 6:WU:211:THR:HG21 | 1.41                     | 1.01              |
| 1:D:62:TYR:HD1   | 2:b:129:VAL:HG13  | 1.25                     | 1.00              |
| 1:O:62:TYR:HD1   | 2:m:129:VAL:HG13  | 1.25                     | 1.00              |
| 1:P:62:TYR:HD1   | 2:n:129:VAL:HG13  | 1.26                     | 1.00              |
| 2:a:80:GLN:NE2   | 3:8:58:GLU:HG3    | 1.74                     | 1.00              |
| 9:Ax:161:GLY:CA  | 6:WE:167:ARG:CD   | 2.38                     | 1.00              |
| 6:WS:200:SER:O   | 6:WT:158:ALA:CB   | 2.09                     | 1.00              |
| 1:J:166:GLU:HB2  | 1:K:35:THR:HG21   | 1.41                     | 1.00              |
| 2:a:101:GLN:NE2  | 2:z:188:GLN:HB3   | 1.75                     | 1.00              |
| 2:a:188:GLN:HB3  | 2:b:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:k:188:GLN:HB3  | 2:l:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:q:188:GLN:HB3  | 2:r:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:r:188:GLN:HB3  | 2:s:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:w:188:GLN:HB3  | 2:x:101:GLN:HE21  | 1.27                     | 1.00              |
| 2:x:188:GLN:HB3  | 2:y:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:x:188:GLN:HB3  | 2:y:101:GLN:HE21  | 1.27                     | 1.00              |
| 4:Za:379:GLN:NE2 | 4:Zf:394:GLN:OE1  | 1.95                     | 1.00              |
| 5:AE:228:GLU:HB3 | 3:AK:258:THR:HG21 | 1.00                     | 1.00              |
| 5:AE:231:MET:HE2 | 3:AJ:257:LEU:HB2  | 1.43                     | 1.00              |
| 6:WA:112:GLY:HA2 | 6:WA:135:ALA:HA   | 1.41                     | 1.00              |
| 1:L:62:TYR:HD1   | 2:j:129:VAL:HG13  | 1.26                     | 1.00              |
| 1:X:62:TYR:HD1   | 2:v:129:VAL:HG13  | 1.26                     | 1.00              |
| 2:m:188:GLN:HB3  | 2:n:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:n:188:GLN:HB3  | 2:o:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:o:188:GLN:HB3  | 2:p:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:o:188:GLN:HB3  | 2:p:101:GLN:HE21  | 1.27                     | 1.00              |
| 2:s:188:GLN:HB3  | 2:t:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:v:188:GLN:HB3  | 2:w:101:GLN:HE21  | 1.27                     | 1.00              |
| 2:y:188:GLN:HB3  | 2:z:101:GLN:HE21  | 1.27                     | 1.00              |
| 2:y:188:GLN:HB3  | 2:z:101:GLN:NE2   | 1.75                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:73:ARG:HD3    | 5:AD:202:MET:SD   | 2.01                     | 1.00              |
| 3:2:58:GLU:HG2    | 5:AA:160:ARG:HH11 | 1.25                     | 1.00              |
| 3:6:218:TYR:OH    | 4:ZH:53:LYS:HG3   | 1.62                     | 1.00              |
| 3:ZD:27:ALA:O     | 4:ZI:52:VAL:CG2   | 2.09                     | 1.00              |
| 4:ZQ:65:THR:HG21  | 4:Zb:4:SER:OG     | 1.62                     | 1.00              |
| 6:UP:62:ASP:OD2   | 6:WV:184:ARG:NH2  | 1.95                     | 1.00              |
| 6:WA:128:GLU:HG3  | 6:WB:126:PHE:CD2  | 1.96                     | 1.00              |
| 2:p:188:GLN:HB3   | 2:q:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:u:188:GLN:HB3   | 2:v:101:GLN:HE21  | 1.27                     | 1.00              |
| 3:1:9:LYS:HE2     | 5:AE:72:ASP:OD1   | 1.59                     | 1.00              |
| 5:AC:70:GLN:HB2   | 3:AN:6:TRP:HE3    | 1.17                     | 1.00              |
| 7:Aq:89:GLY:O     | 6:WW:164:LEU:HD12 | 1.61                     | 1.00              |
| 1:A:62:TYR:HD1    | 2:y:129:VAL:HG13  | 1.26                     | 1.00              |
| 1:B:166:GLU:HB2   | 1:C:35:THR:HG21   | 1.41                     | 1.00              |
| 1:C:166:GLU:HB2   | 1:D:35:THR:HG21   | 1.41                     | 1.00              |
| 1:T:166:GLU:HB2   | 1:U:35:THR:HG21   | 1.41                     | 1.00              |
| 2:a:101:GLN:HE21  | 2:z:188:GLN:HB3   | 1.27                     | 1.00              |
| 2:b:188:GLN:HB3   | 2:c:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:v:188:GLN:HB3   | 2:w:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:w:188:GLN:HB3   | 2:x:101:GLN:NE2   | 1.75                     | 1.00              |
| 3:AJ:62:LEU:CD2   | 12:BF:83:PRO:HD2  | 1.92                     | 1.00              |
| 1:G:62:TYR:HD1    | 2:e:129:VAL:HG13  | 1.26                     | 1.00              |
| 2:d:188:GLN:HB3   | 2:e:101:GLN:NE2   | 1.75                     | 1.00              |
| 2:l:188:GLN:HB3   | 2:m:101:GLN:NE2   | 1.75                     | 1.00              |
| 6:Am:295:SER:HB2  | 11:A7:73:ILE:HG13 | 1.38                     | 1.00              |
| 6:WM:193:ALA:HB1  | 6:WN:213:VAL:HG11 | 1.44                     | 1.00              |
| 1:L:166:GLU:HB2   | 1:M:35:THR:HG21   | 1.41                     | 0.99              |
| 1:Y:166:GLU:HB2   | 1:Z:35:THR:HG21   | 1.41                     | 0.99              |
| 2:n:188:GLN:HB3   | 2:o:101:GLN:HE21  | 1.27                     | 0.99              |
| 3:AK:6:TRP:CE2    | 12:BF:77:VAL:HG11 | 1.97                     | 0.99              |
| 1:G:166:GLU:HB2   | 1:H:35:THR:HG21   | 1.41                     | 0.99              |
| 1:I:62:TYR:HD1    | 2:g:129:VAL:HG13  | 1.25                     | 0.99              |
| 2:t:188:GLN:HB3   | 2:u:101:GLN:NE2   | 1.75                     | 0.99              |
| 3:5:241:GLU:OE2   | 3:ZA:256:LYS:NZ   | 1.94                     | 0.99              |
| 6:WD:200:SER:OG   | 6:WE:175:SER:HB2  | 1.59                     | 0.99              |
| 12:BD:68:ILE:HD11 | 6:BN:312:VAL:CG2  | 1.92                     | 0.99              |
| 2:t:188:GLN:HB3   | 2:u:101:GLN:HE21  | 1.27                     | 0.99              |
| 5:AE:16:LEU:HD23  | 3:AJ:253:MET:HE1  | 1.44                     | 0.99              |
| 3:AK:73:ARG:HD3   | 12:BF:78:TYR:CE2  | 1.96                     | 0.99              |
| 6:AY:299:ASN:HD21 | 11:A9:78:VAL:C    | 1.70                     | 0.99              |
| 11:A7:51:LYS:HE3  | 11:A7:55:ARG:HH12 | 1.25                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:62:TYR:HD1    | 2:q:129:VAL:HG13  | 1.26                     | 0.99              |
| 1:Q:62:TYR:HD1    | 2:o:129:VAL:HG13  | 1.25                     | 0.99              |
| 1:V:62:TYR:HD1    | 2:t:129:VAL:HG13  | 1.26                     | 0.99              |
| 2:s:188:GLN:HB3   | 2:t:101:GLN:HE21  | 1.27                     | 0.99              |
| 6:AS:299:ASN:HD22 | 11:A0:78:VAL:HG11 | 0.86                     | 0.99              |
| 1:D:166:GLU:HB2   | 1:E:35:THR:HG21   | 1.41                     | 0.99              |
| 3:2:58:GLU:HG3    | 5:AA:140:ASP:OD2  | 1.62                     | 0.99              |
| 3:ZB:122:VAL:O    | 4:ZG:322:ASN:CG   | 2.04                     | 0.99              |
| 3:AL:6:TRP:CE2    | 12:BD:77:VAL:HB   | 1.98                     | 0.99              |
| 6:UO:103:GLN:CD   | 6:WU:182:PRO:HB3  | 1.87                     | 0.99              |
| 1:A:166:GLU:HB2   | 1:B:35:THR:HG21   | 1.41                     | 0.99              |
| 2:p:188:GLN:HB3   | 2:q:101:GLN:HE21  | 1.27                     | 0.99              |
| 2:r:188:GLN:HB3   | 2:s:101:GLN:HE21  | 1.27                     | 0.99              |
| 1:N:62:TYR:HD1    | 2:l:129:VAL:HG13  | 1.25                     | 0.99              |
| 1:S:166:GLU:HB2   | 1:T:35:THR:HG21   | 1.41                     | 0.99              |
| 2:u:188:GLN:HB3   | 2:v:101:GLN:NE2   | 1.75                     | 0.99              |
| 7:Ab:8:MET:CE     | 6:WS:124:SER:HB2  | 1.93                     | 0.99              |
| 1:C:62:TYR:HD1    | 2:a:129:VAL:HG13  | 1.26                     | 0.99              |
| 1:K:166:GLU:HB2   | 1:L:35:THR:HG21   | 1.41                     | 0.99              |
| 6:AW:299:ASN:ND2  | 11:A9:55:ARG:NH2  | 2.11                     | 0.99              |
| 6:WD:168:GLU:HG2  | 6:WD:170:LYS:HE3  | 1.42                     | 0.99              |
| 6:Ad:372:ILE:HG21 | 10:A2:11:ILE:HG22 | 1.43                     | 0.98              |
| 3:1:193:ILE:HG21  | 5:AE:152:PRO:CD   | 1.92                     | 0.98              |
| 5:AC:62:PRO:CA    | 3:AH:63:PRO:HG2   | 1.92                     | 0.98              |
| 7:Ab:89:GLY:HA3   | 6:WS:165:PHE:HE1  | 1.24                     | 0.98              |
| 11:A7:51:LYS:HE2  | 11:A7:55:ARG:HH22 | 1.24                     | 0.98              |
| 2:q:188:GLN:HB3   | 2:r:101:GLN:HE21  | 1.27                     | 0.98              |
| 5:AA:200:ARG:NH2  | 3:AG:189:GLU:CB   | 2.23                     | 0.98              |
| 6:Ad:372:ILE:HG21 | 10:A2:11:ILE:CG2  | 1.92                     | 0.98              |
| 3:AL:52:PRO:HG3   | 12:BB:80:PRO:CB   | 1.91                     | 0.98              |
| 6:WE:197:LEU:HD12 | 6:WF:175:SER:OG   | 1.63                     | 0.98              |
| 6:WH:200:SER:O    | 6:WI:158:ALA:HB2  | 1.62                     | 0.98              |
| 6:Ad:372:ILE:CG2  | 10:A2:11:ILE:CG2  | 2.42                     | 0.98              |
| 4:ZT:17:LEU:HD13  | 4:ZY:395:ILE:HD11 | 1.46                     | 0.98              |
| 6:UP:73:MET:CE    | 6:UP:99:ARG:HD3   | 1.93                     | 0.98              |
| 6:WF:197:LEU:CD1  | 6:WG:175:SER:OG   | 2.11                     | 0.98              |
| 3:ZE:56:SER:O     | 3:AM:153:ARG:N    | 1.97                     | 0.98              |
| 6:WI:196:HIS:HB3  | 6:WJ:211:THR:HG21 | 1.45                     | 0.98              |
| 1:I:62:TYR:CD1    | 2:g:129:VAL:HG13  | 1.99                     | 0.98              |
| 1:J:62:TYR:CD1    | 2:h:129:VAL:HG13  | 1.99                     | 0.98              |
| 6:AV:278:THR:HG21 | 10:A3:21:ALA:HB3  | 1.43                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:62:TYR:CD1    | 2:f:129:VAL:HG13  | 1.99                     | 0.98              |
| 1:K:62:TYR:CD1    | 2:i:129:VAL:HG13  | 1.99                     | 0.98              |
| 1:W:62:TYR:HD1    | 2:u:129:VAL:HG13  | 1.25                     | 0.98              |
| 3:6:57:SER:OG     | 3:AK:108:PRO:HG3  | 1.62                     | 0.98              |
| 5:AB:71:LEU:HD23  | 3:AM:44:LEU:HD13  | 1.01                     | 0.98              |
| 1:B:62:TYR:HD1    | 2:z:129:VAL:HG13  | 1.25                     | 0.98              |
| 1:G:62:TYR:CD1    | 2:e:129:VAL:HG13  | 1.99                     | 0.98              |
| 1:M:62:TYR:HD1    | 2:k:129:VAL:HG13  | 1.25                     | 0.98              |
| 4:ZV:181:LYS:HD3  | 4:Zg:129:GLN:NE2  | 1.78                     | 0.98              |
| 6:UN:73:MET:CE    | 6:UN:99:ARG:HD3   | 1.93                     | 0.98              |
| 1:F:62:TYR:CD1    | 2:d:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:M:62:TYR:CD1    | 2:k:129:VAL:HG13  | 1.99                     | 0.97              |
| 4:ZS:181:LYS:HZ3  | 4:Zd:129:GLN:HE21 | 1.07                     | 0.97              |
| 6:UO:73:MET:CE    | 6:UO:99:ARG:HD3   | 1.93                     | 0.97              |
| 6:WJ:197:LEU:CD1  | 6:WK:175:SER:OG   | 2.11                     | 0.97              |
| 1:D:62:TYR:CD1    | 2:b:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:E:62:TYR:CD1    | 2:c:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:L:62:TYR:CD1    | 2:j:129:VAL:HG13  | 1.99                     | 0.97              |
| 5:AA:228:GLU:OE1  | 3:AF:256:LYS:HG2  | 1.64                     | 0.97              |
| 6:UK:207:PRO:HD2  | 6:WE:187:ASP:OD2  | 1.61                     | 0.97              |
| 6:UL:219:LEU:HD22 | 6:BS:247:ARG:NH1  | 1.79                     | 0.97              |
| 6:WA:200:SER:OG   | 6:WB:175:SER:HB2  | 1.64                     | 0.97              |
| 1:F:166:GLU:HB2   | 1:G:35:THR:HG21   | 1.41                     | 0.97              |
| 1:H:62:TYR:HD1    | 2:f:129:VAL:HG13  | 1.26                     | 0.97              |
| 3:ZE:28:ASN:OD1   | 4:ZJ:52:VAL:HB    | 1.62                     | 0.97              |
| 5:AC:70:GLN:CB    | 3:AN:6:TRP:HE3    | 1.76                     | 0.97              |
| 3:AF:44:LEU:HD22  | 12:BA:78:TYR:HB2  | 1.45                     | 0.97              |
| 6:UI:73:MET:CE    | 6:UI:99:ARG:HD3   | 1.93                     | 0.97              |
| 6:UI:125:GLN:O    | 6:UI:129:GLN:N    | 1.97                     | 0.97              |
| 6:UJ:73:MET:CE    | 6:UJ:99:ARG:HD3   | 1.93                     | 0.97              |
| 6:WI:197:LEU:CD1  | 6:WJ:175:SER:OG   | 2.12                     | 0.97              |
| 1:N:62:TYR:CD1    | 2:l:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:W:62:TYR:CD1    | 2:u:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:X:62:TYR:CD1    | 2:v:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:Y:62:TYR:CD1    | 2:w:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:Z:62:TYR:CD1    | 2:x:129:VAL:HG13  | 1.99                     | 0.97              |
| 2:m:188:GLN:HB3   | 2:n:101:GLN:HE21  | 1.27                     | 0.97              |
| 3:AH:44:LEU:CB    | 12:BC:90:TYR:OH   | 2.13                     | 0.97              |
| 6:UM:125:GLN:O    | 6:UM:129:GLN:N    | 1.97                     | 0.97              |
| 1:A:62:TYR:CD1    | 2:y:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:B:62:TYR:CD1    | 2:z:129:VAL:HG13  | 1.99                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:62:TYR:CD1    | 2:a:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:E:166:GLU:HB2   | 1:F:35:THR:HG21   | 1.41                     | 0.97              |
| 1:T:62:TYR:CD1    | 2:r:129:VAL:HG13  | 1.99                     | 0.97              |
| 6:UM:73:MET:CE    | 6:UM:99:ARG:HD3   | 1.93                     | 0.97              |
| 1:H:62:TYR:CD1    | 2:f:129:VAL:CG1   | 2.48                     | 0.97              |
| 1:V:62:TYR:CD1    | 2:t:129:VAL:HG13  | 1.99                     | 0.97              |
| 3:6:231:VAL:HG11  | 3:ZC:9:LYS:HG2    | 1.46                     | 0.97              |
| 10:A4:77:LYS:HE3  | 11:A0:13:GLN:HE22 | 1.23                     | 0.97              |
| 1:S:62:TYR:CD1    | 2:q:129:VAL:CG1   | 2.48                     | 0.97              |
| 1:U:62:TYR:CD1    | 2:s:129:VAL:HG13  | 1.99                     | 0.97              |
| 4:ZV:387:GLN:CD   | 4:Zb:400:VAL:HG13 | 1.89                     | 0.97              |
| 5:AD:26:LEU:HD12  | 3:AI:242:ILE:HG21 | 1.36                     | 0.97              |
| 3:AI:257:LEU:HD13 | 12:BD:99:VAL:HG22 | 1.47                     | 0.97              |
| 6:UJ:125:GLN:O    | 6:UJ:129:GLN:N    | 1.97                     | 0.97              |
| 1:A:35:THR:HG21   | 1:Z:166:GLU:HB2   | 1.41                     | 0.97              |
| 3:0:1:MET:CG      | 5:AD:213:PRO:HG3  | 1.95                     | 0.97              |
| 1:K:62:TYR:CD1    | 2:i:129:VAL:CG1   | 2.48                     | 0.97              |
| 1:O:62:TYR:CD1    | 2:m:129:VAL:HG13  | 1.99                     | 0.97              |
| 1:P:62:TYR:CD1    | 2:n:129:VAL:CG1   | 2.48                     | 0.97              |
| 1:V:62:TYR:CD1    | 2:t:129:VAL:CG1   | 2.48                     | 0.97              |
| 3:ZD:54:ALA:HB1   | 3:AL:150:THR:HG21 | 1.43                     | 0.97              |
| 3:ZD:56:SER:O     | 3:AL:153:ARG:N    | 1.97                     | 0.97              |
| 4:ZN:349:GLY:O    | 4:ZT:89:ASN:ND2   | 1.98                     | 0.97              |
| 6:Aj:372:ILE:CG2  | 10:A1:11:ILE:CG2  | 2.38                     | 0.97              |
| 6:UN:125:GLN:O    | 6:UN:129:GLN:N    | 1.97                     | 0.97              |
| 1:E:62:TYR:CD1    | 2:c:129:VAL:CG1   | 2.48                     | 0.97              |
| 1:F:62:TYR:CD1    | 2:d:129:VAL:CG1   | 2.48                     | 0.97              |
| 1:Q:62:TYR:CD1    | 2:o:129:VAL:CG1   | 2.48                     | 0.97              |
| 3:ZC:240:TYR:CD2  | 4:ZH:395:ILE:CG2  | 2.48                     | 0.97              |
| 3:ZD:76:ALA:CA    | 4:ZI:47:LYS:HE3   | 1.94                     | 0.97              |
| 9:Ax:161:GLY:HA2  | 6:WE:167:ARG:HD3  | 0.98                     | 0.97              |
| 1:N:62:TYR:CD1    | 2:l:129:VAL:CG1   | 2.48                     | 0.96              |
| 1:P:62:TYR:CD1    | 2:n:129:VAL:HG13  | 1.99                     | 0.96              |
| 9:Ay:147:LEU:HD12 | 6:WH:166:VAL:HG11 | 1.47                     | 0.96              |
| 10:A4:14:LEU:HD11 | 6:BX:370:ARG:HH21 | 1.29                     | 0.96              |
| 6:WT:197:LEU:HD12 | 6:WU:175:SER:CB   | 1.94                     | 0.96              |
| 1:C:62:TYR:CD1    | 2:a:129:VAL:CG1   | 2.48                     | 0.96              |
| 1:M:62:TYR:CD1    | 2:k:129:VAL:CG1   | 2.48                     | 0.96              |
| 1:T:62:TYR:CD1    | 2:r:129:VAL:CG1   | 2.48                     | 0.96              |
| 1:X:62:TYR:CD1    | 2:v:129:VAL:CG1   | 2.48                     | 0.96              |
| 2:f:54:GLN:HG2    | 3:AF:168:VAL:HG13 | 1.47                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:ZD:85:ASN:OD1   | 4:ZO:50:LEU:CD1   | 2.12                     | 0.96              |
| 3:AH:44:LEU:HD22  | 12:BC:78:TYR:HB2  | 1.44                     | 0.96              |
| 6:UK:125:GLN:O    | 6:UK:129:GLN:N    | 1.97                     | 0.96              |
| 1:J:62:TYR:CD1    | 2:h:129:VAL:CG1   | 2.48                     | 0.96              |
| 1:U:62:TYR:CD1    | 2:s:129:VAL:CG1   | 2.48                     | 0.96              |
| 3:1:6:TRP:HB2     | 5:AE:70:GLN:CB    | 1.94                     | 0.96              |
| 3:8:36:ARG:HE     | 3:8:38:ARG:HH22   | 1.07                     | 0.96              |
| 6:UO:125:GLN:O    | 6:UO:129:GLN:N    | 1.97                     | 0.96              |
| 6:UP:125:GLN:O    | 6:UP:129:GLN:N    | 1.97                     | 0.96              |
| 1:Q:62:TYR:CD1    | 2:o:129:VAL:HG13  | 1.99                     | 0.96              |
| 1:R:62:TYR:HD1    | 2:p:129:VAL:HG13  | 1.25                     | 0.96              |
| 1:S:62:TYR:CD1    | 2:q:129:VAL:HG13  | 1.99                     | 0.96              |
| 1:I:62:TYR:CD1    | 2:g:129:VAL:CG1   | 2.48                     | 0.96              |
| 3:5:257:LEU:HG    | 3:AI:230:LEU:CD1  | 1.95                     | 0.96              |
| 5:AA:220:MET:HE2  | 3:AF:246:ALA:HA   | 1.47                     | 0.96              |
| 10:A4:21:ALA:HB1  | 6:BV:278:THR:HG21 | 1.43                     | 0.96              |
| 1:A:62:TYR:CD1    | 2:y:129:VAL:CG1   | 2.48                     | 0.96              |
| 1:G:62:TYR:CD1    | 2:e:129:VAL:CG1   | 2.48                     | 0.96              |
| 3:3:55:GLN:O      | 5:AB:138:ALA:CB   | 2.12                     | 0.96              |
| 5:AD:228:GLU:HG2  | 3:AI:256:LYS:HD3  | 1.45                     | 0.96              |
| 6:UL:73:MET:CE    | 6:UL:99:ARG:HD3   | 1.93                     | 0.96              |
| 6:UL:125:GLN:O    | 6:UL:129:GLN:N    | 1.97                     | 0.96              |
| 6:WH:193:ALA:HB1  | 6:WI:213:VAL:HG11 | 1.46                     | 0.96              |
| 1:R:62:TYR:CD1    | 2:p:129:VAL:HG13  | 1.99                     | 0.96              |
| 1:Z:62:TYR:CD1    | 2:x:129:VAL:CG1   | 2.48                     | 0.96              |
| 5:AB:202:MET:HE3  | 3:AM:73:ARG:CZ    | 1.95                     | 0.96              |
| 6:UK:73:MET:CE    | 6:UK:99:ARG:HD3   | 1.93                     | 0.96              |
| 1:R:62:TYR:CD1    | 2:p:129:VAL:CG1   | 2.48                     | 0.96              |
| 3:8:54:ALA:CB     | 3:AG:150:THR:HG21 | 1.94                     | 0.96              |
| 5:AD:74:THR:HG21  | 3:AI:38:ARG:HH12  | 1.21                     | 0.96              |
| 5:AA:72:ASP:HB3   | 3:AL:9:LYS:HZ3    | 0.98                     | 0.96              |
| 5:AA:173:ARG:NH1  | 3:AF:46:TYR:OH    | 1.98                     | 0.96              |
| 9:Ay:147:LEU:HD12 | 6:WH:166:VAL:CG1  | 1.96                     | 0.96              |
| 1:Y:62:TYR:CD1    | 2:w:129:VAL:CG1   | 2.48                     | 0.96              |
| 2:l:188:GLN:HB3   | 2:m:101:GLN:HE21  | 1.27                     | 0.96              |
| 5:AA:225:ARG:NH2  | 3:AG:251:ASP:OD1  | 1.98                     | 0.96              |
| 1:D:62:TYR:CD1    | 2:b:129:VAL:CG1   | 2.48                     | 0.95              |
| 2:p:80:GLN:OE1    | 5:AD:154:THR:CA   | 2.13                     | 0.95              |
| 3:AK:73:ARG:CD    | 12:BF:78:TYR:CE2  | 2.49                     | 0.95              |
| 7:As:52:ILE:CD1   | 9:Ax:206:ALA:HB1  | 1.96                     | 0.95              |
| 1:B:62:TYR:CD1    | 2:z:129:VAL:CG1   | 2.48                     | 0.95              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:L:62:TYR:CD1    | 2:j:129:VAL:CG1    | 2.48                     | 0.95              |
| 4:Za:349:GLY:O    | 4:Zg:89:ASN:ND2    | 1.99                     | 0.95              |
| 5:AB:202:MET:CE   | 3:AM:73:ARG:NH1    | 2.28                     | 0.95              |
| 5:AE:231:MET:HE1  | 3:AJ:257:LEU:HD12  | 1.45                     | 0.95              |
| 6:Ac:278:THR:HG21 | 10:A2:14:LEU:HB3   | 1.45                     | 0.95              |
| 6:Ao:357:SER:OG   | 6:BI:319:GLN:NE2   | 1.98                     | 0.95              |
| 9:Ay:147:LEU:CD1  | 6:WH:166:VAL:HG11  | 1.96                     | 0.95              |
| 6:WI:197:LEU:HD12 | 6:WJ:175:SER:HB3   | 1.47                     | 0.95              |
| 3:0:44:LEU:HD22   | 5:AD:71:LEU:HD22   | 1.48                     | 0.95              |
| 4:ZV:380:ARG:NE   | 4:Zb:393:ASP:OD2   | 1.97                     | 0.95              |
| 7:Aq:2:THR:HG21   | 6:WW:125:GLN:CD    | 1.91                     | 0.95              |
| 9:Au:160:GLN:HB3  | 6:WP:166:VAL:HG22  | 0.96                     | 0.95              |
| 1:O:62:TYR:CD1    | 2:m:129:VAL:CG1    | 2.48                     | 0.95              |
| 1:W:62:TYR:CD1    | 2:u:129:VAL:CG1    | 2.48                     | 0.95              |
| 5:AB:223:ASN:HB3  | 3:AG:253:MET:HE1   | 1.48                     | 0.95              |
| 6:WK:197:LEU:CD1  | 6:WL:175:SER:HB3   | 1.96                     | 0.95              |
| 2:k:188:GLN:HB3   | 2:l:101:GLN:HE21   | 1.27                     | 0.95              |
| 3:8:36:ARG:HE     | 3:8:38:ARG:NH2     | 1.65                     | 0.95              |
| 3:ZB:238:ARG:NH1  | 4:ZH:393:ASP:OD1   | 1.98                     | 0.95              |
| 5:AA:202:MET:HE1  | 3:AL:73:ARG:HH21   | 1.30                     | 0.95              |
| 5:AD:55:THR:OG1   | 12:BE:45:LYS:NZ    | 1.99                     | 0.95              |
| 6:AS:365:ASN:HB3  | 11:A0:72:HIS:HD2   | 0.97                     | 0.95              |
| 6:WT:112:GLY:HA2  | 6:WT:135:ALA:HA    | 1.48                     | 0.95              |
| 3:ZD:185:GLU:OE2  | 4:ZI:46:SER:HB2    | 1.67                     | 0.95              |
| 4:ZT:379:GLN:NE2  | 4:ZY:394:GLN:OE1   | 2.00                     | 0.95              |
| 5:AC:70:GLN:CB    | 3:AN:6:TRP:CE3     | 2.50                     | 0.95              |
| 6:AY:299:ASN:ND2  | 11:A9:78:VAL:O     | 1.99                     | 0.95              |
| 6:Al:365:ASN:HB3  | 11:A7:72:HIS:CE1   | 2.02                     | 0.95              |
| 5:AE:231:MET:CE   | 3:AJ:257:LEU:CA    | 2.24                     | 0.95              |
| 7:As:55:ILE:HD11  | 9:Ax:205:MET:HE1   | 0.95                     | 0.95              |
| 3:1:193:ILE:HG22  | 5:AE:152:PRO:HG2   | 1.47                     | 0.95              |
| 3:AF:44:LEU:CD2   | 12:BA:78:TYR:HB2   | 1.96                     | 0.95              |
| 6:Ak:372:ILE:CG2  | 10:A1:4:ILE:CG1    | 2.44                     | 0.95              |
| 3:4:76:ALA:HB1    | 3:9:64:SER:O       | 1.65                     | 0.95              |
| 5:AB:9:MET:HB2    | 12:BB:103:VAL:HG21 | 1.49                     | 0.95              |
| 6:UM:62:ASP:OD2   | 6:WP:184:ARG:NH2   | 1.99                     | 0.94              |
| 3:2:179:MET:HE3   | 3:AL:144:ALA:HA    | 1.46                     | 0.94              |
| 4:ZS:65:THR:HG21  | 4:Zd:4:SER:OG      | 1.66                     | 0.94              |
| 7:Ab:81:PHE:O     | 7:Ab:85:PRO:HD2    | 1.67                     | 0.94              |
| 6:UI:133:GLN:NE2  | 6:UI:157:LEU:O     | 2.00                     | 0.94              |
| 6:UN:133:GLN:NE2  | 6:UN:157:LEU:O     | 2.00                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UO:133:GLN:NE2  | 6:UO:157:LEU:O    | 2.00                     | 0.94              |
| 6:WC:200:SER:O    | 6:WD:158:ALA:HB2  | 1.64                     | 0.94              |
| 6:WH:200:SER:OG   | 6:WI:175:SER:HB2  | 1.67                     | 0.94              |
| 2:f:188:GLN:HB3   | 2:g:101:GLN:HE21  | 1.27                     | 0.94              |
| 2:g:188:GLN:HB3   | 2:h:101:GLN:HE21  | 1.27                     | 0.94              |
| 2:j:188:GLN:HB3   | 2:k:101:GLN:HE21  | 1.27                     | 0.94              |
| 3:7:235:GLN:HE22  | 3:ZD:9:LYS:HD2    | 1.29                     | 0.94              |
| 6:Ag:295:SER:HB3  | 11:A8:72:HIS:HB2  | 1.48                     | 0.94              |
| 6:UL:133:GLN:NE2  | 6:UL:157:LEU:O    | 2.00                     | 0.94              |
| 3:2:55:GLN:O      | 5:AA:138:ALA:HB2  | 1.68                     | 0.94              |
| 3:7:235:GLN:NE2   | 3:ZD:9:LYS:HD2    | 1.82                     | 0.94              |
| 3:ZE:31:THR:HG22  | 4:ZJ:39:PHE:CB    | 1.97                     | 0.94              |
| 4:ZI:373:VAL:HG21 | 4:ZO:10:LEU:CD2   | 1.97                     | 0.94              |
| 6:AQ:295:SER:HB2  | 11:A6:65:LEU:HD22 | 1.49                     | 0.94              |
| 1:L:101:LYS:HZ3   | 3:6:168:VAL:CG1   | 1.76                     | 0.94              |
| 1:L:101:LYS:HZ3   | 3:6:168:VAL:HG11  | 1.14                     | 0.94              |
| 3:ZC:54:ALA:HB1   | 3:AK:150:THR:HG21 | 1.47                     | 0.94              |
| 4:ZU:65:THR:HG21  | 4:Zf:4:SER:HB3    | 1.50                     | 0.94              |
| 5:AB:213:PRO:HD2  | 3:AM:2:ILE:HD11   | 1.49                     | 0.94              |
| 6:WT:200:SER:O    | 6:WU:158:ALA:CB   | 2.15                     | 0.94              |
| 2:e:188:GLN:HB3   | 2:f:101:GLN:HE21  | 1.27                     | 0.94              |
| 3:ZD:207:GLY:O    | 4:ZJ:89:ASN:ND2   | 2.01                     | 0.94              |
| 5:AB:70:GLN:NE2   | 3:AM:1:MET:N      | 2.16                     | 0.94              |
| 6:UK:133:GLN:NE2  | 6:UK:157:LEU:O    | 2.00                     | 0.94              |
| 2:i:188:GLN:HB3   | 2:j:101:GLN:HE21  | 1.27                     | 0.94              |
| 5:AE:215:GLU:HG2  | 3:AK:9:LYS:HE3    | 1.46                     | 0.94              |
| 9:Au:38:TRP:HB2   | 10:A1:46:SER:OG   | 1.67                     | 0.94              |
| 6:UJ:133:GLN:NE2  | 6:UJ:157:LEU:O    | 2.00                     | 0.94              |
| 6:UM:103:GLN:CD   | 6:WQ:182:PRO:HB3  | 1.93                     | 0.94              |
| 6:UM:133:GLN:NE2  | 6:UM:157:LEU:O    | 2.00                     | 0.94              |
| 6:WS:112:GLY:CA   | 6:WS:135:ALA:HA   | 1.97                     | 0.93              |
| 2:h:188:GLN:HB3   | 2:i:101:GLN:HE21  | 1.27                     | 0.93              |
| 7:Ab:52:ILE:HD11  | 9:Au:206:ALA:CB   | 1.98                     | 0.93              |
| 6:UP:133:GLN:NE2  | 6:UP:157:LEU:O    | 2.00                     | 0.93              |
| 6:WE:200:SER:OG   | 6:WF:175:SER:HB2  | 1.67                     | 0.93              |
| 6:WS:112:GLY:HA2  | 6:WS:135:ALA:CA   | 1.99                     | 0.93              |
| 6:Ak:372:ILE:CB   | 10:A1:4:ILE:HG12  | 1.99                     | 0.93              |
| 3:1:258:THR:HA    | 5:AE:217:MET:HE2  | 1.49                     | 0.93              |
| 2:s:80:GLN:NE2    | 3:AI:141:THR:CG2  | 2.32                     | 0.93              |
| 3:ZB:28:ASN:ND2   | 4:ZG:52:VAL:HG23  | 1.84                     | 0.93              |
| 4:ZX:331:ASP:HA   | 4:Zc:40:ALA:HB1   | 1.50                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:At:145:TRP:CD1  | 6:WJ:164:LEU:CD1  | 2.52                     | 0.93              |
| 3:8:111:THR:HG21  | 3:AL:163:GLY:HA2  | 1.51                     | 0.93              |
| 5:AB:202:MET:CE   | 3:AM:73:ARG:NE    | 2.31                     | 0.93              |
| 5:AC:21:VAL:HG23  | 3:AH:68:ILE:HG22  | 1.47                     | 0.93              |
| 2:a:188:GLN:HB3   | 2:b:101:GLN:HE21  | 1.27                     | 0.93              |
| 4:Za:331:ASP:CA   | 4:Zf:40:ALA:HB1   | 1.98                     | 0.93              |
| 6:WP:200:SER:OG   | 6:WQ:175:SER:HB2  | 1.69                     | 0.93              |
| 4:ZW:42:MET:HE3   | 4:ZW:53:LYS:HB3   | 1.50                     | 0.92              |
| 4:ZW:183:THR:HG22 | 4:Zh:131:GLY:O    | 1.68                     | 0.92              |
| 5:AB:202:MET:HE3  | 3:AM:73:ARG:HH11  | 1.17                     | 0.92              |
| 3:ZA:20:ASP:OD1   | 4:ZF:2:SER:CB     | 2.13                     | 0.92              |
| 3:AK:73:ARG:HD3   | 12:BF:78:TYR:CZ   | 2.05                     | 0.92              |
| 2:d:188:GLN:HB3   | 2:e:101:GLN:HE21  | 1.27                     | 0.92              |
| 5:AC:71:LEU:HD13  | 3:AN:70:THR:CG2   | 1.99                     | 0.92              |
| 6:UK:207:PRO:CG   | 6:WE:187:ASP:OD1  | 2.16                     | 0.92              |
| 3:6:28:ASN:ND2    | 3:ZB:43:ASP:OD1   | 2.03                     | 0.92              |
| 1:L:101:LYS:HZ1   | 3:6:168:VAL:HG11  | 1.24                     | 0.92              |
| 5:AD:26:LEU:HD12  | 3:AI:242:ILE:HG22 | 1.51                     | 0.92              |
| 5:AE:227:PHE:CE2  | 3:AJ:253:MET:O    | 2.22                     | 0.92              |
| 3:ZD:76:ALA:HB1   | 4:ZI:47:LYS:CE    | 2.00                     | 0.92              |
| 3:5:257:LEU:CG    | 3:AI:230:LEU:HD12 | 1.98                     | 0.92              |
| 5:AA:202:MET:HG3  | 3:AL:45:LEU:CD1   | 1.98                     | 0.92              |
| 6:WR:112:GLY:CA   | 6:WR:135:ALA:HA   | 2.00                     | 0.92              |
| 4:ZY:269:GLN:OE1  | 4:Ze:286:PRO:HB3  | 1.69                     | 0.92              |
| 5:AB:223:ASN:C    | 3:AG:253:MET:HE2  | 1.94                     | 0.92              |
| 5:AE:231:MET:SD   | 3:AJ:260:LEU:HD23 | 2.10                     | 0.92              |
| 3:0:44:LEU:HD22   | 5:AD:71:LEU:CD2   | 1.98                     | 0.92              |
| 8:At:145:TRP:HE1  | 6:WJ:164:LEU:HB2  | 1.29                     | 0.92              |
| 6:WQ:181:GLU:CB   | 6:WQ:184:ARG:HG3  | 2.00                     | 0.92              |
| 3:1:258:THR:CA    | 5:AE:217:MET:CE   | 2.48                     | 0.92              |
| 4:ZQ:380:ARG:NH2  | 4:ZW:393:ASP:OD1  | 2.02                     | 0.92              |
| 6:UN:62:ASP:OD2   | 6:WR:184:ARG:NH2  | 2.02                     | 0.92              |
| 6:WA:197:LEU:HD12 | 6:WB:175:SER:CB   | 1.99                     | 0.92              |
| 5:AB:26:LEU:HD22  | 3:AG:242:ILE:CG2  | 1.99                     | 0.91              |
| 8:At:158:PRO:HG2  | 8:At:162:ASN:HD21 | 1.35                     | 0.91              |
| 6:WF:181:GLU:CB   | 6:WF:184:ARG:HG3  | 2.00                     | 0.91              |
| 5:AA:76:ARG:HD3   | 3:AF:80:LEU:HD11  | 1.51                     | 0.91              |
| 5:AD:16:LEU:CD2   | 3:AI:253:MET:HE2  | 2.00                     | 0.91              |
| 6:WK:181:GLU:CB   | 6:WK:184:ARG:HG3  | 2.00                     | 0.91              |
| 6:WN:181:GLU:CB   | 6:WN:184:ARG:HG3  | 2.01                     | 0.91              |
| 6:WU:181:GLU:CB   | 6:WU:184:ARG:HG3  | 2.01                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:ZC:234:ILE:HG21 | 4:ZI:393:ASP:OD2  | 1.69                     | 0.91              |
| 5:AB:70:GLN:CB    | 3:AM:6:TRP:CD1    | 2.53                     | 0.91              |
| 6:WG:181:GLU:CB   | 6:WG:184:ARG:HG3  | 2.01                     | 0.91              |
| 5:AC:71:LEU:CD1   | 3:AN:70:THR:HG21  | 2.00                     | 0.91              |
| 7:Ar:14:MET:HE3   | 7:As:63:ILE:CD1   | 2.00                     | 0.91              |
| 6:WO:181:GLU:CB   | 6:WO:184:ARG:HG3  | 2.00                     | 0.91              |
| 3:O:2:ILE:CG2     | 5:AD:211:VAL:O    | 2.14                     | 0.91              |
| 6:Ao:357:SER:OG   | 6:BI:319:GLN:CD   | 2.13                     | 0.91              |
| 6:Aj:370:ARG:HH21 | 10:A1:14:LEU:CD2  | 1.83                     | 0.91              |
| 6:WR:181:GLU:CB   | 6:WR:184:ARG:HG3  | 2.01                     | 0.91              |
| 3:O:2:ILE:HG22    | 5:AD:211:VAL:C    | 1.95                     | 0.91              |
| 4:ZY:373:VAL:HG11 | 4:Ze:7:VAL:HG22   | 1.52                     | 0.91              |
| 4:Za:331:ASP:HA   | 4:Zf:40:ALA:CB    | 2.00                     | 0.91              |
| 5:AA:202:MET:CE   | 3:AL:73:ARG:HH21  | 1.84                     | 0.91              |
| 6:An:278:THR:HG21 | 10:Az:14:LEU:CD2  | 2.01                     | 0.91              |
| 6:WD:181:GLU:CB   | 6:WD:184:ARG:HG3  | 2.01                     | 0.91              |
| 5:AA:217:MET:HE2  | 3:AL:257:LEU:O    | 1.71                     | 0.91              |
| 6:WL:181:GLU:CB   | 6:WL:184:ARG:HG3  | 2.01                     | 0.91              |
| 6:WV:181:GLU:CB   | 6:WV:184:ARG:HG3  | 2.01                     | 0.91              |
| 2:c:188:GLN:HB3   | 2:d:101:GLN:HE21  | 1.27                     | 0.91              |
| 3:ZC:31:THR:HG22  | 4:ZH:39:PHE:HB2   | 1.53                     | 0.91              |
| 4:Za:18:ASP:OD2   | 4:Zf:2:SER:N      | 2.03                     | 0.91              |
| 6:Ag:297:GLN:HB2  | 11:A8:73:ILE:HD13 | 1.53                     | 0.91              |
| 6:WJ:128:GLU:CG   | 6:WK:126:PHE:HD2  | 1.84                     | 0.91              |
| 6:WM:181:GLU:CB   | 6:WM:184:ARG:HG3  | 2.00                     | 0.91              |
| 3:ZA:145:ASN:HA   | 4:ZF:352:ASN:HD22 | 1.36                     | 0.91              |
| 4:ZU:183:THR:HB   | 4:Zf:132:ALA:HA   | 1.53                     | 0.91              |
| 3:AG:257:LEU:HD11 | 12:BB:102:MET:SD  | 2.10                     | 0.91              |
| 3:AI:50:ARG:CG    | 6:BN:322:PRO:HG3  | 2.01                     | 0.91              |
| 3:5:226:VAL:CG1   | 3:ZA:242:ILE:HD13 | 2.01                     | 0.90              |
| 2:m:80:GLN:HE22   | 3:AJ:204:SER:HA   | 1.32                     | 0.90              |
| 3:ZA:145:ASN:OD1  | 4:ZF:352:ASN:ND2  | 2.05                     | 0.90              |
| 3:ZB:248:SER:HB3  | 4:ZG:402:LEU:HD22 | 1.51                     | 0.90              |
| 7:Ab:8:MET:HE2    | 6:WS:124:SER:CA   | 2.01                     | 0.90              |
| 3:1:6:TRP:HB2     | 5:AE:70:GLN:HB2   | 1.54                     | 0.90              |
| 3:AK:73:ARG:CD    | 12:BF:78:TYR:CZ   | 2.54                     | 0.90              |
| 10:A4:14:LEU:HB3  | 6:BW:278:THR:HG21 | 1.52                     | 0.90              |
| 6:WD:168:GLU:HG2  | 6:WD:170:LYS:CE   | 2.00                     | 0.90              |
| 6:WH:181:GLU:CB   | 6:WH:184:ARG:HG3  | 2.00                     | 0.90              |
| 6:WS:181:GLU:CB   | 6:WS:184:ARG:HG3  | 2.00                     | 0.90              |
| 3:ZB:31:THR:HG22  | 4:ZG:39:PHE:CB    | 2.02                     | 0.90              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:Ak:372:ILE:HG22 | 10:A1:4:ILE:HD11   | 1.49                     | 0.90              |
| 5:AB:223:ASN:O    | 3:AG:253:MET:HE2   | 1.71                     | 0.90              |
| 6:Ai:303:GLN:HE22 | 6:BK:319:GLN:HB3   | 0.76                     | 0.90              |
| 10:A4:7:ILE:CB    | 6:BX:278:THR:HG21  | 2.01                     | 0.90              |
| 3:1:73:ARG:NH1    | 5:AE:202:MET:HE2   | 1.86                     | 0.90              |
| 5:AA:26:LEU:HD22  | 3:AF:242:ILE:HG21  | 1.52                     | 0.90              |
| 5:AE:238:ASP:OD1  | 12:BE:110:ARG:NH1  | 2.05                     | 0.90              |
| 8:At:145:TRP:CD1  | 6:WJ:164:LEU:CG    | 2.54                     | 0.90              |
| 5:AB:28:ASN:OD1   | 3:AG:72:VAL:CG2    | 2.19                     | 0.90              |
| 6:WR:197:LEU:HD12 | 6:WS:175:SER:HB3   | 1.54                     | 0.90              |
| 2:b:188:GLN:HB3   | 2:c:101:GLN:HE21   | 1.27                     | 0.89              |
| 3:0:44:LEU:HD21   | 5:AD:205:VAL:HG11  | 1.52                     | 0.89              |
| 3:ZD:20:ASP:OD1   | 4:ZI:2:SER:HB2     | 1.71                     | 0.89              |
| 6:WS:121:PHE:HE1  | 6:WT:120:LYS:HZ3   | 0.94                     | 0.89              |
| 6:WW:181:GLU:CB   | 6:WW:184:ARG:HG3   | 2.01                     | 0.89              |
| 2:k:80:GLN:OE1    | 5:AE:157:PRO:HD2   | 1.70                     | 0.89              |
| 3:5:241:GLU:HG2   | 3:ZA:256:LYS:HE3   | 1.53                     | 0.89              |
| 5:AB:70:GLN:HE21  | 3:AM:1:MET:H1      | 1.18                     | 0.89              |
| 9:Ay:148:ALA:CB   | 6:WI:164:LEU:HD22  | 2.02                     | 0.89              |
| 6:WB:197:LEU:HD12 | 6:WC:175:SER:OG    | 1.72                     | 0.89              |
| 3:7:85:ASN:ND2    | 4:ZI:4:SER:OG      | 2.05                     | 0.89              |
| 4:ZY:380:ARG:HB3  | 4:Ze:396:LEU:HD23  | 1.54                     | 0.89              |
| 5:AB:72:ASP:HB2   | 3:AM:9:LYS:HZ3     | 1.35                     | 0.89              |
| 5:AB:223:ASN:C    | 3:AG:253:MET:CE    | 2.46                     | 0.89              |
| 5:AB:71:LEU:HD22  | 3:AM:70:THR:HG21   | 1.52                     | 0.89              |
| 4:Za:331:ASP:N    | 4:Zf:41:ASP:O      | 2.05                     | 0.89              |
| 5:AD:243:ARG:NE   | 12:BE:113:GLN:HB2  | 1.88                     | 0.89              |
| 3:AF:44:LEU:CD2   | 12:BA:78:TYR:CG    | 2.56                     | 0.89              |
| 7:As:7:MET:HE2    | 8:At:233:MET:C     | 1.97                     | 0.89              |
| 6:WP:181:GLU:CB   | 6:WP:184:ARG:HG3   | 2.01                     | 0.89              |
| 5:AA:247:LEU:CB   | 12:BB:120:ASN:HD21 | 1.85                     | 0.89              |
| 9:Aw:162:PRO:HD3  | 6:WA:167:ARG:HH21  | 1.38                     | 0.89              |
| 2:c:78:ASN:ND2    | 3:AG:145:ASN:ND2   | 2.20                     | 0.89              |
| 3:5:58:GLU:OE2    | 5:AD:160:ARG:NH2   | 2.06                     | 0.89              |
| 6:AV:355:PRO:HB2  | 6:BO:319:GLN:NE2   | 1.87                     | 0.89              |
| 6:WE:181:GLU:CB   | 6:WE:184:ARG:HG3   | 2.01                     | 0.89              |
| 6:WJ:181:GLU:CB   | 6:WJ:184:ARG:HG3   | 2.01                     | 0.89              |
| 3:AM:52:PRO:C     | 12:BC:87:ALA:O     | 2.16                     | 0.89              |
| 9:Ax:144:GLU:HG2  | 6:WD:164:LEU:O     | 1.73                     | 0.89              |
| 12:BC:6:ILE:HG21  | 12:BC:122:VAL:HG21 | 1.55                     | 0.89              |
| 4:ZR:375:MET:HE1  | 4:ZW:388:THR:HG23  | 1.54                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AJ:2:ILE:CD1    | 12:BE:32:ASP:OD1  | 2.21                     | 0.89              |
| 10:A4:21:ALA:HB3  | 6:BV:278:THR:HG21 | 1.53                     | 0.89              |
| 3:ZE:31:THR:HG22  | 4:ZJ:39:PHE:HB2   | 1.52                     | 0.88              |
| 6:WM:197:LEU:HD12 | 6:WN:175:SER:OG   | 1.72                     | 0.88              |
| 3:ZA:57:SER:HA    | 3:AI:154:ASP:HB3  | 1.55                     | 0.88              |
| 4:ZI:382:TYR:CE1  | 4:ZN:395:ILE:HG23 | 2.06                     | 0.88              |
| 6:Af:295:SER:CB   | 11:A8:65:LEU:HB2  | 2.03                     | 0.88              |
| 2:i:54:GLN:OE1    | 3:AK:106:MET:SD   | 2.31                     | 0.88              |
| 3:ZA:240:TYR:CD2  | 4:ZF:395:ILE:HG23 | 2.09                     | 0.88              |
| 3:ZD:248:SER:HB2  | 4:ZI:402:LEU:HD22 | 1.54                     | 0.88              |
| 4:ZK:379:GLN:HG3  | 4:ZP:391:THR:HG23 | 1.52                     | 0.88              |
| 5:AA:26:LEU:CD1   | 3:AF:242:ILE:CG2  | 2.52                     | 0.88              |
| 5:AE:26:LEU:HD22  | 3:AJ:242:ILE:HG23 | 1.55                     | 0.88              |
| 8:At:145:TRP:HD1  | 6:WJ:164:LEU:CG   | 1.86                     | 0.88              |
| 6:WD:200:SER:O    | 6:WE:158:ALA:CB   | 2.20                     | 0.88              |
| 3:5:55:GLN:O      | 5:AD:138:ALA:HB2  | 1.72                     | 0.88              |
| 6:AY:365:ASN:CB   | 11:A9:72:HIS:HD2  | 1.87                     | 0.88              |
| 7:Ar:40:ALA:HB2   | 7:As:44:ILE:HD13  | 1.55                     | 0.88              |
| 2:s:80:GLN:NE2    | 3:AI:141:THR:HG21 | 1.88                     | 0.88              |
| 4:ZU:183:THR:CB   | 4:Zf:132:ALA:HA   | 2.04                     | 0.88              |
| 6:WB:181:GLU:CB   | 6:WB:184:ARG:HG3  | 2.01                     | 0.88              |
| 4:ZQ:181:LYS:HZ3  | 4:Zb:129:GLN:HE21 | 1.20                     | 0.88              |
| 8:At:114:VAL:HG21 | 9:Ax:211:MET:HE1  | 1.53                     | 0.88              |
| 6:UP:126:PHE:CE1  | 6:UP:130:VAL:HG21 | 2.09                     | 0.88              |
| 6:WA:181:GLU:CB   | 6:WA:184:ARG:HG3  | 2.01                     | 0.88              |
| 6:WT:181:GLU:CB   | 6:WT:184:ARG:HG3  | 2.01                     | 0.88              |
| 4:ZG:380:ARG:NE   | 4:ZM:393:ASP:OD2  | 2.07                     | 0.88              |
| 6:UN:126:PHE:CE1  | 6:UN:130:VAL:HG21 | 2.09                     | 0.88              |
| 3:ZD:28:ASN:OD1   | 4:ZI:52:VAL:HG13  | 1.73                     | 0.88              |
| 6:WD:115:LEU:HD22 | 6:WD:134:ARG:HD2  | 1.54                     | 0.88              |
| 6:WI:181:GLU:CB   | 6:WI:184:ARG:HG3  | 2.01                     | 0.88              |
| 6:WR:196:HIS:HB3  | 6:WS:211:THR:HG21 | 1.56                     | 0.88              |
| 4:ZH:160:SER:O    | 4:ZN:252:ASN:ND2  | 2.07                     | 0.87              |
| 4:ZY:349:GLY:O    | 4:Ze:89:ASN:ND2   | 2.07                     | 0.87              |
| 6:UM:126:PHE:O    | 6:UM:130:VAL:N    | 2.07                     | 0.87              |
| 6:WT:121:PHE:CZ   | 6:WU:122:GLY:O    | 2.27                     | 0.87              |
| 3:7:70:THR:HG23   | 3:AK:85:ASN:OD1   | 1.73                     | 0.87              |
| 6:UO:126:PHE:CE1  | 6:UO:130:VAL:HG21 | 2.09                     | 0.87              |
| 3:5:245:LYS:HE3   | 3:ZB:258:THR:O    | 1.75                     | 0.87              |
| 4:ZL:18:ASP:OD1   | 4:ZQ:2:SER:N      | 2.07                     | 0.87              |
| 6:UK:126:PHE:CE1  | 6:UK:130:VAL:HG21 | 2.09                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UN:126:PHE:O    | 6:UN:130:VAL:N    | 2.07                     | 0.87              |
| 12:BA:22:ASN:HB2  | 6:BG:315:ALA:HB2  | 1.54                     | 0.87              |
| 2:i:273:CYS:HA    | 2:j:328:LEU:HD21  | 1.57                     | 0.87              |
| 3:ZC:122:VAL:O    | 4:ZH:322:ASN:CB   | 2.22                     | 0.87              |
| 5:AC:70:GLN:OE1   | 3:AN:2:ILE:O      | 1.90                     | 0.87              |
| 3:AF:73:ARG:HD2   | 12:BA:78:TYR:CZ   | 2.10                     | 0.87              |
| 9:Ax:162:PRO:HD3  | 6:WE:167:ARG:HH21 | 1.39                     | 0.87              |
| 9:Ay:160:GLN:O    | 6:WI:167:ARG:HG3  | 1.75                     | 0.87              |
| 11:A7:51:LYS:HB3  | 11:A7:55:ARG:HH22 | 1.13                     | 0.87              |
| 6:UJ:103:GLN:CB   | 6:WD:182:PRO:HB3  | 2.04                     | 0.87              |
| 6:UO:126:PHE:O    | 6:UO:130:VAL:N    | 2.07                     | 0.87              |
| 2:j:273:CYS:HA    | 2:k:328:LEU:HD21  | 1.57                     | 0.87              |
| 2:l:273:CYS:HA    | 2:m:328:LEU:HD21  | 1.57                     | 0.87              |
| 4:ZT:17:LEU:HD13  | 4:ZY:395:ILE:CD1  | 2.03                     | 0.87              |
| 7:Aq:59:PHE:HZ    | 9:Av:198:LEU:HD21 | 1.39                     | 0.87              |
| 6:UI:126:PHE:O    | 6:UI:130:VAL:N    | 2.07                     | 0.87              |
| 6:WV:200:SER:O    | 6:WW:158:ALA:HB2  | 1.73                     | 0.87              |
| 2:h:273:CYS:HA    | 2:i:328:LEU:HD21  | 1.57                     | 0.87              |
| 2:k:273:CYS:HA    | 2:l:328:LEU:HD21  | 1.57                     | 0.87              |
| 2:m:273:CYS:HA    | 2:n:328:LEU:HD21  | 1.57                     | 0.87              |
| 5:AA:70:GLN:CB    | 3:AL:6:TRP:HB2    | 2.05                     | 0.87              |
| 5:AA:72:ASP:HB3   | 3:AL:9:LYS:HZ1    | 1.34                     | 0.87              |
| 6:AS:365:ASN:CB   | 11:A0:72:HIS:HD2  | 1.87                     | 0.87              |
| 6:AX:361:ASN:HD22 | 11:A9:78:VAL:HG12 | 1.40                     | 0.87              |
| 6:UI:126:PHE:CE1  | 6:UI:130:VAL:HG21 | 2.09                     | 0.87              |
| 6:WD:203:ALA:HB1  | 6:WE:160:PRO:HB3  | 1.57                     | 0.87              |
| 2:g:273:CYS:HA    | 2:h:328:LEU:HD21  | 1.57                     | 0.87              |
| 2:n:273:CYS:HA    | 2:o:328:LEU:HD21  | 1.57                     | 0.87              |
| 4:ZT:99:GLN:NE2   | 4:ZY:58:THR:HG21  | 1.89                     | 0.87              |
| 6:UJ:126:PHE:CE1  | 6:UJ:130:VAL:HG21 | 2.09                     | 0.87              |
| 6:WC:200:SER:O    | 6:WD:158:ALA:CB   | 2.23                     | 0.87              |
| 9:Ax:162:PRO:CD   | 6:WE:167:ARG:HH21 | 1.87                     | 0.87              |
| 6:WM:197:LEU:HD12 | 6:WN:175:SER:CB   | 2.05                     | 0.87              |
| 4:ZI:379:GLN:HG3  | 4:ZN:391:THR:HG23 | 1.56                     | 0.86              |
| 5:AC:62:PRO:HA    | 3:AH:63:PRO:CG    | 2.05                     | 0.86              |
| 3:AJ:257:LEU:HD21 | 12:BE:98:VAL:HG12 | 1.57                     | 0.86              |
| 6:UL:126:PHE:CE1  | 6:UL:130:VAL:HG21 | 2.09                     | 0.86              |
| 2:o:273:CYS:HA    | 2:p:328:LEU:HD21  | 1.57                     | 0.86              |
| 6:UM:126:PHE:CE1  | 6:UM:130:VAL:HG21 | 2.09                     | 0.86              |
| 3:0:251:ASP:OD1   | 3:AI:238:ARG:NH2  | 2.07                     | 0.86              |
| 3:1:45:LEU:HD13   | 5:AE:83:GLN:HA    | 1.55                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Ak:372:ILE:HB   | 10:A1:4:ILE:HG12  | 1.55                     | 0.86              |
| 6:UJ:126:PHE:O    | 6:UJ:130:VAL:N    | 2.07                     | 0.86              |
| 6:WA:196:HIS:HB3  | 6:WB:211:THR:HG21 | 1.57                     | 0.86              |
| 4:Za:157:ASN:ND2  | 4:Zg:143:LEU:HD13 | 1.90                     | 0.86              |
| 6:Am:278:THR:HG21 | 10:Az:21:ALA:HB1  | 1.56                     | 0.86              |
| 6:UK:126:PHE:O    | 6:UK:130:VAL:N    | 2.07                     | 0.86              |
| 2:f:273:CYS:HA    | 2:g:328:LEU:HD21  | 1.57                     | 0.86              |
| 4:ZH:331:ASP:HA   | 4:ZM:40:ALA:HB1   | 1.57                     | 0.86              |
| 6:WK:132:TYR:HB2  | 6:WL:126:PHE:HZ   | 1.40                     | 0.86              |
| 2:e:273:CYS:HA    | 2:f:328:LEU:HD21  | 1.57                     | 0.86              |
| 2:p:53:THR:HG21   | 5:AD:154:THR:HG22 | 1.58                     | 0.86              |
| 2:p:273:CYS:HA    | 2:q:328:LEU:HD21  | 1.57                     | 0.86              |
| 3:1:258:THR:HA    | 5:AE:217:MET:HE3  | 1.55                     | 0.86              |
| 5:AA:72:ASP:CB    | 3:AL:9:LYS:NZ     | 2.36                     | 0.86              |
| 3:AI:46:TYR:HA    | 3:AI:69:GLY:HA2   | 1.56                     | 0.86              |
| 7:Ab:89:GLY:HA3   | 6:WS:165:PHE:CE1  | 2.09                     | 0.86              |
| 6:UP:126:PHE:O    | 6:UP:130:VAL:N    | 2.07                     | 0.86              |
| 6:WM:139:GLU:HB3  | 6:WN:154:ARG:HH21 | 1.39                     | 0.86              |
| 4:ZU:66:THR:HB    | 4:Zf:42:MET:CE    | 2.05                     | 0.86              |
| 6:WV:120:LYS:HZ3  | 6:WV:123:ILE:HD11 | 1.40                     | 0.86              |
| 3:ZC:234:ILE:CG2  | 4:ZI:393:ASP:OD2  | 2.22                     | 0.86              |
| 5:AD:104:ASN:HD21 | 3:AI:38:ARG:HH21  | 1.18                     | 0.86              |
| 6:WB:200:SER:OG   | 6:WC:175:SER:HB2  | 1.76                     | 0.86              |
| 2:q:273:CYS:HA    | 2:r:328:LEU:HD21  | 1.57                     | 0.86              |
| 3:1:163:GLY:HA2   | 3:ZC:111:THR:HG21 | 1.57                     | 0.86              |
| 3:4:86:LEU:HD12   | 4:ZF:42:MET:HE2   | 1.57                     | 0.86              |
| 6:An:278:THR:HG22 | 10:Az:14:LEU:HD23 | 1.54                     | 0.86              |
| 2:g:80:GLN:NE2    | 3:AF:168:VAL:HG11 | 1.90                     | 0.86              |
| 5:AD:217:MET:HE1  | 3:AI:242:ILE:HD13 | 1.56                     | 0.86              |
| 6:UL:126:PHE:O    | 6:UL:130:VAL:N    | 2.07                     | 0.86              |
| 5:AB:16:LEU:HD22  | 3:AG:2:ILE:CD1    | 2.05                     | 0.85              |
| 6:AV:357:SER:OG   | 6:BO:318:ASN:ND2  | 2.09                     | 0.85              |
| 6:Ak:372:ILE:HG21 | 10:A1:4:ILE:CG1   | 2.04                     | 0.85              |
| 3:0:180:ASN:ND2   | 3:AJ:122:VAL:O    | 2.09                     | 0.85              |
| 4:ZU:372:LEU:HD12 | 4:Zf:396:LEU:HD21 | 1.58                     | 0.85              |
| 4:ZW:382:TYR:CE1  | 4:Zb:395:ILE:HG23 | 2.11                     | 0.85              |
| 6:WK:200:SER:O    | 6:WL:158:ALA:HB3  | 1.75                     | 0.85              |
| 12:BD:68:ILE:HD11 | 6:BN:312:VAL:HG21 | 1.56                     | 0.85              |
| 2:d:273:CYS:HA    | 2:e:328:LEU:HD21  | 1.57                     | 0.85              |
| 4:ZH:157:ASN:ND2  | 4:ZN:143:LEU:HD13 | 1.91                     | 0.85              |
| 4:ZY:331:ASP:HA   | 4:Zd:40:ALA:HB1   | 1.59                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AD:59:ALA:O     | 3:AI:66:LEU:HD13  | 1.76                     | 0.85              |
| 6:Ag:297:GLN:HB2  | 11:A8:73:ILE:HD12 | 1.57                     | 0.85              |
| 2:r:273:CYS:HA    | 2:s:328:LEU:HD21  | 1.57                     | 0.85              |
| 5:AC:21:VAL:HG22  | 3:AH:68:ILE:HG22  | 1.56                     | 0.85              |
| 5:AE:49:LEU:HB3   | 11:A0:90:PRO:HG2  | 1.58                     | 0.85              |
| 3:ZB:244:SER:HB2  | 4:ZG:399:LEU:CD2  | 2.07                     | 0.85              |
| 5:AC:217:MET:SD   | 3:AH:245:LYS:HD2  | 2.16                     | 0.85              |
| 10:A4:68:LEU:HD23 | 12:BE:126:MET:HE2 | 1.57                     | 0.85              |
| 6:WA:175:SER:HB2  | 6:WW:200:SER:OG   | 1.76                     | 0.85              |
| 6:WR:200:SER:O    | 6:WS:158:ALA:CB   | 2.24                     | 0.85              |
| 3:1:193:ILE:CG2   | 5:AE:152:PRO:HG2  | 2.04                     | 0.85              |
| 3:1:258:THR:HA    | 5:AE:217:MET:HE1  | 1.56                     | 0.85              |
| 4:ZZ:269:GLN:OE1  | 4:Zf:286:PRO:HG3  | 1.76                     | 0.85              |
| 6:Aj:370:ARG:NH2  | 10:A1:14:LEU:HD21 | 1.91                     | 0.85              |
| 7:Aq:2:THR:CG2    | 6:WW:125:GLN:OE1  | 2.25                     | 0.85              |
| 6:UL:126:PHE:O    | 6:UL:130:VAL:HG23 | 1.77                     | 0.85              |
| 6:UM:103:GLN:CG   | 6:WQ:182:PRO:HB3  | 2.07                     | 0.85              |
| 1:L:101:LYS:HZ1   | 3:6:168:VAL:CG1   | 1.85                     | 0.85              |
| 2:x:273:CYS:HA    | 2:y:328:LEU:HD21  | 1.57                     | 0.85              |
| 3:2:76:ALA:HB1    | 3:7:64:SER:O      | 1.75                     | 0.85              |
| 5:AB:211:VAL:O    | 3:AM:1:MET:HA     | 1.77                     | 0.85              |
| 2:c:273:CYS:HA    | 2:d:328:LEU:HD21  | 1.57                     | 0.85              |
| 2:y:273:CYS:HA    | 2:z:328:LEU:HD21  | 1.57                     | 0.85              |
| 3:0:73:ARG:CD     | 5:AD:202:MET:SD   | 2.65                     | 0.85              |
| 3:3:238:ARG:NH2   | 3:9:251:ASP:OD2   | 2.09                     | 0.85              |
| 5:AA:220:MET:CE   | 3:AF:246:ALA:HB2  | 2.06                     | 0.85              |
| 6:AS:297:GLN:HB2  | 11:A0:65:LEU:HD22 | 1.57                     | 0.85              |
| 6:UK:126:PHE:O    | 6:UK:130:VAL:HG23 | 1.77                     | 0.85              |
| 6:WH:200:SER:O    | 6:WI:158:ALA:CB   | 2.23                     | 0.85              |
| 6:WK:193:ALA:HB1  | 6:WL:213:VAL:CG2  | 2.06                     | 0.85              |
| 6:WS:121:PHE:HE1  | 6:WT:120:LYS:NZ   | 1.74                     | 0.85              |
| 6:WT:200:SER:O    | 6:WU:158:ALA:HB2  | 1.77                     | 0.85              |
| 2:s:273:CYS:HA    | 2:t:328:LEU:HD21  | 1.57                     | 0.85              |
| 4:ZJ:370:LYS:HE2  | 4:ZP:11:ASN:ND2   | 1.92                     | 0.85              |
| 5:AE:16:LEU:CD2   | 3:AJ:253:MET:CE   | 2.55                     | 0.85              |
| 9:Au:160:GLN:O    | 6:WP:165:PHE:HB3  | 1.77                     | 0.85              |
| 9:Ax:143:ARG:HA   | 6:WD:165:PHE:HB2  | 1.59                     | 0.85              |
| 9:Ax:241:GLN:CG   | 6:WC:164:LEU:O    | 2.23                     | 0.85              |
| 2:m:80:GLN:HE22   | 3:AJ:204:SER:N    | 1.74                     | 0.85              |
| 2:w:273:CYS:HA    | 2:x:328:LEU:HD21  | 1.57                     | 0.85              |
| 3:0:226:VAL:HB    | 3:ZB:2:ILE:HD11   | 1.59                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Za:24:ILE:HD13  | 4:Zf:384:SER:OG   | 1.77                     | 0.85              |
| 11:A6:88:ARG:NH1  | 11:A6:105:GLU:OE1 | 2.10                     | 0.85              |
| 6:UJ:126:PHE:O    | 6:UJ:130:VAL:HG23 | 1.77                     | 0.85              |
| 6:WU:197:LEU:HD12 | 6:WV:175:SER:CB   | 2.07                     | 0.85              |
| 6:WV:200:SER:O    | 6:WW:158:ALA:CB   | 2.25                     | 0.85              |
| 2:v:273:CYS:HA    | 2:w:328:LEU:HD21  | 1.57                     | 0.84              |
| 4:ZU:17:LEU:HD13  | 4:ZZ:395:ILE:HD11 | 1.59                     | 0.84              |
| 12:BB:3:LEU:N     | 12:BB:8:ASP:OD1   | 2.09                     | 0.84              |
| 2:a:328:LEU:HD21  | 2:z:273:CYS:HA    | 1.57                     | 0.84              |
| 4:Zc:18:ASP:HA    | 4:Zh:5:GLN:HE22   | 1.41                     | 0.84              |
| 7:As:52:ILE:HD13  | 9:Ax:206:ALA:HB1  | 1.58                     | 0.84              |
| 6:UN:126:PHE:O    | 6:UN:130:VAL:HG23 | 1.77                     | 0.84              |
| 2:j:159:GLN:CD    | 2:k:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:t:273:CYS:HA    | 2:u:328:LEU:HD21  | 1.57                     | 0.84              |
| 3:6:56:SER:CA     | 5:AE:138:ALA:CB   | 2.36                     | 0.84              |
| 5:AC:27:ALA:O     | 3:AH:72:VAL:HG11  | 1.77                     | 0.84              |
| 6:UJ:167:ARG:NH2  | 6:WB:188:GLU:HB3  | 1.92                     | 0.84              |
| 2:l:159:GLN:CD    | 2:m:46:ASP:OD1    | 2.21                     | 0.84              |
| 3:ZC:56:SER:O     | 3:AK:153:ARG:N    | 2.11                     | 0.84              |
| 4:ZK:27:SER:OG    | 4:ZP:381:ASN:ND2  | 2.10                     | 0.84              |
| 12:BE:47:VAL:O    | 6:BP:313:PRO:HD2  | 1.76                     | 0.84              |
| 2:d:54:GLN:OE1    | 3:AL:110:GLY:O    | 1.94                     | 0.84              |
| 2:g:159:GLN:CD    | 2:h:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:h:159:GLN:CD    | 2:i:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:u:273:CYS:HA    | 2:v:328:LEU:HD21  | 1.57                     | 0.84              |
| 3:ZB:244:SER:HB2  | 4:ZG:399:LEU:HD23 | 1.60                     | 0.84              |
| 6:UO:103:GLN:NE2  | 6:WU:182:PRO:HB3  | 1.92                     | 0.84              |
| 6:UP:126:PHE:O    | 6:UP:130:VAL:HG23 | 1.77                     | 0.84              |
| 2:a:273:CYS:HA    | 2:b:328:LEU:HD21  | 1.57                     | 0.84              |
| 2:f:159:GLN:CD    | 2:g:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:y:159:GLN:CD    | 2:z:46:ASP:OD1    | 2.21                     | 0.84              |
| 3:5:94:ASP:OD2    | 3:ZA:38:ARG:NH1   | 2.10                     | 0.84              |
| 3:6:57:SER:CB     | 3:AK:108:PRO:HG3  | 2.07                     | 0.84              |
| 3:ZE:248:SER:CB   | 4:ZJ:402:LEU:HD22 | 2.07                     | 0.84              |
| 3:AI:45:LEU:HD23  | 12:BD:76:LEU:HD12 | 1.60                     | 0.84              |
| 7:Ar:14:MET:HE3   | 7:As:63:ILE:HD13  | 1.58                     | 0.84              |
| 2:a:159:GLN:CD    | 2:b:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:r:54:GLN:OE1    | 3:AI:139:ALA:CB   | 2.25                     | 0.84              |
| 3:0:2:ILE:CG2     | 5:AD:212:LYS:HA   | 2.07                     | 0.84              |
| 9:Aw:152:ARG:HD2  | 6:WB:166:VAL:O    | 1.77                     | 0.84              |
| 9:Ax:160:GLN:C    | 6:WE:167:ARG:HG3  | 2.03                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UK:207:PRO:CD   | 6:WE:187:ASP:CG   | 2.51                     | 0.84              |
| 2:b:159:GLN:CD    | 2:c:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:b:273:CYS:HA    | 2:c:328:LEU:HD21  | 1.57                     | 0.84              |
| 2:d:159:GLN:CD    | 2:e:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:s:159:GLN:CD    | 2:t:46:ASP:OD1    | 2.21                     | 0.84              |
| 3:O:193:ILE:CD1   | 5:AD:152:PRO:HD3  | 2.07                     | 0.84              |
| 4:ZS:183:THR:HB   | 4:Zd:131:GLY:O    | 1.76                     | 0.84              |
| 5:AA:70:GLN:HB3   | 3:AL:6:TRP:HB2    | 1.55                     | 0.84              |
| 6:WA:175:SER:CB   | 6:WW:197:LEU:HD12 | 2.08                     | 0.84              |
| 1:O:47:ALA:HB3    | 2:l:178:GLN:HG3   | 1.60                     | 0.84              |
| 1:Q:47:ALA:HB3    | 2:n:178:GLN:HG3   | 1.60                     | 0.84              |
| 2:c:159:GLN:CD    | 2:d:46:ASP:OD1    | 2.21                     | 0.84              |
| 2:w:159:GLN:CD    | 2:x:46:ASP:OD1    | 2.21                     | 0.84              |
| 6:Af:297:GLN:OE1  | 11:A8:76:GLN:O    | 1.96                     | 0.84              |
| 6:UI:126:PHE:O    | 6:UI:130:VAL:HG23 | 1.77                     | 0.84              |
| 1:F:47:ALA:HB3    | 2:c:178:GLN:HG3   | 1.60                     | 0.84              |
| 1:R:47:ALA:HB3    | 2:o:178:GLN:HG3   | 1.60                     | 0.84              |
| 2:a:46:ASP:OD1    | 2:z:159:GLN:CD    | 2.21                     | 0.84              |
| 2:n:159:GLN:CD    | 2:o:46:ASP:OD1    | 2.21                     | 0.84              |
| 3:O:128:LEU:HD12  | 3:O:140:ILE:HD12  | 1.59                     | 0.84              |
| 1:N:47:ALA:HB3    | 2:k:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:e:110:MET:SD    | 2:f:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:p:159:GLN:CD    | 2:q:46:ASP:OD1    | 2.21                     | 0.83              |
| 2:s:110:MET:SD    | 2:t:62:LEU:HD11   | 2.18                     | 0.83              |
| 3:ZA:235:GLN:HE22 | 4:ZG:3:PHE:HB3    | 1.41                     | 0.83              |
| 6:Ak:372:ILE:HG22 | 10:A1:4:ILE:CD1   | 2.08                     | 0.83              |
| 6:WQ:200:SER:OG   | 6:WR:175:SER:HB2  | 1.78                     | 0.83              |
| 1:C:47:ALA:HB3    | 2:z:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:a:80:GLN:CD     | 3:8:58:GLU:HG3    | 2.03                     | 0.83              |
| 2:q:110:MET:SD    | 2:r:62:LEU:HD11   | 2.18                     | 0.83              |
| 4:ZP:18:ASP:O     | 4:ZU:5:GLN:NE2    | 2.11                     | 0.83              |
| 4:ZS:181:LYS:NZ   | 4:Zd:129:GLN:NE2  | 2.26                     | 0.83              |
| 9:Ay:162:PRO:HG3  | 6:WH:167:ARG:HH22 | 1.41                     | 0.83              |
| 1:E:47:ALA:HB3    | 2:b:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:G:47:ALA:HB3    | 2:d:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:I:47:ALA:HB3    | 2:f:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:J:47:ALA:HB3    | 2:g:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:T:47:ALA:HB3    | 2:q:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:e:159:GLN:CD    | 2:f:46:ASP:OD1    | 2.21                     | 0.83              |
| 2:o:159:GLN:CD    | 2:p:46:ASP:OD1    | 2.21                     | 0.83              |
| 2:r:159:GLN:CD    | 2:s:46:ASP:OD1    | 2.21                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:v:159:GLN:CD    | 2:w:46:ASP:OD1    | 2.21                     | 0.83              |
| 3:6:86:LEU:HD12   | 4:ZH:42:MET:HE3   | 0.87                     | 0.83              |
| 5:AE:231:MET:HE3  | 3:AJ:257:LEU:CB   | 2.00                     | 0.83              |
| 7:Ab:37:ILE:HD13  | 7:Aq:44:ILE:HD11  | 1.59                     | 0.83              |
| 1:B:47:ALA:HB3    | 2:y:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:D:47:ALA:HB3    | 2:a:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:U:47:ALA:HB3    | 2:r:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:b:110:MET:SD    | 2:c:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:g:110:MET:SD    | 2:h:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:t:159:GLN:CD    | 2:u:46:ASP:OD1    | 2.21                     | 0.83              |
| 2:x:110:MET:SD    | 2:y:62:LEU:HD11   | 2.18                     | 0.83              |
| 5:AC:34:PHE:HE1   | 3:AH:46:TYR:OH    | 1.59                     | 0.83              |
| 1:M:47:ALA:HB3    | 2:j:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:Z:47:ALA:HB3    | 2:w:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:a:62:LEU:HD11   | 2:z:110:MET:SD    | 2.18                     | 0.83              |
| 2:c:110:MET:SD    | 2:d:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:j:110:MET:SD    | 2:k:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:k:110:MET:SD    | 2:l:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:u:159:GLN:CD    | 2:v:46:ASP:OD1    | 2.21                     | 0.83              |
| 2:x:188:GLN:CB    | 2:y:101:GLN:HE21  | 1.91                     | 0.83              |
| 2:y:188:GLN:CB    | 2:z:101:GLN:HE21  | 1.91                     | 0.83              |
| 5:AC:59:ALA:HB3   | 3:AH:66:LEU:HD21  | 1.61                     | 0.83              |
| 7:Ab:8:MET:HE3    | 6:WS:124:SER:HB2  | 1.61                     | 0.83              |
| 9:Ax:143:ARG:CA   | 6:WD:165:PHE:CB   | 2.54                     | 0.83              |
| 9:Ay:138:MET:HE1  | 9:Ay:171:LEU:HD23 | 1.60                     | 0.83              |
| 1:K:47:ALA:HB3    | 2:h:178:GLN:HG3   | 1.60                     | 0.83              |
| 1:S:47:ALA:HB3    | 2:p:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:i:110:MET:SD    | 2:j:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:k:159:GLN:CD    | 2:l:46:ASP:OD1    | 2.21                     | 0.83              |
| 2:l:110:MET:SD    | 2:m:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:u:110:MET:SD    | 2:v:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:w:188:GLN:CB    | 2:x:101:GLN:HE21  | 1.91                     | 0.83              |
| 2:y:110:MET:SD    | 2:z:62:LEU:HD11   | 2.18                     | 0.83              |
| 4:ZK:270:ASN:HD22 | 4:ZQ:192:ASN:HA   | 1.44                     | 0.83              |
| 5:AA:173:ARG:HD3  | 3:AF:46:TYR:CE2   | 2.13                     | 0.83              |
| 3:AK:44:LEU:HD22  | 12:BF:78:TYR:HB2  | 1.59                     | 0.83              |
| 1:X:47:ALA:HB3    | 2:u:178:GLN:HG3   | 1.60                     | 0.83              |
| 2:a:101:GLN:HE21  | 2:z:188:GLN:CB    | 1.91                     | 0.83              |
| 2:a:110:MET:SD    | 2:b:62:LEU:HD11   | 2.18                     | 0.83              |
| 2:a:188:GLN:CB    | 2:b:101:GLN:HE21  | 1.91                     | 0.83              |
| 2:h:110:MET:SD    | 2:i:62:LEU:HD11   | 2.18                     | 0.83              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:v:110:MET:SD   | 2:w:62:LEU:HD11    | 2.18                     | 0.83              |
| 2:v:188:GLN:CB   | 2:w:101:GLN:HE21   | 1.91                     | 0.83              |
| 2:x:159:GLN:CD   | 2:y:46:ASP:OD1     | 2.21                     | 0.83              |
| 1:A:47:ALA:HB3   | 2:x:178:GLN:HG3    | 1.60                     | 0.83              |
| 1:H:47:ALA:HB3   | 2:e:178:GLN:HG3    | 1.60                     | 0.83              |
| 1:P:47:ALA:HB3   | 2:m:178:GLN:HG3    | 1.60                     | 0.83              |
| 1:W:47:ALA:HB3   | 2:t:178:GLN:HG3    | 1.60                     | 0.83              |
| 2:d:110:MET:SD   | 2:e:62:LEU:HD11    | 2.18                     | 0.83              |
| 2:i:159:GLN:CD   | 2:j:46:ASP:OD1     | 2.21                     | 0.83              |
| 2:o:110:MET:SD   | 2:p:62:LEU:HD11    | 2.18                     | 0.83              |
| 2:w:110:MET:SD   | 2:x:62:LEU:HD11    | 2.18                     | 0.83              |
| 3:AH:44:LEU:CD2  | 12:BC:78:TYR:CB    | 2.54                     | 0.83              |
| 3:AJ:260:LEU:CD1 | 12:BE:106:MET:SD   | 2.67                     | 0.83              |
| 8:At:248:PHE:HB3 | 6:WK:164:LEU:HD12  | 1.59                     | 0.83              |
| 6:UM:103:GLN:HG2 | 6:WQ:182:PRO:HB3   | 1.61                     | 0.83              |
| 1:L:47:ALA:HB3   | 2:i:178:GLN:HG3    | 1.60                     | 0.83              |
| 2:m:159:GLN:CD   | 2:n:46:ASP:OD1     | 2.21                     | 0.83              |
| 2:u:188:GLN:CB   | 2:v:101:GLN:HE21   | 1.91                     | 0.83              |
| 6:UN:94:HIS:HB3  | 6:UN:146:THR:HG21  | 1.60                     | 0.83              |
| 1:Y:47:ALA:HB3   | 2:v:178:GLN:HG3    | 1.60                     | 0.83              |
| 2:b:188:GLN:CB   | 2:c:101:GLN:HE21   | 1.91                     | 0.83              |
| 2:m:110:MET:SD   | 2:n:62:LEU:HD11    | 2.18                     | 0.83              |
| 2:q:159:GLN:CD   | 2:r:46:ASP:OD1     | 2.21                     | 0.83              |
| 2:t:110:MET:SD   | 2:u:62:LEU:HD11    | 2.18                     | 0.83              |
| 3:ZE:26:LEU:HD22 | 4:ZJ:384:SER:OG    | 1.78                     | 0.83              |
| 3:AJ:3:SER:CB    | 12:BE:75:LYS:NZ    | 2.40                     | 0.83              |
| 6:UP:94:HIS:HB3  | 6:UP:146:THR:HG21  | 1.61                     | 0.83              |
| 12:BE:6:ILE:HG21 | 12:BE:122:VAL:HG11 | 1.59                     | 0.83              |
| 2:c:188:GLN:CB   | 2:d:101:GLN:HE21   | 1.91                     | 0.82              |
| 2:n:110:MET:SD   | 2:o:62:LEU:HD11    | 2.18                     | 0.82              |
| 3:O:44:LEU:HD23  | 5:AD:202:MET:SD    | 2.18                     | 0.82              |
| 3:1:83:GLN:HE21  | 3:ZC:45:LEU:HD12   | 1.43                     | 0.82              |
| 5:AD:82:LEU:HD21 | 5:AD:88:LEU:HG     | 1.60                     | 0.82              |
| 6:UM:126:PHE:O   | 6:UM:130:VAL:HG23  | 1.77                     | 0.82              |
| 6:WG:200:SER:O   | 6:WH:158:ALA:HB2   | 1.79                     | 0.82              |
| 1:V:47:ALA:HB3   | 2:s:178:GLN:HG3    | 1.60                     | 0.82              |
| 2:f:188:GLN:CB   | 2:g:101:GLN:HE21   | 1.91                     | 0.82              |
| 2:g:188:GLN:CB   | 2:h:101:GLN:HE21   | 1.91                     | 0.82              |
| 2:h:188:GLN:CB   | 2:i:101:GLN:HE21   | 1.91                     | 0.82              |
| 2:t:188:GLN:CB   | 2:u:101:GLN:HE21   | 1.91                     | 0.82              |
| 3:6:2:ILE:HD13   | 3:AJ:226:VAL:HG22  | 1.61                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:5:ILE:HD11   | 12:BB:106:MET:HE2 | 1.62                     | 0.82              |
| 11:A7:51:LYS:HE3  | 11:A7:55:ARG:NH1  | 1.93                     | 0.82              |
| 6:UJ:103:GLN:OE1  | 6:WD:182:PRO:CB   | 2.26                     | 0.82              |
| 6:WT:197:LEU:CD1  | 6:WU:175:SER:OG   | 2.27                     | 0.82              |
| 1:I:136:GLY:HA3   | 1:K:213:ILE:HG23  | 1.62                     | 0.82              |
| 1:J:136:GLY:HA3   | 1:L:213:ILE:HG23  | 1.62                     | 0.82              |
| 2:d:188:GLN:CB    | 2:e:101:GLN:HE21  | 1.91                     | 0.82              |
| 2:f:110:MET:SD    | 2:g:62:LEU:HD11   | 2.18                     | 0.82              |
| 2:i:188:GLN:CB    | 2:j:101:GLN:HE21  | 1.91                     | 0.82              |
| 2:s:188:GLN:CB    | 2:t:101:GLN:HE21  | 1.91                     | 0.82              |
| 3:9:57:SER:HA     | 3:AH:154:ASP:HB2  | 1.59                     | 0.82              |
| 4:ZS:181:LYS:HZ3  | 4:Zd:129:GLN:NE2  | 1.77                     | 0.82              |
| 3:AH:1:MET:HG3    | 12:BC:93:MET:HE3  | 1.60                     | 0.82              |
| 6:Ak:370:ARG:CZ   | 10:A1:7:ILE:HD11  | 2.08                     | 0.82              |
| 7:As:36:SER:OG    | 8:At:211:LEU:O    | 1.97                     | 0.82              |
| 6:UJ:94:HIS:HB3   | 6:UJ:146:THR:HG21 | 1.60                     | 0.82              |
| 1:G:136:GLY:HA3   | 1:I:213:ILE:HG23  | 1.62                     | 0.82              |
| 1:H:136:GLY:HA3   | 1:J:213:ILE:HG23  | 1.62                     | 0.82              |
| 2:e:188:GLN:CB    | 2:f:101:GLN:HE21  | 1.91                     | 0.82              |
| 3:ZE:207:GLY:O    | 4:ZK:89:ASN:ND2   | 2.13                     | 0.82              |
| 4:Za:382:TYR:CD1  | 4:Zf:395:ILE:HD12 | 2.14                     | 0.82              |
| 3:AG:44:LEU:HD13  | 12:BB:78:TYR:HB2  | 1.61                     | 0.82              |
| 6:AS:299:ASN:ND2  | 11:A0:78:VAL:HG12 | 1.93                     | 0.82              |
| 6:UO:126:PHE:O    | 6:UO:130:VAL:HG23 | 1.77                     | 0.82              |
| 1:F:136:GLY:HA3   | 1:H:213:ILE:HG23  | 1.62                     | 0.82              |
| 1:K:136:GLY:HA3   | 1:M:213:ILE:HG23  | 1.62                     | 0.82              |
| 2:j:188:GLN:CB    | 2:k:101:GLN:HE21  | 1.91                     | 0.82              |
| 5:AA:202:MET:CG   | 3:AL:45:LEU:HD11  | 2.07                     | 0.82              |
| 10:A4:14:LEU:HD23 | 6:BW:278:THR:CG2  | 2.09                     | 0.82              |
| 10:A4:48:ARG:NH2  | 11:A0:6:ASP:OD1   | 2.12                     | 0.82              |
| 2:r:110:MET:SD    | 2:s:62:LEU:HD11   | 2.18                     | 0.82              |
| 2:r:188:GLN:CB    | 2:s:101:GLN:HE21  | 1.91                     | 0.82              |
| 3:5:44:LEU:HD22   | 3:AI:86:LEU:HD12  | 1.62                     | 0.82              |
| 3:9:56:SER:O      | 3:AH:153:ARG:N    | 2.13                     | 0.82              |
| 5:AB:107:VAL:O    | 3:AG:180:ASN:ND2  | 2.13                     | 0.82              |
| 6:AR:278:THR:HG21 | 10:A2:21:ALA:HB1  | 1.62                     | 0.82              |
| 6:UI:94:HIS:HB3   | 6:UI:146:THR:HG21 | 1.61                     | 0.82              |
| 2:m:188:GLN:CB    | 2:n:101:GLN:HE21  | 1.91                     | 0.82              |
| 2:o:188:GLN:CB    | 2:p:101:GLN:HE21  | 1.91                     | 0.82              |
| 3:1:78:GLU:HG2    | 3:AK:121:GLN:NE2  | 1.95                     | 0.82              |
| 5:AC:228:GLU:HG2  | 3:AH:256:LYS:HG3  | 1.61                     | 0.82              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:As:84:LEU:HD21 | 9:Ay:185:ILE:HG23 | 1.59                     | 0.82              |
| 6:UK:207:PRO:CD  | 6:WE:187:ASP:OD1  | 2.27                     | 0.82              |
| 1:L:136:GLY:HA3  | 1:N:213:ILE:HG23  | 1.62                     | 0.82              |
| 2:l:188:GLN:CB   | 2:m:101:GLN:HE21  | 1.91                     | 0.82              |
| 2:n:188:GLN:CB   | 2:o:101:GLN:HE21  | 1.91                     | 0.82              |
| 2:p:188:GLN:CB   | 2:q:101:GLN:HE21  | 1.91                     | 0.82              |
| 3:4:2:ILE:HD13   | 3:4:250:THR:HG23  | 1.59                     | 0.82              |
| 3:5:189:GLU:HA   | 3:ZA:42:GLU:OE1   | 1.79                     | 0.82              |
| 3:8:1:MET:HE3    | 3:AL:226:VAL:HG21 | 1.61                     | 0.82              |
| 3:9:109:ASP:OD1  | 3:AM:162:GLN:NE2  | 2.12                     | 0.82              |
| 5:AC:28:ASN:ND2  | 3:AH:43:ASP:HB3   | 1.94                     | 0.82              |
| 5:AD:74:THR:HG21 | 3:AI:38:ARG:HH11  | 1.01                     | 0.82              |
| 3:AG:238:ARG:NH2 | 3:AM:251:ASP:OD1  | 2.12                     | 0.82              |
| 6:Ad:278:THR:CG2 | 10:A2:7:ILE:HB    | 2.06                     | 0.82              |
| 6:UO:94:HIS:HB3  | 6:UO:146:THR:HG21 | 1.60                     | 0.82              |
| 2:k:188:GLN:CB   | 2:l:101:GLN:HE21  | 1.91                     | 0.82              |
| 2:p:110:MET:SD   | 2:q:62:LEU:HD11   | 2.18                     | 0.82              |
| 3:1:6:TRP:CB     | 5:AE:70:GLN:HB2   | 2.10                     | 0.82              |
| 3:7:257:LEU:HG   | 3:AK:230:LEU:HD12 | 1.61                     | 0.82              |
| 5:AE:231:MET:SD  | 3:AJ:260:LEU:CD2  | 2.68                     | 0.82              |
| 7:As:74:LEU:HD11 | 9:Ay:228:LEU:CD1  | 2.09                     | 0.82              |
| 9:Ax:161:GLY:CA  | 6:WE:167:ARG:HD2  | 2.08                     | 0.82              |
| 9:Ay:162:PRO:CG  | 6:WH:167:ARG:HH22 | 1.92                     | 0.82              |
| 1:E:136:GLY:HA3  | 1:G:213:ILE:HG23  | 1.62                     | 0.82              |
| 1:F:228:ASN:ND2  | 1:H:24:TRP:CZ2    | 2.48                     | 0.82              |
| 1:J:228:ASN:ND2  | 1:L:24:TRP:CZ2    | 2.48                     | 0.82              |
| 1:K:228:ASN:ND2  | 1:M:24:TRP:CZ2    | 2.48                     | 0.82              |
| 2:q:188:GLN:CB   | 2:r:101:GLN:HE21  | 1.91                     | 0.82              |
| 6:Al:365:ASN:CB  | 11:A7:72:HIS:ND1  | 2.40                     | 0.82              |
| 7:As:7:MET:HE1   | 8:At:233:MET:HB3  | 1.62                     | 0.82              |
| 1:I:228:ASN:ND2  | 1:K:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:N:228:ASN:ND2  | 1:P:24:TRP:CZ2    | 2.48                     | 0.81              |
| 2:q:51:GLN:HG3   | 3:AI:209:ASN:ND2  | 1.94                     | 0.81              |
| 3:ZD:76:ALA:CB   | 4:ZI:47:LYS:CE    | 2.58                     | 0.81              |
| 6:UM:127:SER:O   | 6:UM:131:ASN:N    | 2.13                     | 0.81              |
| 1:D:228:ASN:ND2  | 1:F:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:M:136:GLY:HA3  | 1:O:213:ILE:HG23  | 1.62                     | 0.81              |
| 1:P:228:ASN:ND2  | 1:R:24:TRP:CZ2    | 2.48                     | 0.81              |
| 2:h:80:GLN:OE1   | 3:AK:202:ASN:ND2  | 2.12                     | 0.81              |
| 3:ZA:240:TYR:CE2 | 4:ZF:395:ILE:CG2  | 2.62                     | 0.81              |
| 5:AE:231:MET:HE1 | 3:AJ:257:LEU:HD13 | 1.61                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Aw:140:ARG:O    | 6:WW:167:ARG:HD2  | 1.80                     | 0.81              |
| 6:UK:94:HIS:HB3   | 6:UK:146:THR:HG21 | 1.61                     | 0.81              |
| 6:UK:127:SER:O    | 6:UK:131:ASN:N    | 2.13                     | 0.81              |
| 1:D:136:GLY:HA3   | 1:F:213:ILE:HG23  | 1.62                     | 0.81              |
| 1:E:228:ASN:ND2   | 1:G:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:G:228:ASN:ND2   | 1:I:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:H:228:ASN:ND2   | 1:J:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:M:228:ASN:ND2   | 1:O:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:O:228:ASN:ND2   | 1:Q:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:Q:65:LEU:HG     | 2:p:65:MET:HG3    | 1.62                     | 0.81              |
| 1:R:65:LEU:HG     | 2:q:65:MET:HG3    | 1.62                     | 0.81              |
| 1:S:131:SER:O     | 1:U:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:T:131:SER:O     | 1:V:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:U:65:LEU:HG     | 2:t:65:MET:HG3    | 1.62                     | 0.81              |
| 3:O:193:ILE:CD1   | 5:AD:152:PRO:CD   | 2.58                     | 0.81              |
| 3:5:238:ARG:NE    | 3:ZB:251:ASP:OD1  | 2.11                     | 0.81              |
| 3:ZB:28:ASN:ND2   | 4:ZG:52:VAL:CG2   | 2.42                     | 0.81              |
| 5:AE:215:GLU:OE1  | 3:AK:9:LYS:NZ     | 2.12                     | 0.81              |
| 6:AX:372:ILE:HD12 | 10:A3:11:ILE:HG22 | 1.62                     | 0.81              |
| 7:Ab:17:ALA:HB2   | 9:Av:195:ILE:HD12 | 1.62                     | 0.81              |
| 9:Aw:140:ARG:O    | 6:WW:167:ARG:CD   | 2.28                     | 0.81              |
| 11:A7:51:LYS:CE   | 11:A7:55:ARG:HH22 | 1.93                     | 0.81              |
| 6:UL:127:SER:O    | 6:UL:131:ASN:N    | 2.13                     | 0.81              |
| 6:UM:73:MET:HE1   | 6:UM:99:ARG:HD3   | 1.62                     | 0.81              |
| 6:UN:127:SER:O    | 6:UN:131:ASN:N    | 2.13                     | 0.81              |
| 6:UO:73:MET:HE1   | 6:UO:99:ARG:HD3   | 1.62                     | 0.81              |
| 1:L:228:ASN:ND2   | 1:N:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:P:65:LEU:HG     | 2:o:65:MET:HG3    | 1.62                     | 0.81              |
| 1:V:131:SER:O     | 1:X:223:GLN:NE2   | 2.14                     | 0.81              |
| 2:c:159:GLN:OE1   | 2:d:46:ASP:OD1    | 1.99                     | 0.81              |
| 2:e:159:GLN:OE1   | 2:f:46:ASP:OD1    | 1.99                     | 0.81              |
| 4:ZS:181:LYS:NZ   | 4:Zd:129:GLN:HE21 | 1.79                     | 0.81              |
| 3:AK:260:LEU:HB3  | 12:BF:106:MET:HE1 | 1.61                     | 0.81              |
| 6:UO:127:SER:O    | 6:UO:131:ASN:N    | 2.13                     | 0.81              |
| 6:WI:200:SER:O    | 6:WJ:158:ALA:CB   | 2.29                     | 0.81              |
| 1:O:131:SER:O     | 1:Q:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:R:131:SER:O     | 1:T:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:T:65:LEU:HG     | 2:s:65:MET:HG3    | 1.62                     | 0.81              |
| 2:g:159:GLN:OE1   | 2:h:46:ASP:OD1    | 1.99                     | 0.81              |
| 3:ZE:255:GLN:HG3  | 3:ZE:259:GLN:HE21 | 1.46                     | 0.81              |
| 4:ZY:373:VAL:CG1  | 4:Ze:7:VAL:HG22   | 2.10                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AD:104:ASN:ND2  | 3:AI:38:ARG:HH21  | 1.75                     | 0.81              |
| 3:AG:73:ARG:CG    | 12:BB:78:TYR:CE2  | 2.63                     | 0.81              |
| 3:AH:2:ILE:HG13   | 3:AH:254:LEU:HD11 | 1.62                     | 0.81              |
| 6:UJ:167:ARG:HH22 | 6:WB:188:GLU:HB3  | 1.43                     | 0.81              |
| 6:WP:200:SER:O    | 6:WQ:158:ALA:HB2  | 1.80                     | 0.81              |
| 1:A:223:GLN:NE2   | 1:Y:131:SER:O     | 2.14                     | 0.81              |
| 1:V:65:LEU:HG     | 2:u:65:MET:HG3    | 1.62                     | 0.81              |
| 2:f:159:GLN:OE1   | 2:g:46:ASP:OD1    | 1.99                     | 0.81              |
| 3:ZA:77:THR:H     | 4:ZF:47:LYS:HD2   | 1.43                     | 0.81              |
| 4:ZH:390:LYS:HB2  | 4:ZM:402:LEU:HD22 | 1.61                     | 0.81              |
| 5:AE:131:GLU:CB   | 3:AJ:179:MET:SD   | 2.60                     | 0.81              |
| 3:AK:35:LYS:HD2   | 3:AK:81:HIS:HA    | 1.62                     | 0.81              |
| 7:Ar:28:ALA:HB1   | 7:Ar:54:LYS:HE3   | 1.60                     | 0.81              |
| 1:B:228:ASN:ND2   | 1:D:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:P:131:SER:O     | 1:R:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:S:65:LEU:HG     | 2:r:65:MET:HG3    | 1.62                     | 0.81              |
| 2:h:159:GLN:OE1   | 2:i:46:ASP:OD1    | 1.99                     | 0.81              |
| 3:4:85:ASN:OD1    | 4:ZF:50:LEU:CD2   | 2.29                     | 0.81              |
| 3:ZD:24:ASN:ND2   | 4:ZI:49:GLY:HA3   | 1.94                     | 0.81              |
| 5:AA:220:MET:HE2  | 3:AF:246:ALA:CA   | 2.11                     | 0.81              |
| 1:N:136:GLY:HA3   | 1:P:213:ILE:HG23  | 1.62                     | 0.81              |
| 1:W:131:SER:O     | 1:Y:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:X:228:ASN:ND2   | 1:Z:24:TRP:CZ2    | 2.48                     | 0.81              |
| 2:a:159:GLN:OE1   | 2:b:46:ASP:OD1    | 1.99                     | 0.81              |
| 2:b:159:GLN:OE1   | 2:c:46:ASP:OD1    | 1.99                     | 0.81              |
| 2:k:80:GLN:OE1    | 5:AE:157:PRO:HD3  | 1.79                     | 0.81              |
| 6:UP:127:SER:O    | 6:UP:131:ASN:N    | 2.13                     | 0.81              |
| 1:B:223:GLN:NE2   | 1:Z:131:SER:O     | 2.14                     | 0.81              |
| 1:I:63:GLN:OE1    | 2:g:131:SER:OG    | 1.99                     | 0.81              |
| 1:U:131:SER:O     | 1:W:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:U:228:ASN:ND2   | 1:W:24:TRP:CZ2    | 2.48                     | 0.81              |
| 2:d:159:GLN:OE1   | 2:e:46:ASP:OD1    | 1.99                     | 0.81              |
| 2:j:159:GLN:OE1   | 2:k:46:ASP:OD1    | 1.99                     | 0.81              |
| 4:ZN:379:GLN:HG3  | 4:ZS:391:THR:HG23 | 1.62                     | 0.81              |
| 4:ZY:101:LYS:HD2  | 4:Zd:324:GLU:OE2  | 1.79                     | 0.81              |
| 5:AE:26:LEU:HD22  | 3:AJ:242:ILE:CG2  | 2.11                     | 0.81              |
| 11:A9:68:THR:HG1  | 11:A9:72:HIS:CE1  | 1.95                     | 0.81              |
| 6:UK:73:MET:HE1   | 6:UK:99:ARG:HD3   | 1.62                     | 0.81              |
| 6:UM:128:GLU:O    | 6:UM:132:TYR:N    | 2.13                     | 0.81              |
| 6:WK:143:THR:CB   | 6:WL:156:HIS:HE2  | 1.94                     | 0.81              |
| 6:WT:121:PHE:CE1  | 6:WU:122:GLY:O    | 2.34                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:136:GLY:HA3   | 1:E:213:ILE:HG23  | 1.62                     | 0.81              |
| 1:C:228:ASN:ND2   | 1:E:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:E:63:GLN:OE1    | 2:c:131:SER:OG    | 1.99                     | 0.81              |
| 1:H:65:LEU:HG     | 2:g:65:MET:HG3    | 1.62                     | 0.81              |
| 1:L:131:SER:O     | 1:N:223:GLN:NE2   | 2.14                     | 0.81              |
| 1:O:65:LEU:HG     | 2:n:65:MET:HG3    | 1.62                     | 0.81              |
| 1:R:228:ASN:ND2   | 1:T:24:TRP:CZ2    | 2.48                     | 0.81              |
| 1:U:63:GLN:OE1    | 2:s:131:SER:OG    | 1.99                     | 0.81              |
| 2:a:46:ASP:OD1    | 2:z:159:GLN:OE1   | 1.99                     | 0.81              |
| 2:i:159:GLN:OE1   | 2:j:46:ASP:OD1    | 1.99                     | 0.81              |
| 3:3:242:ILE:CD1   | 3:9:1:MET:HE1     | 2.11                     | 0.81              |
| 3:ZD:27:ALA:HB1   | 4:ZI:52:VAL:HG23  | 1.63                     | 0.81              |
| 4:ZQ:181:LYS:NZ   | 4:Zb:129:GLN:NE2  | 2.29                     | 0.81              |
| 5:AD:243:ARG:HE   | 12:BE:113:GLN:HB2 | 1.42                     | 0.81              |
| 7:Ab:8:MET:HE2    | 6:WS:124:SER:HB2  | 1.61                     | 0.81              |
| 7:Ab:74:LEU:HD13  | 7:Ab:78:ARG:HH22  | 1.44                     | 0.81              |
| 6:WF:200:SER:OG   | 6:WG:175:SER:HB2  | 1.81                     | 0.81              |
| 1:A:65:LEU:HG     | 2:z:65:MET:HG3    | 1.62                     | 0.80              |
| 1:B:24:TRP:CZ2    | 1:Z:228:ASN:ND2   | 2.48                     | 0.80              |
| 1:B:65:LEU:HG     | 2:a:65:MET:HG3    | 1.62                     | 0.80              |
| 1:C:65:LEU:HG     | 2:b:65:MET:HG3    | 1.62                     | 0.80              |
| 1:I:65:LEU:HG     | 2:h:65:MET:HG3    | 1.62                     | 0.80              |
| 1:Q:131:SER:O     | 1:S:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:S:228:ASN:ND2   | 1:U:24:TRP:CZ2    | 2.48                     | 0.80              |
| 1:V:228:ASN:ND2   | 1:X:24:TRP:CZ2    | 2.48                     | 0.80              |
| 11:A0:33:ALA:O    | 11:A0:98:ASN:ND2  | 2.13                     | 0.80              |
| 6:UL:73:MET:HE1   | 6:UL:99:ARG:HD3   | 1.62                     | 0.80              |
| 1:J:65:LEU:HG     | 2:i:65:MET:HG3    | 1.62                     | 0.80              |
| 1:T:63:GLN:OE1    | 2:r:131:SER:OG    | 1.99                     | 0.80              |
| 1:W:65:LEU:HG     | 2:v:65:MET:HG3    | 1.62                     | 0.80              |
| 1:X:63:GLN:OE1    | 2:v:131:SER:OG    | 2.00                     | 0.80              |
| 3:AF:62:LEU:CD2   | 12:BB:83:PRO:HG2  | 2.11                     | 0.80              |
| 7:As:29:LEU:HD12  | 8:At:216:ILE:HG13 | 1.62                     | 0.80              |
| 10:A2:68:LEU:HD13 | 11:A7:118:MET:SD  | 2.21                     | 0.80              |
| 6:WJ:197:LEU:HD12 | 6:WK:175:SER:HB3  | 1.63                     | 0.80              |
| 1:A:228:ASN:ND2   | 1:C:24:TRP:CZ2    | 2.48                     | 0.80              |
| 1:B:63:GLN:OE1    | 2:z:131:SER:OG    | 1.99                     | 0.80              |
| 1:F:63:GLN:OE1    | 2:d:131:SER:OG    | 1.99                     | 0.80              |
| 1:M:131:SER:O     | 1:O:223:GLN:NE2   | 2.14                     | 0.80              |
| 3:3:76:ALA:HB1    | 3:8:64:SER:O      | 1.81                     | 0.80              |
| 3:4:238:ARG:NH2   | 3:ZA:251:ASP:OD2  | 2.14                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UI:127:SER:O    | 6:UI:131:ASN:N    | 2.13                     | 0.80              |
| 1:B:131:SER:O     | 1:D:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:M:65:LEU:HG     | 2:l:65:MET:HG3    | 1.62                     | 0.80              |
| 1:Q:63:GLN:OE1    | 2:o:131:SER:OG    | 1.99                     | 0.80              |
| 1:W:136:GLY:HA3   | 1:Y:213:ILE:HG23  | 1.61                     | 0.80              |
| 1:W:228:ASN:ND2   | 1:Y:24:TRP:CZ2    | 2.48                     | 0.80              |
| 2:k:159:GLN:OE1   | 2:l:46:ASP:OD1    | 1.99                     | 0.80              |
| 6:AK:372:ILE:HG21 | 10:A1:4:ILE:HG12  | 1.57                     | 0.80              |
| 6:UJ:127:SER:O    | 6:UJ:131:ASN:N    | 2.13                     | 0.80              |
| 6:WB:181:GLU:HB2  | 6:WB:184:ARG:CG   | 2.07                     | 0.80              |
| 1:A:131:SER:O     | 1:C:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:G:65:LEU:HG     | 2:f:65:MET:HG3    | 1.62                     | 0.80              |
| 1:H:63:GLN:OE1    | 2:f:131:SER:OG    | 2.00                     | 0.80              |
| 1:N:65:LEU:HG     | 2:m:65:MET:HG3    | 1.62                     | 0.80              |
| 1:O:136:GLY:HA3   | 1:Q:213:ILE:HG23  | 1.62                     | 0.80              |
| 1:Q:228:ASN:ND2   | 1:S:24:TRP:CZ2    | 2.48                     | 0.80              |
| 1:V:136:GLY:HA3   | 1:X:213:ILE:HG23  | 1.62                     | 0.80              |
| 1:X:131:SER:O     | 1:Z:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:Y:63:GLN:OE1    | 2:w:131:SER:OG    | 1.99                     | 0.80              |
| 2:q:159:GLN:OE1   | 2:r:46:ASP:OD1    | 1.99                     | 0.80              |
| 2:x:159:GLN:OE1   | 2:y:46:ASP:OD1    | 1.99                     | 0.80              |
| 4:ZO:236:GLY:HA2  | 4:ZO:268:GLN:H    | 1.46                     | 0.80              |
| 5:AA:76:ARG:HD3   | 3:AF:80:LEU:CD1   | 2.11                     | 0.80              |
| 5:AC:175:ASP:O    | 3:AH:45:LEU:HD12  | 1.82                     | 0.80              |
| 5:AE:213:PRO:HB3  | 3:AJ:242:ILE:HD13 | 1.64                     | 0.80              |
| 6:WA:197:LEU:CD1  | 6:WB:175:SER:OG   | 2.28                     | 0.80              |
| 1:A:24:TRP:CZ2    | 1:Y:228:ASN:ND2   | 2.48                     | 0.80              |
| 1:C:131:SER:O     | 1:E:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:H:131:SER:O     | 1:J:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:K:65:LEU:HG     | 2:j:65:MET:HG3    | 1.62                     | 0.80              |
| 1:M:63:GLN:OE1    | 2:k:131:SER:OG    | 1.99                     | 0.80              |
| 1:U:136:GLY:HA3   | 1:W:213:ILE:HG23  | 1.62                     | 0.80              |
| 1:Z:65:LEU:HG     | 2:y:65:MET:HG3    | 1.62                     | 0.80              |
| 2:g:346:MET:CE    | 2:i:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:l:159:GLN:OE1   | 2:m:46:ASP:OD1    | 1.99                     | 0.80              |
| 2:s:159:GLN:OE1   | 2:t:46:ASP:OD1    | 1.99                     | 0.80              |
| 6:UL:94:HIS:HB3   | 6:UL:146:THR:HG21 | 1.60                     | 0.80              |
| 1:E:131:SER:O     | 1:G:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:I:131:SER:O     | 1:K:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:J:63:GLN:OE1    | 2:h:131:SER:OG    | 1.99                     | 0.80              |
| 1:L:63:GLN:OE1    | 2:j:131:SER:OG    | 1.99                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:131:SER:O     | 1:P:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:P:63:GLN:OE1    | 2:n:131:SER:OG    | 1.99                     | 0.80              |
| 1:S:136:GLY:HA3   | 1:U:213:ILE:HG23  | 1.62                     | 0.80              |
| 1:T:136:GLY:HA3   | 1:V:213:ILE:HG23  | 1.62                     | 0.80              |
| 2:f:346:MET:CE    | 2:h:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:w:346:MET:CE    | 2:y:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:x:346:MET:CE    | 2:z:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:y:159:GLN:OE1   | 2:z:46:ASP:OD1    | 1.99                     | 0.80              |
| 3:4:54:ALA:HB1    | 5:AC:136:THR:HG21 | 1.64                     | 0.80              |
| 5:AB:229:MET:HG3  | 3:AH:258:THR:HG22 | 1.62                     | 0.80              |
| 3:AI:62:LEU:CD2   | 12:BE:84:LEU:HD23 | 2.12                     | 0.80              |
| 3:AI:185:GLU:HG3  | 3:AN:67:GLN:HE22  | 1.45                     | 0.80              |
| 6:UI:73:MET:HE1   | 6:UI:99:ARG:HD3   | 1.62                     | 0.80              |
| 6:UL:128:GLU:O    | 6:UL:132:TYR:N    | 2.13                     | 0.80              |
| 6:WG:197:LEU:HD12 | 6:WH:175:SER:OG   | 1.82                     | 0.80              |
| 1:D:65:LEU:HG     | 2:c:65:MET:HG3    | 1.62                     | 0.80              |
| 1:L:65:LEU:HG     | 2:k:65:MET:HG3    | 1.62                     | 0.80              |
| 1:X:65:LEU:HG     | 2:w:65:MET:HG3    | 1.62                     | 0.80              |
| 1:X:136:GLY:HA3   | 1:Z:213:ILE:HG23  | 1.62                     | 0.80              |
| 2:e:346:MET:CE    | 2:g:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:r:159:GLN:OE1   | 2:s:46:ASP:OD1    | 1.99                     | 0.80              |
| 2:v:346:MET:CE    | 2:x:142:LEU:HD11  | 2.12                     | 0.80              |
| 6:WG:181:GLU:HB2  | 6:WG:184:ARG:CG   | 2.07                     | 0.80              |
| 6:WU:200:SER:OG   | 6:WV:175:SER:HB2  | 1.82                     | 0.80              |
| 1:B:136:GLY:HA3   | 1:D:213:ILE:HG23  | 1.62                     | 0.80              |
| 1:F:131:SER:O     | 1:H:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:J:131:SER:O     | 1:L:223:GLN:NE2   | 2.14                     | 0.80              |
| 2:m:159:GLN:OE1   | 2:n:46:ASP:OD1    | 1.99                     | 0.80              |
| 2:p:346:MET:CE    | 2:r:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:q:346:MET:CE    | 2:s:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:u:159:GLN:OE1   | 2:v:46:ASP:OD1    | 1.99                     | 0.80              |
| 3:0:76:ALA:HB1    | 3:5:64:SER:O      | 1.82                     | 0.80              |
| 3:5:257:LEU:CD2   | 3:AI:230:LEU:HD12 | 2.12                     | 0.80              |
| 3:8:54:ALA:HB1    | 3:AG:150:THR:CG2  | 2.09                     | 0.80              |
| 4:ZR:390:LYS:HB2  | 4:ZW:402:LEU:HD22 | 1.64                     | 0.80              |
| 5:AB:203:SER:O    | 3:AM:73:ARG:NH2   | 2.14                     | 0.80              |
| 9:Au:139:LEU:O    | 6:WO:166:VAL:HG23 | 1.81                     | 0.80              |
| 6:UM:94:HIS:HB3   | 6:UM:146:THR:HG21 | 1.61                     | 0.80              |
| 1:A:213:ILE:HG23  | 1:Y:136:GLY:HA3   | 1.62                     | 0.80              |
| 1:G:131:SER:O     | 1:I:223:GLN:NE2   | 2.14                     | 0.80              |
| 1:K:131:SER:O     | 1:M:223:GLN:NE2   | 2.14                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:136:GLY:HA3   | 1:T:213:ILE:HG23  | 1.62                     | 0.80              |
| 1:T:228:ASN:ND2   | 1:V:24:TRP:CZ2    | 2.48                     | 0.80              |
| 2:h:346:MET:CE    | 2:j:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:k:346:MET:CE    | 2:m:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:l:346:MET:CE    | 2:n:142:LEU:HD11  | 2.12                     | 0.80              |
| 2:p:159:GLN:OE1   | 2:q:46:ASP:OD1    | 1.99                     | 0.80              |
| 3:ZC:240:TYR:CD2  | 4:ZH:395:ILE:HG21 | 2.16                     | 0.80              |
| 7:As:58:VAL:CG1   | 9:Ay:207:LEU:HD11 | 2.02                     | 0.80              |
| 9:Au:141:GLN:HE22 | 9:Au:243:PHE:HB3  | 1.48                     | 0.80              |
| 10:A5:7:ILE:CG2   | 6:BR:278:THR:CG2  | 2.52                     | 0.80              |
| 6:UJ:73:MET:HE1   | 6:UJ:99:ARG:HD3   | 1.62                     | 0.80              |
| 6:UK:128:GLU:O    | 6:UK:132:TYR:N    | 2.13                     | 0.80              |
| 6:UN:167:ARG:HH22 | 6:WQ:188:GLU:HB3  | 1.47                     | 0.80              |
| 6:WK:196:HIS:CB   | 6:WL:211:THR:HG21 | 2.10                     | 0.80              |
| 1:F:65:LEU:HG     | 2:e:65:MET:HG3    | 1.62                     | 0.79              |
| 1:V:63:GLN:OE1    | 2:t:131:SER:OG    | 1.99                     | 0.79              |
| 1:Y:65:LEU:HG     | 2:x:65:MET:HG3    | 1.62                     | 0.79              |
| 2:o:159:GLN:OE1   | 2:p:46:ASP:OD1    | 1.99                     | 0.79              |
| 2:t:159:GLN:OE1   | 2:u:46:ASP:OD1    | 1.99                     | 0.79              |
| 2:u:346:MET:CE    | 2:w:142:LEU:HD11  | 2.12                     | 0.79              |
| 3:4:54:ALA:CB     | 5:AC:136:THR:HG21 | 2.12                     | 0.79              |
| 3:5:55:GLN:O      | 5:AD:138:ALA:CB   | 2.30                     | 0.79              |
| 3:5:219:VAL:HG11  | 3:ZA:38:ARG:HH22  | 1.47                     | 0.79              |
| 3:6:86:LEU:CD1    | 4:ZH:42:MET:CE    | 2.50                     | 0.79              |
| 3:ZA:45:LEU:HD13  | 3:AN:83:GLN:HG2   | 1.63                     | 0.79              |
| 3:ZE:85:ASN:ND2   | 4:ZP:50:LEU:HD22  | 1.97                     | 0.79              |
| 5:AD:16:LEU:CD2   | 3:AI:253:MET:HE3  | 2.10                     | 0.79              |
| 7:Ab:52:ILE:HD11  | 9:Au:206:ALA:HB2  | 1.64                     | 0.79              |
| 6:Ae:370:ARG:HE   | 10:A2:7:ILE:HD11  | 1.46                     | 0.79              |
| 8:At:242:HIS:ND1  | 6:WJ:125:GLN:HG3  | 1.95                     | 0.79              |
| 6:UJ:128:GLU:O    | 6:UJ:132:TYR:N    | 2.13                     | 0.79              |
| 1:C:63:GLN:OE1    | 2:a:131:SER:OG    | 1.99                     | 0.79              |
| 1:R:63:GLN:OE1    | 2:p:131:SER:OG    | 1.99                     | 0.79              |
| 2:a:142:LEU:HD11  | 2:y:346:MET:CE    | 2.12                     | 0.79              |
| 2:w:159:GLN:OE1   | 2:x:46:ASP:OD1    | 1.99                     | 0.79              |
| 3:0:51:GLN:HB3    | 3:0:52:PRO:HD2    | 1.62                     | 0.79              |
| 3:0:153:ARG:HD2   | 3:0:213:LEU:HD13  | 1.63                     | 0.79              |
| 3:8:56:SER:O      | 3:AG:153:ARG:N    | 2.16                     | 0.79              |
| 3:ZB:233:MET:SD   | 4:ZG:388:THR:HA   | 2.22                     | 0.79              |
| 3:ZE:248:SER:CB   | 4:ZJ:402:LEU:CD2  | 2.58                     | 0.79              |
| 8:At:248:PHE:CB   | 6:WK:164:LEU:HD12 | 2.12                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AU:43:GLN:OE1    | 11:A6:4:ARG:NH1    | 2.14                     | 0.79              |
| 6:WH:143:THR:OG1   | 6:WI:154:ARG:HG2   | 1.82                     | 0.79              |
| 1:Q:136:GLY:HA3    | 1:S:213:ILE:HG23   | 1.62                     | 0.79              |
| 2:m:80:GLN:NE2     | 3:AJ:204:SER:HA    | 1.97                     | 0.79              |
| 3:O:108:PRO:HG2    | 3:AI:153:ARG:HH21  | 1.46                     | 0.79              |
| 3:5:9:LYS:HB2      | 3:AN:231:VAL:HG11  | 1.65                     | 0.79              |
| 5:AC:104:ASN:ND2   | 3:AH:38:ARG:HH21   | 1.81                     | 0.79              |
| 6:Ad:372:ILE:CB    | 10:A2:11:ILE:HG22  | 2.11                     | 0.79              |
| 1:B:213:ILE:HG23   | 1:Z:136:GLY:HA3    | 1.62                     | 0.79              |
| 1:N:63:GLN:OE1     | 2:l:131:SER:OG     | 1.99                     | 0.79              |
| 1:P:136:GLY:HA3    | 1:R:213:ILE:HG23   | 1.62                     | 0.79              |
| 2:d:346:MET:CE     | 2:f:142:LEU:HD11   | 2.12                     | 0.79              |
| 2:i:346:MET:CE     | 2:k:142:LEU:HD11   | 2.12                     | 0.79              |
| 2:q:53:THR:HB      | 3:AI:208:LEU:HD13  | 1.64                     | 0.79              |
| 2:r:346:MET:CE     | 2:t:142:LEU:HD11   | 2.12                     | 0.79              |
| 3:2:124:GLN:O      | 3:7:179:MET:HE3    | 1.83                     | 0.79              |
| 6:Ao:278:THR:CG2   | 10:Az:7:ILE:CG2    | 2.53                     | 0.79              |
| 6:WA:175:SER:OG    | 6:WW:197:LEU:HD12  | 1.83                     | 0.79              |
| 6:WD:181:GLU:HB2   | 6:WD:184:ARG:CG    | 2.07                     | 0.79              |
| 6:WE:181:GLU:HB2   | 6:WE:184:ARG:CG    | 2.07                     | 0.79              |
| 2:g:273:CYS:HA     | 2:h:328:LEU:CD2    | 2.13                     | 0.79              |
| 2:j:346:MET:CE     | 2:l:142:LEU:HD11   | 2.12                     | 0.79              |
| 2:m:346:MET:CE     | 2:o:142:LEU:HD11   | 2.12                     | 0.79              |
| 2:n:159:GLN:OE1    | 2:o:46:ASP:OD1     | 1.99                     | 0.79              |
| 2:o:346:MET:CE     | 2:q:142:LEU:HD11   | 2.12                     | 0.79              |
| 2:v:159:GLN:OE1    | 2:w:46:ASP:OD1     | 1.99                     | 0.79              |
| 4:ZR:87:ASP:OD2    | 4:ZR:88:SER:N      | 2.15                     | 0.79              |
| 3:AF:44:LEU:HD21   | 12:BA:78:TYR:CB    | 2.13                     | 0.79              |
| 2:b:346:MET:CE     | 2:d:142:LEU:HD11   | 2.12                     | 0.79              |
| 2:e:273:CYS:HA     | 2:f:328:LEU:CD2    | 2.13                     | 0.79              |
| 2:i:273:CYS:HA     | 2:j:328:LEU:CD2    | 2.13                     | 0.79              |
| 2:r:273:CYS:HA     | 2:s:328:LEU:CD2    | 2.13                     | 0.79              |
| 2:t:346:MET:CE     | 2:v:142:LEU:HD11   | 2.12                     | 0.79              |
| 4:ZT:102:LEU:O     | 4:ZY:322:ASN:HB2   | 1.83                     | 0.79              |
| 4:Zb:387:GLN:NE2   | 4:Zh:400:VAL:O     | 2.15                     | 0.79              |
| 5:AB:28:ASN:OD1    | 3:AG:72:VAL:HB     | 1.81                     | 0.79              |
| 5:AC:215:GLU:HG2   | 3:AI:9:LYS:HE3     | 1.63                     | 0.79              |
| 8:At:145:TRP:CD1   | 6:WJ:164:LEU:HB2   | 2.18                     | 0.79              |
| 11:A0:123:LEU:HD23 | 12:BE:132:LEU:HD11 | 1.63                     | 0.79              |
| 6:UO:128:GLU:O     | 6:UO:132:TYR:N     | 2.13                     | 0.79              |
| 6:WF:181:GLU:HB2   | 6:WF:184:ARG:CG    | 2.07                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:65:LEU:HG     | 2:d:65:MET:HG3    | 1.62                     | 0.79              |
| 2:a:346:MET:CE    | 2:c:142:LEU:HD11  | 2.12                     | 0.79              |
| 2:f:273:CYS:HA    | 2:g:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:h:273:CYS:HA    | 2:i:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:s:273:CYS:HA    | 2:t:328:LEU:CD2   | 2.13                     | 0.79              |
| 7:As:52:ILE:HD11  | 9:Ax:206:ALA:HB1  | 1.63                     | 0.79              |
| 6:WA:181:GLU:HB2  | 6:WA:184:ARG:CG   | 2.07                     | 0.79              |
| 6:WQ:197:LEU:CD1  | 6:WR:175:SER:OG   | 2.26                     | 0.79              |
| 6:WW:181:GLU:HB2  | 6:WW:184:ARG:CG   | 2.07                     | 0.79              |
| 1:A:136:GLY:HA3   | 1:C:213:ILE:HG23  | 1.62                     | 0.79              |
| 1:D:131:SER:O     | 1:F:223:GLN:NE2   | 2.14                     | 0.79              |
| 1:G:63:GLN:OE1    | 2:e:131:SER:OG    | 1.99                     | 0.79              |
| 2:d:273:CYS:HA    | 2:e:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:j:273:CYS:HA    | 2:k:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:q:273:CYS:HA    | 2:r:328:LEU:CD2   | 2.13                     | 0.79              |
| 5:AC:229:MET:HG2  | 12:BD:102:MET:HE3 | 1.65                     | 0.79              |
| 3:AF:44:LEU:CD2   | 12:BA:78:TYR:CB   | 2.61                     | 0.79              |
| 3:AI:6:TRP:CZ2    | 12:BD:77:VAL:HB   | 2.17                     | 0.79              |
| 6:AQ:278:THR:HG21 | 10:A5:14:LEU:HB3  | 1.64                     | 0.79              |
| 9:Ax:194:LEU:HD11 | 9:Ay:220:PRO:HG2  | 1.63                     | 0.79              |
| 2:b:142:LEU:HD11  | 2:z:346:MET:CE    | 2.12                     | 0.79              |
| 2:c:346:MET:CE    | 2:e:142:LEU:HD11  | 2.12                     | 0.79              |
| 2:n:216:LEU:O     | 2:o:229:ASN:OD1   | 2.01                     | 0.79              |
| 2:o:273:CYS:HA    | 2:p:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:t:273:CYS:HA    | 2:u:328:LEU:CD2   | 2.13                     | 0.79              |
| 3:AL:52:PRO:CD    | 12:BB:80:PRO:HB3  | 2.13                     | 0.79              |
| 7:Aq:39:GLN:NE2   | 7:Aq:46:GLU:O     | 2.13                     | 0.79              |
| 6:UI:128:GLU:O    | 6:UI:132:TYR:N    | 2.13                     | 0.79              |
| 2:k:273:CYS:HA    | 2:l:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:l:273:CYS:HA    | 2:m:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:p:216:LEU:O     | 2:q:229:ASN:OD1   | 2.01                     | 0.79              |
| 2:p:273:CYS:HA    | 2:q:328:LEU:CD2   | 2.13                     | 0.79              |
| 2:r:216:LEU:O     | 2:s:229:ASN:OD1   | 2.01                     | 0.79              |
| 2:u:273:CYS:HA    | 2:v:328:LEU:CD2   | 2.13                     | 0.79              |
| 3:O:42:GLU:OE2    | 3:AJ:189:GLU:HG2  | 1.83                     | 0.79              |
| 3:ZA:57:SER:HA    | 3:AI:154:ASP:CB   | 2.13                     | 0.79              |
| 3:ZE:20:ASP:OD2   | 4:ZJ:2:SER:HB2    | 1.83                     | 0.79              |
| 4:ZH:270:ASN:N    | 4:ZN:190:GLN:O    | 2.16                     | 0.79              |
| 4:ZT:375:MET:SD   | 4:ZY:388:THR:HA   | 2.23                     | 0.79              |
| 5:AB:59:ALA:O     | 3:AG:66:LEU:HD13  | 1.83                     | 0.79              |
| 3:AF:62:LEU:CD1   | 12:BB:84:LEU:HD11 | 2.13                     | 0.79              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WP:197:LEU:HD12 | 6:WQ:175:SER:OG    | 1.83                     | 0.79              |
| 12:BD:6:ILE:HG21  | 12:BD:122:VAL:HG21 | 1.62                     | 0.79              |
| 2:c:273:CYS:HA    | 2:d:328:LEU:CD2    | 2.13                     | 0.78              |
| 2:l:216:LEU:O     | 2:m:229:ASN:OD1    | 2.01                     | 0.78              |
| 2:m:273:CYS:HA    | 2:n:328:LEU:CD2    | 2.13                     | 0.78              |
| 2:n:273:CYS:HA    | 2:o:328:LEU:CD2    | 2.13                     | 0.78              |
| 2:o:216:LEU:O     | 2:p:229:ASN:OD1    | 2.01                     | 0.78              |
| 2:s:346:MET:CE    | 2:u:142:LEU:HD11   | 2.12                     | 0.78              |
| 2:t:216:LEU:O     | 2:u:229:ASN:OD1    | 2.01                     | 0.78              |
| 3:ZA:122:VAL:O    | 4:ZF:322:ASN:CG    | 2.25                     | 0.78              |
| 6:AP:299:ASN:HD22 | 12:BA:55:PRO:HB2   | 1.46                     | 0.78              |
| 11:A7:51:LYS:CE   | 11:A7:55:ARG:HH12  | 1.96                     | 0.78              |
| 6:WU:181:GLU:HB2  | 6:WU:184:ARG:CG    | 2.07                     | 0.78              |
| 1:Z:63:GLN:OE1    | 2:x:131:SER:OG     | 1.99                     | 0.78              |
| 2:v:273:CYS:HA    | 2:w:328:LEU:CD2    | 2.13                     | 0.78              |
| 4:ZQ:160:SER:HA   | 4:ZQ:268:GLN:HE21  | 1.48                     | 0.78              |
| 5:AA:109:PRO:HG3  | 3:AF:197:SER:O     | 1.84                     | 0.78              |
| 9:Ay:162:PRO:HG2  | 6:WH:167:ARG:NH2   | 1.98                     | 0.78              |
| 11:A7:67:LEU:HD11 | 11:A7:74:PRO:HA    | 1.64                     | 0.78              |
| 6:UN:128:GLU:O    | 6:UN:132:TYR:N     | 2.13                     | 0.78              |
| 6:UP:73:MET:HE1   | 6:UP:99:ARG:HD3    | 1.62                     | 0.78              |
| 6:WS:200:SER:OG   | 6:WT:175:SER:HB2   | 1.83                     | 0.78              |
| 6:WV:181:GLU:HB2  | 6:WV:184:ARG:CG    | 2.07                     | 0.78              |
| 2:n:346:MET:CE    | 2:p:142:LEU:HD11   | 2.12                     | 0.78              |
| 2:q:216:LEU:O     | 2:r:229:ASN:OD1    | 2.01                     | 0.78              |
| 2:s:216:LEU:O     | 2:t:229:ASN:OD1    | 2.01                     | 0.78              |
| 6:AP:278:THR:CG2  | 10:A5:21:ALA:HB1   | 2.10                     | 0.78              |
| 6:UM:98:LEU:HD22  | 6:UM:147:LEU:HD21  | 1.66                     | 0.78              |
| 6:UN:73:MET:HE1   | 6:UN:99:ARG:HD3    | 1.62                     | 0.78              |
| 2:a:273:CYS:HA    | 2:b:328:LEU:CD2    | 2.13                     | 0.78              |
| 2:k:216:LEU:O     | 2:l:229:ASN:OD1    | 2.01                     | 0.78              |
| 2:m:216:LEU:O     | 2:n:229:ASN:OD1    | 2.02                     | 0.78              |
| 2:v:216:LEU:O     | 2:w:229:ASN:OD1    | 2.01                     | 0.78              |
| 3:2:56:SER:C      | 5:AA:138:ALA:CB    | 2.52                     | 0.78              |
| 4:Zc:331:ASP:HA   | 4:Zh:40:ALA:HB1    | 1.66                     | 0.78              |
| 5:AC:84:GLN:OE1   | 3:AN:48:THR:HG22   | 1.83                     | 0.78              |
| 3:AK:73:ARG:HD2   | 12:BF:78:TYR:CZ    | 2.18                     | 0.78              |
| 6:WG:143:THR:OG1  | 6:WH:154:ARG:HG2   | 1.83                     | 0.78              |
| 1:F:165:GLY:C     | 1:G:35:THR:CG2     | 2.57                     | 0.78              |
| 1:H:165:GLY:C     | 1:I:35:THR:CG2     | 2.57                     | 0.78              |
| 1:K:63:GLN:OE1    | 2:i:131:SER:OG     | 1.99                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:165:GLY:C     | 1:N:35:THR:CG2    | 2.57                     | 0.78              |
| 2:b:273:CYS:HA    | 2:c:328:LEU:CD2   | 2.13                     | 0.78              |
| 2:w:273:CYS:HA    | 2:x:328:LEU:CD2   | 2.13                     | 0.78              |
| 3:2:231:VAL:HG11  | 3:8:9:LYS:HG3     | 1.66                     | 0.78              |
| 3:4:85:ASN:OD1    | 4:ZF:50:LEU:HD22  | 1.84                     | 0.78              |
| 3:6:1:MET:HE2     | 3:AJ:226:VAL:HG11 | 1.64                     | 0.78              |
| 5:AE:131:GLU:HB3  | 3:AJ:179:MET:CE   | 2.12                     | 0.78              |
| 3:AI:50:ARG:HD3   | 6:BN:322:PRO:HG3  | 1.64                     | 0.78              |
| 7:As:25:LEU:HD23  | 9:Ay:206:ALA:HB2  | 1.64                     | 0.78              |
| 6:WV:197:LEU:HD12 | 6:WW:175:SER:CB   | 2.12                     | 0.78              |
| 1:K:165:GLY:C     | 1:L:35:THR:CG2    | 2.57                     | 0.78              |
| 1:R:165:GLY:C     | 1:S:35:THR:CG2    | 2.57                     | 0.78              |
| 1:T:165:GLY:C     | 1:U:35:THR:CG2    | 2.57                     | 0.78              |
| 2:j:216:LEU:O     | 2:k:229:ASN:OD1   | 2.02                     | 0.78              |
| 2:u:216:LEU:O     | 2:v:229:ASN:OD1   | 2.02                     | 0.78              |
| 4:ZQ:65:THR:HA    | 4:Zb:50:LEU:HD13  | 1.65                     | 0.78              |
| 5:AC:71:LEU:HB2   | 3:AN:70:THR:CG2   | 2.13                     | 0.78              |
| 5:AE:175:ASP:OD2  | 3:AJ:46:TYR:O     | 2.00                     | 0.78              |
| 6:WA:167:ARG:NH2  | 6:WA:168:GLU:OE2  | 2.17                     | 0.78              |
| 6:WF:128:GLU:HG2  | 6:WG:126:PHE:HD2  | 1.48                     | 0.78              |
| 6:WK:197:LEU:CD1  | 6:WL:175:SER:CB   | 2.58                     | 0.78              |
| 6:WP:200:SER:O    | 6:WQ:158:ALA:CB   | 2.31                     | 0.78              |
| 1:C:165:GLY:C     | 1:D:35:THR:CG2    | 2.57                     | 0.78              |
| 1:V:165:GLY:C     | 1:W:35:THR:CG2    | 2.57                     | 0.78              |
| 2:x:273:CYS:HA    | 2:y:328:LEU:CD2   | 2.13                     | 0.78              |
| 3:1:52:PRO:HG3    | 12:BF:80:PRO:HB3  | 1.65                     | 0.78              |
| 3:ZC:218:TYR:OH   | 4:ZN:53:LYS:HD2   | 1.84                     | 0.78              |
| 5:AB:202:MET:CE   | 3:AM:73:ARG:HD2   | 2.01                     | 0.78              |
| 5:AB:217:MET:HE1  | 3:AM:258:THR:HA   | 1.66                     | 0.78              |
| 6:Ag:295:SER:OG   | 11:A8:72:HIS:HA   | 1.83                     | 0.78              |
| 6:Ao:303:GLN:CD   | 6:BI:319:GLN:OE1  | 2.26                     | 0.78              |
| 10:A2:77:LYS:NZ   | 11:A8:13:GLN:OE1  | 2.16                     | 0.78              |
| 6:WH:181:GLU:HB2  | 6:WH:184:ARG:CG   | 2.07                     | 0.78              |
| 6:WQ:113:PHE:HB3  | 6:WR:134:ARG:HE   | 1.48                     | 0.78              |
| 1:D:165:GLY:C     | 1:E:35:THR:CG2    | 2.57                     | 0.78              |
| 2:i:216:LEU:O     | 2:j:229:ASN:OD1   | 2.01                     | 0.78              |
| 4:ZU:183:THR:HB   | 4:Zf:131:GLY:O    | 1.84                     | 0.78              |
| 7:Ab:48:THR:HG21  | 9:Au:208:GLY:HA2  | 1.65                     | 0.78              |
| 9:Ax:143:ARG:CA   | 6:WD:165:PHE:HB3  | 2.00                     | 0.78              |
| 1:A:165:GLY:C     | 1:B:35:THR:CG2    | 2.57                     | 0.78              |
| 1:S:63:GLN:OE1    | 2:q:131:SER:OG    | 1.99                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:X:165:GLY:C     | 1:Y:35:THR:CG2    | 2.57                     | 0.78              |
| 2:x:216:LEU:O     | 2:y:229:ASN:OD1   | 2.01                     | 0.78              |
| 3:ZA:121:GLN:OE1  | 4:ZF:324:GLU:HG3  | 1.83                     | 0.78              |
| 7:As:7:MET:CE     | 8:At:233:MET:HB3  | 2.14                     | 0.78              |
| 9:Ay:38:TRP:NE1   | 10:A5:43:ASP:OD1  | 2.16                     | 0.78              |
| 10:A2:61:LEU:HD13 | 11:A7:50:LYS:NZ   | 1.99                     | 0.78              |
| 6:WV:120:LYS:NZ   | 6:WV:123:ILE:HD11 | 1.99                     | 0.78              |
| 1:I:165:GLY:C     | 1:J:35:THR:CG2    | 2.57                     | 0.78              |
| 1:J:165:GLY:C     | 1:K:35:THR:CG2    | 2.57                     | 0.78              |
| 1:W:165:GLY:C     | 1:X:35:THR:CG2    | 2.57                     | 0.78              |
| 1:Y:165:GLY:C     | 1:Z:35:THR:CG2    | 2.57                     | 0.78              |
| 2:a:328:LEU:CD2   | 2:z:273:CYS:HA    | 2.13                     | 0.78              |
| 5:AE:16:LEU:CD2   | 3:AJ:253:MET:HE3  | 2.13                     | 0.78              |
| 3:AJ:62:LEU:HD21  | 12:BF:83:PRO:HD2  | 1.62                     | 0.78              |
| 7:Ar:29:LEU:HB2   | 7:As:52:ILE:HG21  | 1.66                     | 0.78              |
| 9:Ay:62:THR:HG23  | 9:Ay:101:MET:HE2  | 1.65                     | 0.78              |
| 11:A0:103:ASP:OD1 | 12:BF:112:TYR:OH  | 2.00                     | 0.78              |
| 6:UP:128:GLU:O    | 6:UP:132:TYR:N    | 2.13                     | 0.78              |
| 1:E:165:GLY:C     | 1:F:35:THR:CG2    | 2.57                     | 0.77              |
| 1:N:165:GLY:C     | 1:O:35:THR:CG2    | 2.57                     | 0.77              |
| 1:O:63:GLN:OE1    | 2:m:131:SER:OG    | 1.99                     | 0.77              |
| 1:P:165:GLY:C     | 1:Q:35:THR:CG2    | 2.57                     | 0.77              |
| 1:U:165:GLY:C     | 1:V:35:THR:CG2    | 2.57                     | 0.77              |
| 2:h:216:LEU:O     | 2:i:229:ASN:OD1   | 2.01                     | 0.77              |
| 2:w:216:LEU:O     | 2:x:229:ASN:OD1   | 2.01                     | 0.77              |
| 2:y:273:CYS:HA    | 2:z:328:LEU:CD2   | 2.13                     | 0.77              |
| 3:ZA:44:LEU:HD22  | 3:AN:86:LEU:HD12  | 1.66                     | 0.77              |
| 5:AA:46:VAL:HG12  | 11:A6:93:PRO:HB2  | 1.64                     | 0.77              |
| 5:AB:175:ASP:O    | 3:AG:45:LEU:HD12  | 1.83                     | 0.77              |
| 10:A1:77:LYS:NZ   | 11:A7:13:GLN:OE1  | 2.14                     | 0.77              |
| 6:UJ:103:GLN:HB3  | 6:WD:182:PRO:CA   | 2.13                     | 0.77              |
| 6:UK:207:PRO:CD   | 6:WE:187:ASP:OD2  | 2.31                     | 0.77              |
| 6:WU:197:LEU:CD1  | 6:WV:175:SER:OG   | 2.29                     | 0.77              |
| 1:A:35:THR:CG2    | 1:Z:165:GLY:C     | 2.57                     | 0.77              |
| 1:O:165:GLY:C     | 1:P:35:THR:CG2    | 2.57                     | 0.77              |
| 3:ZA:248:SER:HB2  | 4:ZF:402:LEU:HD22 | 1.64                     | 0.77              |
| 4:ZQ:2:SER:OG     | 4:ZQ:3:PHE:N      | 2.17                     | 0.77              |
| 5:AA:54:ARG:HE    | 12:BB:22:ASN:ND2  | 1.81                     | 0.77              |
| 6:AX:372:ILE:CD1  | 10:A3:11:ILE:HG22 | 2.14                     | 0.77              |
| 9:Av:116:PHE:CE2  | 11:A7:4:ARG:CZ    | 2.66                     | 0.77              |
| 6:UK:98:LEU:HD22  | 6:UK:147:LEU:HD21 | 1.66                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:UL:98:LEU:HD22  | 6:UL:147:LEU:HD21  | 1.66                     | 0.77              |
| 6:WA:175:SER:HB3  | 6:WW:197:LEU:HD12  | 1.64                     | 0.77              |
| 6:WB:163:SER:HB2  | 6:WB:166:VAL:HG22  | 1.66                     | 0.77              |
| 1:W:63:GLN:OE1    | 2:u:131:SER:OG     | 1.99                     | 0.77              |
| 2:g:216:LEU:O     | 2:h:229:ASN:OD1    | 2.01                     | 0.77              |
| 5:AD:241:GLU:CD   | 11:A9:106:ARG:HH22 | 1.92                     | 0.77              |
| 9:Aw:152:ARG:HH21 | 6:WC:165:PHE:HD2   | 1.28                     | 0.77              |
| 6:UJ:98:LEU:HD22  | 6:UJ:147:LEU:HD21  | 1.66                     | 0.77              |
| 6:WF:187:ASP:HB3  | 6:WF:190:GLN:HG3   | 1.66                     | 0.77              |
| 6:WJ:143:THR:OG1  | 6:WK:154:ARG:HG2   | 1.83                     | 0.77              |
| 6:WL:181:GLU:HB2  | 6:WL:184:ARG:CG    | 2.07                     | 0.77              |
| 1:D:63:GLN:OE1    | 2:b:131:SER:OG     | 1.99                     | 0.77              |
| 3:3:218:TYR:CE1   | 3:ZE:73:ARG:HD2    | 2.19                     | 0.77              |
| 6:WM:181:GLU:HB2  | 6:WM:184:ARG:CG    | 2.07                     | 0.77              |
| 6:WO:203:ALA:HB1  | 6:WP:160:PRO:HB3   | 1.67                     | 0.77              |
| 6:WT:200:SER:O    | 6:WU:158:ALA:HB3   | 1.84                     | 0.77              |
| 1:C:165:GLY:C     | 1:D:35:THR:HG22    | 2.10                     | 0.77              |
| 1:D:165:GLY:C     | 1:E:35:THR:HG22    | 2.10                     | 0.77              |
| 1:I:165:GLY:C     | 1:J:35:THR:HG22    | 2.10                     | 0.77              |
| 1:M:165:GLY:C     | 1:N:35:THR:HG22    | 2.10                     | 0.77              |
| 3:7:235:GLN:HG2   | 3:ZD:5:LEU:HD21    | 1.64                     | 0.77              |
| 5:AA:72:ASP:OD1   | 3:AL:6:TRP:CD2     | 2.38                     | 0.77              |
| 5:AC:165:LYS:HG3  | 5:AC:199:ILE:HD11  | 1.67                     | 0.77              |
| 7:Ab:8:MET:HE2    | 6:WS:124:SER:CB    | 2.14                     | 0.77              |
| 6:UN:98:LEU:HD22  | 6:UN:147:LEU:HD21  | 1.66                     | 0.77              |
| 6:WJ:181:GLU:HB2  | 6:WJ:184:ARG:CG    | 2.07                     | 0.77              |
| 1:E:165:GLY:C     | 1:F:35:THR:HG22    | 2.10                     | 0.77              |
| 1:G:165:GLY:C     | 1:H:35:THR:CG2     | 2.57                     | 0.77              |
| 1:G:165:GLY:C     | 1:H:35:THR:HG22    | 2.10                     | 0.77              |
| 1:S:165:GLY:C     | 1:T:35:THR:CG2     | 2.57                     | 0.77              |
| 1:U:165:GLY:C     | 1:V:35:THR:HG22    | 2.10                     | 0.77              |
| 2:a:229:ASN:OD1   | 2:z:216:LEU:O      | 2.02                     | 0.77              |
| 2:y:216:LEU:O     | 2:z:229:ASN:OD1    | 2.01                     | 0.77              |
| 3:5:231:VAL:HG11  | 3:ZB:9:LYS:HG2     | 1.66                     | 0.77              |
| 3:6:56:SER:HA     | 5:AE:138:ALA:HB2   | 1.60                     | 0.77              |
| 3:6:57:SER:HB3    | 3:AK:108:PRO:CG    | 2.14                     | 0.77              |
| 6:AV:278:THR:HG21 | 10:A3:21:ALA:HB1   | 1.65                     | 0.77              |
| 9:Ay:240:ALA:CB   | 6:WG:165:PHE:CE1   | 2.67                     | 0.77              |
| 6:UO:98:LEU:HD22  | 6:UO:147:LEU:HD21  | 1.65                     | 0.77              |
| 6:WT:160:PRO:HD3  | 6:WT:172:PRO:HA    | 1.66                     | 0.77              |
| 1:B:165:GLY:C     | 1:C:35:THR:HG22    | 2.10                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:165:GLY:C     | 1:M:35:THR:HG22   | 2.10                     | 0.77              |
| 2:c:216:LEU:O     | 2:d:229:ASN:OD1   | 2.01                     | 0.77              |
| 9:Aw:162:PRO:CD   | 6:WA:167:ARG:HH21 | 1.98                     | 0.77              |
| 6:WJ:128:GLU:CG   | 6:WK:126:PHE:CD2  | 2.67                     | 0.77              |
| 1:B:165:GLY:C     | 1:C:35:THR:CG2    | 2.57                     | 0.77              |
| 1:K:165:GLY:C     | 1:L:35:THR:HG22   | 2.10                     | 0.77              |
| 1:L:165:GLY:C     | 1:M:35:THR:CG2    | 2.57                     | 0.77              |
| 1:N:165:GLY:C     | 1:O:35:THR:HG22   | 2.10                     | 0.77              |
| 1:T:165:GLY:C     | 1:U:35:THR:HG22   | 2.10                     | 0.77              |
| 2:e:216:LEU:O     | 2:f:229:ASN:OD1   | 2.01                     | 0.77              |
| 3:8:36:ARG:NE     | 3:8:38:ARG:NH2    | 2.24                     | 0.77              |
| 5:AA:248:LEU:O    | 5:AA:249:SER:C    | 2.28                     | 0.77              |
| 7:Aq:2:THR:HG23   | 6:WW:125:GLN:OE1  | 1.84                     | 0.77              |
| 9:Av:59:LEU:HD11  | 10:A1:102:MET:HE1 | 1.67                     | 0.77              |
| 6:WI:181:GLU:HB2  | 6:WI:184:ARG:CG   | 2.07                     | 0.77              |
| 6:WN:201:ALA:CA   | 6:WO:158:ALA:HB2  | 2.13                     | 0.77              |
| 1:F:47:ALA:CB     | 2:c:178:GLN:HG3   | 2.15                     | 0.77              |
| 1:L:47:ALA:CB     | 2:i:178:GLN:HG3   | 2.15                     | 0.77              |
| 1:V:165:GLY:C     | 1:W:35:THR:HG22   | 2.10                     | 0.77              |
| 2:b:216:LEU:O     | 2:c:229:ASN:OD1   | 2.01                     | 0.77              |
| 2:f:216:LEU:O     | 2:g:229:ASN:OD1   | 2.01                     | 0.77              |
| 3:ZB:122:VAL:O    | 4:ZG:322:ASN:ND2  | 2.18                     | 0.77              |
| 4:ZM:18:ASP:O     | 4:ZR:5:GLN:NE2    | 2.18                     | 0.77              |
| 5:AB:49:LEU:HB3   | 11:A7:90:PRO:HG2  | 1.66                     | 0.77              |
| 12:BD:37:PRO:HB2  | 6:BM:330:THR:CG2  | 2.14                     | 0.77              |
| 1:F:165:GLY:C     | 1:G:35:THR:HG22   | 2.10                     | 0.77              |
| 1:G:47:ALA:CB     | 2:d:178:GLN:HG3   | 2.15                     | 0.77              |
| 1:K:47:ALA:CB     | 2:h:178:GLN:HG3   | 2.15                     | 0.77              |
| 1:O:165:GLY:C     | 1:P:35:THR:HG22   | 2.10                     | 0.77              |
| 1:Q:165:GLY:C     | 1:R:35:THR:CG2    | 2.57                     | 0.77              |
| 1:W:165:GLY:C     | 1:X:35:THR:HG22   | 2.10                     | 0.77              |
| 2:a:216:LEU:O     | 2:b:229:ASN:OD1   | 2.01                     | 0.77              |
| 3:ZA:233:MET:SD   | 4:ZF:388:THR:HB   | 2.25                     | 0.77              |
| 4:ZL:29:THR:HG22  | 4:ZQ:39:PHE:HB2   | 1.67                     | 0.77              |
| 6:Ag:297:GLN:HB2  | 11:A8:73:ILE:HD11 | 1.63                     | 0.77              |
| 11:A7:51:LYS:CB   | 11:A7:55:ARG:HH22 | 1.86                     | 0.77              |
| 6:WF:196:HIS:HB3  | 6:WG:211:THR:HG21 | 1.67                     | 0.77              |
| 6:WM:197:LEU:HD12 | 6:WN:175:SER:HB3  | 1.67                     | 0.77              |
| 1:A:47:ALA:CB     | 2:x:178:GLN:HG3   | 2.15                     | 0.76              |
| 1:E:47:ALA:CB     | 2:b:178:GLN:HG3   | 2.15                     | 0.76              |
| 1:S:165:GLY:C     | 1:T:35:THR:HG22   | 2.10                     | 0.76              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:d:216:LEU:O     | 2:e:229:ASN:OD1    | 2.02                     | 0.76              |
| 4:ZF:181:LYS:NZ   | 4:ZQ:129:GLN:OE1   | 2.13                     | 0.76              |
| 4:ZX:387:GLN:NE2  | 4:Zd:400:VAL:O     | 2.18                     | 0.76              |
| 5:AB:9:MET:CB     | 12:BB:103:VAL:HG21 | 2.15                     | 0.76              |
| 5:AD:74:THR:CG2   | 3:AI:38:ARG:HH11   | 1.89                     | 0.76              |
| 6:AT:236:LYS:NZ   | 6:UJ:167:ARG:HH11  | 1.83                     | 0.76              |
| 6:WD:197:LEU:HD12 | 6:WE:175:SER:OG    | 1.85                     | 0.76              |
| 1:A:165:GLY:C     | 1:B:35:THR:HG22    | 2.10                     | 0.76              |
| 1:X:47:ALA:CB     | 2:u:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:Z:47:ALA:CB     | 2:w:178:GLN:HG3    | 2.15                     | 0.76              |
| 3:4:111:THR:HG21  | 3:AH:163:GLY:HA2   | 1.67                     | 0.76              |
| 5:AB:53:THR:OG1   | 11:A7:92:GLN:HG2   | 1.85                     | 0.76              |
| 6:AT:295:SER:HB2  | 11:A0:73:ILE:HG13  | 1.67                     | 0.76              |
| 6:UJ:261:LEU:HB3  | 6:UJ:270:THR:HG23  | 1.67                     | 0.76              |
| 6:WN:200:SER:HA   | 6:WO:173:SER:OG    | 1.85                     | 0.76              |
| 1:M:47:ALA:CB     | 2:j:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:Q:47:ALA:CB     | 2:n:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:R:165:GLY:C     | 1:S:35:THR:HG22    | 2.10                     | 0.76              |
| 2:f:54:GLN:OE1    | 3:AF:168:VAL:CG1   | 2.33                     | 0.76              |
| 3:0:47:GLN:HB2    | 5:AD:68:PRO:HG2    | 1.68                     | 0.76              |
| 3:ZC:240:TYR:CD2  | 4:ZH:395:ILE:HG23  | 2.19                     | 0.76              |
| 5:AA:153:ASN:ND2  | 3:AL:194:GLU:OE2   | 2.18                     | 0.76              |
| 3:AL:73:ARG:HH12  | 3:AL:75:VAL:HG13   | 1.50                     | 0.76              |
| 7:Aq:89:GLY:O     | 6:WW:164:LEU:CD1   | 2.32                     | 0.76              |
| 12:BA:128:LYS:O   | 12:BA:131:THR:N    | 2.18                     | 0.76              |
| 1:B:47:ALA:CB     | 2:y:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:J:47:ALA:CB     | 2:g:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:J:165:GLY:C     | 1:K:35:THR:HG22    | 2.10                     | 0.76              |
| 1:R:47:ALA:CB     | 2:o:178:GLN:HG3    | 2.15                     | 0.76              |
| 6:UP:98:LEU:HD22  | 6:UP:147:LEU:HD21  | 1.66                     | 0.76              |
| 6:WD:112:GLY:HA2  | 6:WD:135:ALA:HA    | 1.68                     | 0.76              |
| 1:P:47:ALA:CB     | 2:m:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:S:47:ALA:CB     | 2:p:178:GLN:HG3    | 2.15                     | 0.76              |
| 1:X:165:GLY:C     | 1:Y:35:THR:HG22    | 2.10                     | 0.76              |
| 1:Y:47:ALA:CB     | 2:v:178:GLN:HG3    | 2.15                     | 0.76              |
| 3:9:218:TYR:OH    | 4:ZK:53:LYS:HB2    | 1.85                     | 0.76              |
| 5:AA:58:THR:OG1   | 6:BH:320:PRO:HG2   | 1.85                     | 0.76              |
| 6:Am:295:SER:CB   | 11:A7:73:ILE:HG13  | 2.14                     | 0.76              |
| 10:A4:14:LEU:HD23 | 6:BW:278:THR:HG22  | 1.66                     | 0.76              |
| 6:WN:181:GLU:HB2  | 6:WN:184:ARG:CG    | 2.07                     | 0.76              |
| 4:ZM:380:ARG:NH2  | 4:ZS:393:ASP:OD1   | 2.19                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZQ:332:ASN:N    | 4:ZV:41:ASP:OD2   | 2.18                     | 0.76              |
| 3:AI:47:GLN:HE22  | 12:BD:75:LYS:HA   | 1.50                     | 0.76              |
| 1:H:47:ALA:CB     | 2:e:178:GLN:HG3   | 2.15                     | 0.76              |
| 3:1:78:GLU:HG2    | 3:AK:121:GLN:HE22 | 1.50                     | 0.76              |
| 3:5:52:PRO:HB3    | 3:5:65:GLY:H      | 1.49                     | 0.76              |
| 6:UM:212:LEU:HB3  | 6:UM:221:THR:HG23 | 1.67                     | 0.76              |
| 6:WN:197:LEU:HD12 | 6:WO:175:SER:HB3  | 1.68                     | 0.76              |
| 1:D:47:ALA:CB     | 2:a:178:GLN:HG3   | 2.15                     | 0.76              |
| 1:P:165:GLY:C     | 1:Q:35:THR:HG22   | 2.10                     | 0.76              |
| 2:f:54:GLN:OE1    | 3:AF:169:GLN:O    | 2.04                     | 0.76              |
| 3:ZC:240:TYR:HD2  | 4:ZH:395:ILE:HG23 | 1.50                     | 0.76              |
| 5:AD:104:ASN:HD22 | 3:AI:38:ARG:NH2   | 1.82                     | 0.76              |
| 5:AE:248:LEU:O    | 12:BE:121:THR:OG1 | 2.04                     | 0.76              |
| 3:AF:9:LYS:HE3    | 12:BF:100:GLY:HA2 | 1.66                     | 0.76              |
| 6:UI:98:LEU:HD22  | 6:UI:147:LEU:HD21 | 1.66                     | 0.76              |
| 1:A:35:THR:HG22   | 1:Z:165:GLY:C     | 2.10                     | 0.76              |
| 1:O:47:ALA:CB     | 2:l:178:GLN:HG3   | 2.15                     | 0.76              |
| 1:Q:165:GLY:C     | 1:R:35:THR:HG22   | 2.10                     | 0.76              |
| 1:T:47:ALA:CB     | 2:q:178:GLN:HG3   | 2.15                     | 0.76              |
| 4:Zc:379:GLN:NE2  | 4:Zh:394:GLN:HE21 | 1.83                     | 0.76              |
| 5:AD:49:LEU:CB    | 11:A9:90:PRO:HG2  | 2.16                     | 0.76              |
| 9:Ax:160:GLN:N    | 6:WE:166:VAL:HG22 | 1.99                     | 0.76              |
| 10:A1:48:ARG:HH22 | 11:A7:6:ASP:CG    | 1.93                     | 0.76              |
| 10:A5:61:LEU:HD21 | 11:A0:50:LYS:HZ3  | 1.51                     | 0.76              |
| 6:WT:181:GLU:HB2  | 6:WT:184:ARG:CG   | 2.07                     | 0.76              |
| 1:N:47:ALA:CB     | 2:k:178:GLN:HG3   | 2.15                     | 0.76              |
| 1:Y:165:GLY:C     | 1:Z:35:THR:HG22   | 2.10                     | 0.76              |
| 3:3:56:SER:C      | 5:AB:138:ALA:HB1  | 2.11                     | 0.76              |
| 3:ZB:233:MET:CE   | 4:ZG:388:THR:OG1  | 2.29                     | 0.76              |
| 4:ZK:401:ASN:O    | 4:ZK:402:LEU:C    | 2.28                     | 0.76              |
| 5:AB:71:LEU:HD22  | 3:AM:70:THR:CG2   | 2.15                     | 0.76              |
| 6:WE:199:SER:HA   | 6:WE:205:LEU:HD23 | 1.68                     | 0.76              |
| 6:WR:181:GLU:HB2  | 6:WR:184:ARG:CG   | 2.07                     | 0.76              |
| 1:A:63:GLN:OE1    | 2:y:131:SER:OG    | 1.99                     | 0.75              |
| 3:2:58:GLU:CG     | 5:AA:160:ARG:NH1  | 2.48                     | 0.75              |
| 4:ZH:18:ASP:HB3   | 4:ZM:5:GLN:HE22   | 1.50                     | 0.75              |
| 5:AD:26:LEU:HD11  | 3:AI:242:ILE:CG2  | 2.05                     | 0.75              |
| 6:Am:278:THR:CG2  | 10:Az:21:ALA:CB   | 2.64                     | 0.75              |
| 10:A5:4:ILE:CD1   | 6:BS:374:HIS:HB2  | 2.16                     | 0.75              |
| 6:WS:181:GLU:HB2  | 6:WS:184:ARG:CG   | 2.07                     | 0.75              |
| 1:C:47:ALA:CB     | 2:z:178:GLN:HG3   | 2.15                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:165:GLY:C     | 1:I:35:THR:HG22   | 2.10                     | 0.75              |
| 4:Zh:196:MET:HE3  | 4:Zh:259:PHE:HZ   | 1.51                     | 0.75              |
| 3:AI:50:ARG:CD    | 6:BN:322:PRO:HG3  | 2.16                     | 0.75              |
| 6:AX:278:THR:HG21 | 10:A3:7:ILE:CG2   | 2.17                     | 0.75              |
| 9:Ax:106:ASP:OD2  | 10:A3:32:VAL:HG23 | 1.86                     | 0.75              |
| 6:WA:128:GLU:CG   | 6:WB:126:PHE:CE2  | 2.64                     | 0.75              |
| 6:WD:199:SER:HA   | 6:WD:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WK:199:SER:HA   | 6:WK:205:LEU:HD23 | 1.68                     | 0.75              |
| 1:I:47:ALA:CB     | 2:f:178:GLN:HG3   | 2.15                     | 0.75              |
| 3:6:86:LEU:CB     | 4:ZH:42:MET:HE1   | 2.16                     | 0.75              |
| 6:AX:278:THR:CG2  | 10:A3:7:ILE:HG21  | 2.15                     | 0.75              |
| 6:WA:199:SER:HA   | 6:WA:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WD:193:ALA:HB1  | 6:WE:213:VAL:HG11 | 1.67                     | 0.75              |
| 1:U:47:ALA:CB     | 2:r:178:GLN:HG3   | 2.15                     | 0.75              |
| 3:ZE:248:SER:HB2  | 4:ZJ:402:LEU:HD21 | 1.63                     | 0.75              |
| 5:AA:72:ASP:CB    | 3:AL:9:LYS:HZ3    | 1.92                     | 0.75              |
| 6:AR:278:THR:HG21 | 10:A2:21:ALA:CB   | 2.16                     | 0.75              |
| 6:WF:199:SER:HA   | 6:WF:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WT:197:LEU:HD12 | 6:WU:175:SER:HB3  | 1.65                     | 0.75              |
| 1:W:47:ALA:CB     | 2:t:178:GLN:HG3   | 2.16                     | 0.75              |
| 3:0:80:LEU:HD13   | 3:AJ:91:ASN:HB2   | 1.68                     | 0.75              |
| 3:ZC:10:THR:CG2   | 3:ZC:71:GLY:HA3   | 2.17                     | 0.75              |
| 4:ZQ:181:LYS:HZ3  | 4:Zb:129:GLN:NE2  | 1.85                     | 0.75              |
| 4:ZR:382:TYR:CE1  | 4:ZW:395:ILE:HG23 | 2.22                     | 0.75              |
| 4:Zh:112:GLN:HE21 | 4:Zh:331:ASP:HB2  | 1.51                     | 0.75              |
| 5:AD:243:ARG:CZ   | 12:BE:113:GLN:HB2 | 2.17                     | 0.75              |
| 3:AF:62:LEU:HG    | 12:BB:84:LEU:HD11 | 1.68                     | 0.75              |
| 6:AW:299:ASN:HD21 | 11:A9:55:ARG:NH2  | 1.81                     | 0.75              |
| 6:Ae:372:ILE:HB   | 10:A2:4:ILE:HG12  | 1.68                     | 0.75              |
| 6:Am:278:THR:CG2  | 10:Az:21:ALA:HB1  | 2.17                     | 0.75              |
| 6:AP:276:GLU:OE2  | 10:A5:19:MET:CA   | 2.32                     | 0.75              |
| 6:WP:199:SER:HA   | 6:WP:205:LEU:HD23 | 1.69                     | 0.75              |
| 3:0:47:GLN:NE2    | 5:AD:67:THR:HG23  | 2.02                     | 0.75              |
| 4:ZJ:331:ASP:HA   | 4:ZO:40:ALA:HB1   | 1.68                     | 0.75              |
| 5:AB:28:ASN:OD1   | 3:AG:72:VAL:HG23  | 1.86                     | 0.75              |
| 5:AD:53:THR:OG1   | 11:A9:92:GLN:OE1  | 2.04                     | 0.75              |
| 5:AE:227:PHE:HE2  | 3:AJ:253:MET:O    | 1.70                     | 0.75              |
| 3:AG:147:LEU:HD11 | 3:AG:162:GLN:HG2  | 1.68                     | 0.75              |
| 3:AH:50:ARG:NH1   | 6:BM:328:ILE:HG21 | 2.02                     | 0.75              |
| 6:Af:365:ASN:CB   | 11:A8:72:HIS:ND1  | 2.47                     | 0.75              |
| 9:Ax:142:THR:C    | 6:WD:165:PHE:HB2  | 2.11                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UL:167:ARG:NH1  | 6:WF:188:GLU:OE2  | 2.19                     | 0.75              |
| 6:UL:212:LEU:HB3  | 6:UL:221:THR:HG23 | 1.67                     | 0.75              |
| 6:UO:212:LEU:HB3  | 6:UO:221:THR:HG23 | 1.67                     | 0.75              |
| 6:UP:212:LEU:HB3  | 6:UP:221:THR:HG23 | 1.67                     | 0.75              |
| 6:WC:193:ALA:HB1  | 6:WD:213:VAL:HG11 | 1.68                     | 0.75              |
| 6:WC:199:SER:HA   | 6:WC:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WO:199:SER:HA   | 6:WO:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WQ:181:GLU:HB2  | 6:WQ:184:ARG:CG   | 2.07                     | 0.75              |
| 6:WW:199:SER:HA   | 6:WW:205:LEU:HD23 | 1.69                     | 0.75              |
| 4:ZT:99:GLN:HE21  | 4:ZY:58:THR:HG21  | 1.52                     | 0.75              |
| 5:AB:202:MET:CE   | 3:AM:73:ARG:HD3   | 1.99                     | 0.75              |
| 5:AC:61:THR:N     | 3:AH:65:GLY:O     | 2.17                     | 0.75              |
| 3:AK:45:LEU:HD23  | 12:BF:90:TYR:CZ   | 2.21                     | 0.75              |
| 3:AK:73:ARG:HD3   | 12:BF:78:TYR:CD2  | 2.22                     | 0.75              |
| 6:UK:212:LEU:HB3  | 6:UK:221:THR:HG23 | 1.67                     | 0.75              |
| 6:WC:200:SER:OG   | 6:WD:175:SER:HB2  | 1.85                     | 0.75              |
| 6:WG:199:SER:HA   | 6:WG:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WP:196:HIS:HB3  | 6:WQ:211:THR:HG21 | 1.66                     | 0.75              |
| 6:WQ:199:SER:HA   | 6:WQ:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WR:199:SER:HA   | 6:WR:205:LEU:HD23 | 1.69                     | 0.75              |
| 3:2:56:SER:CA     | 5:AA:138:ALA:HB1  | 2.16                     | 0.75              |
| 3:AJ:2:ILE:HD13   | 12:BE:32:ASP:OD1  | 1.85                     | 0.75              |
| 6:Ae:374:HIS:HB2  | 10:A2:4:ILE:HD12  | 1.68                     | 0.75              |
| 6:UI:212:LEU:HB3  | 6:UI:221:THR:HG23 | 1.67                     | 0.75              |
| 1:V:47:ALA:CB     | 2:s:178:GLN:HG3   | 2.15                     | 0.75              |
| 4:ZS:17:LEU:HD13  | 4:ZX:395:ILE:HD11 | 1.69                     | 0.75              |
| 5:AC:53:THR:OG1   | 11:A8:92:GLN:HG2  | 1.87                     | 0.75              |
| 5:AD:243:ARG:NH2  | 12:BE:109:SER:O   | 2.20                     | 0.75              |
| 9:Ay:148:ALA:HB2  | 6:WI:164:LEU:HD22 | 1.66                     | 0.75              |
| 6:UN:139:GLU:OE1  | 6:UN:142:ARG:NH2  | 2.20                     | 0.75              |
| 6:WA:211:THR:HG21 | 6:WW:196:HIS:HB3  | 1.67                     | 0.75              |
| 6:WM:199:SER:HA   | 6:WM:205:LEU:HD23 | 1.69                     | 0.75              |
| 6:WS:199:SER:HA   | 6:WS:205:LEU:HD23 | 1.69                     | 0.75              |
| 3:ZD:31:THR:HG22  | 4:ZI:39:PHE:HB2   | 1.69                     | 0.74              |
| 4:ZI:144:MET:HE2  | 4:ZI:310:GLN:HE21 | 1.50                     | 0.74              |
| 4:ZR:269:GLN:HB3  | 4:ZX:286:PRO:HG3  | 1.68                     | 0.74              |
| 4:ZV:181:LYS:CD   | 4:Zg:129:GLN:HE21 | 1.96                     | 0.74              |
| 6:Ag:297:GLN:CB   | 11:A8:73:ILE:CD1  | 2.56                     | 0.74              |
| 9:Ay:162:PRO:CG   | 6:WH:167:ARG:NH2  | 2.50                     | 0.74              |
| 6:UO:139:GLU:OE1  | 6:UO:142:ARG:NH2  | 2.20                     | 0.74              |
| 6:WT:199:SER:HA   | 6:WT:205:LEU:HD23 | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:BD:37:PRO:HB2  | 6:BM:330:THR:HG23 | 1.69                     | 0.74              |
| 4:Zc:101:LYS:HE2  | 4:Zh:322:ASN:HD21 | 1.52                     | 0.74              |
| 6:UK:103:GLN:NE2  | 6:WF:182:PRO:HB3  | 2.01                     | 0.74              |
| 6:UP:139:GLU:OE1  | 6:UP:142:ARG:NH2  | 2.20                     | 0.74              |
| 6:WK:193:ALA:CB   | 6:WL:213:VAL:HG21 | 2.13                     | 0.74              |
| 3:5:145:ASN:HB3   | 3:ZA:209:ASN:O    | 1.87                     | 0.74              |
| 3:7:231:VAL:HG11  | 3:ZD:9:LYS:HG2    | 1.68                     | 0.74              |
| 3:ZD:185:GLU:CD   | 4:ZI:46:SER:HB2   | 2.12                     | 0.74              |
| 6:Ao:303:GLN:OE1  | 6:BI:319:GLN:OE1  | 2.05                     | 0.74              |
| 9:Av:135:ARG:NH2  | 9:Av:165:VAL:O    | 2.21                     | 0.74              |
| 6:UK:73:MET:HE1   | 6:UK:99:ARG:CD    | 2.17                     | 0.74              |
| 3:ZB:122:VAL:HG21 | 4:ZG:321:ALA:O    | 1.86                     | 0.74              |
| 4:ZV:387:GLN:CG   | 4:Zb:400:VAL:HG13 | 2.15                     | 0.74              |
| 3:AI:47:GLN:NE2   | 12:BD:75:LYS:HA   | 2.01                     | 0.74              |
| 10:A3:57:GLU:HG2  | 11:A8:11:PHE:CE2  | 2.22                     | 0.74              |
| 10:A4:14:LEU:HD11 | 6:BX:370:ARG:NH2  | 2.02                     | 0.74              |
| 6:UJ:73:MET:HE1   | 6:UJ:99:ARG:CD    | 2.17                     | 0.74              |
| 6:UN:212:LEU:HB3  | 6:UN:221:THR:HG23 | 1.67                     | 0.74              |
| 6:WA:158:ALA:HB3  | 6:WW:200:SER:O    | 1.87                     | 0.74              |
| 6:WK:181:GLU:HB2  | 6:WK:184:ARG:CG   | 2.07                     | 0.74              |
| 6:WL:199:SER:HA   | 6:WL:205:LEU:HD23 | 1.69                     | 0.74              |
| 6:WN:199:SER:HA   | 6:WN:205:LEU:HD23 | 1.69                     | 0.74              |
| 2:m:80:GLN:NE2    | 3:AJ:204:SER:CA   | 2.46                     | 0.74              |
| 2:n:80:GLN:OE1    | 3:AJ:137:GLN:HG3  | 1.87                     | 0.74              |
| 3:ZB:122:VAL:O    | 4:ZG:322:ASN:CB   | 2.36                     | 0.74              |
| 4:ZH:160:SER:OG   | 4:ZN:192:ASN:OD1  | 2.04                     | 0.74              |
| 4:ZI:2:SER:HB3    | 4:ZI:392:GLN:HE21 | 1.51                     | 0.74              |
| 5:AA:200:ARG:HH22 | 3:AG:189:GLU:HB2  | 1.52                     | 0.74              |
| 9:Aw:152:ARG:HD3  | 6:WB:164:LEU:O    | 1.88                     | 0.74              |
| 10:A5:61:LEU:HD21 | 11:A0:50:LYS:NZ   | 2.02                     | 0.74              |
| 3:9:37:GLN:HE21   | 3:9:79:ARG:HH12   | 1.34                     | 0.74              |
| 3:AG:62:LEU:CD1   | 12:BC:84:LEU:HD11 | 2.17                     | 0.74              |
| 3:AH:44:LEU:HD21  | 12:BC:78:TYR:CB   | 2.17                     | 0.74              |
| 3:AI:6:TRP:NE1    | 12:BD:77:VAL:HB   | 2.02                     | 0.74              |
| 11:A8:103:ASP:OD1 | 12:BD:112:TYR:OH  | 2.06                     | 0.74              |
| 6:UI:139:GLU:OE1  | 6:UI:142:ARG:NH2  | 2.20                     | 0.74              |
| 6:UL:73:MET:HE1   | 6:UL:99:ARG:CD    | 2.17                     | 0.74              |
| 6:WB:199:SER:HA   | 6:WB:205:LEU:HD23 | 1.68                     | 0.74              |
| 6:WK:132:TYR:HB2  | 6:WL:126:PHE:CZ   | 2.23                     | 0.74              |
| 6:WR:200:SER:O    | 6:WS:158:ALA:HB2  | 1.87                     | 0.74              |
| 6:WU:199:SER:HA   | 6:WU:205:LEU:HD23 | 1.68                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WV:199:SER:HA   | 6:WV:205:LEU:HD23 | 1.69                     | 0.74              |
| 6:BJ:312:VAL:O    | 6:BJ:317:SER:OG   | 2.05                     | 0.74              |
| 2:l:258:ARG:HH12  | 2:n:140:ASN:ND2   | 1.86                     | 0.74              |
| 2:q:258:ARG:HH12  | 2:s:140:ASN:ND2   | 1.86                     | 0.74              |
| 4:ZN:401:ASN:O    | 4:ZN:402:LEU:C    | 2.31                     | 0.74              |
| 4:ZQ:355:LYS:NZ   | 4:ZW:87:ASP:OD1   | 2.20                     | 0.74              |
| 4:ZW:181:LYS:NZ   | 4:Zh:129:GLN:HE21 | 1.85                     | 0.74              |
| 5:AE:173:ARG:HD2  | 3:AJ:46:TYR:CE1   | 2.22                     | 0.74              |
| 9:Au:160:GLN:CB   | 6:WP:166:VAL:CG2  | 2.48                     | 0.74              |
| 6:WB:163:SER:HB3  | 6:WB:169:GLN:HG2  | 1.70                     | 0.74              |
| 2:m:258:ARG:HH12  | 2:o:140:ASN:ND2   | 1.86                     | 0.74              |
| 3:0:70:THR:CG2    | 5:AD:71:LEU:HD13  | 2.06                     | 0.74              |
| 3:ZA:76:ALA:HA    | 4:ZF:47:LYS:NZ    | 2.03                     | 0.74              |
| 4:ZF:118:GLY:HA2  | 4:ZF:316:VAL:HG12 | 1.68                     | 0.74              |
| 4:ZV:234:GLU:HB3  | 4:Zb:255:THR:CG2  | 2.18                     | 0.74              |
| 6:AS:294:ARG:CD   | 11:A0:68:THR:CG2  | 2.65                     | 0.74              |
| 9:Au:160:GLN:O    | 6:WP:165:PHE:HA   | 1.87                     | 0.74              |
| 6:UL:94:HIS:CB    | 6:UL:146:THR:HG21 | 2.17                     | 0.74              |
| 2:p:258:ARG:HH12  | 2:r:140:ASN:ND2   | 1.86                     | 0.74              |
| 4:ZR:18:ASP:CB    | 4:ZW:5:GLN:HE22   | 2.01                     | 0.74              |
| 4:ZR:183:THR:OG1  | 4:Zc:131:GLY:O    | 2.03                     | 0.74              |
| 3:AK:6:TRP:NE1    | 12:BF:77:VAL:CG1  | 2.51                     | 0.74              |
| 8:At:66:PHE:CE1   | 11:A6:5:LEU:HD13  | 2.23                     | 0.74              |
| 6:UJ:94:HIS:CB    | 6:UJ:146:THR:HG21 | 2.17                     | 0.74              |
| 6:WV:197:LEU:HD12 | 6:WW:175:SER:OG   | 1.88                     | 0.74              |
| 2:h:258:ARG:HH12  | 2:j:140:ASN:ND2   | 1.86                     | 0.74              |
| 3:0:17:THR:HG23   | 3:5:68:ILE:HD11   | 1.69                     | 0.74              |
| 3:1:9:LYS:CE      | 5:AE:72:ASP:OD1   | 2.36                     | 0.74              |
| 4:ZW:69:THR:HG21  | 4:ZW:361:LEU:HD12 | 1.69                     | 0.74              |
| 4:ZX:382:TYR:CE1  | 4:Zc:395:ILE:HG23 | 2.23                     | 0.74              |
| 4:ZY:71:ARG:NH1   | 4:ZY:74:ASP:OD1   | 2.20                     | 0.74              |
| 5:AB:172:GLN:NE2  | 3:AG:52:PRO:HG3   | 1.99                     | 0.74              |
| 5:AE:228:GLU:C    | 3:AK:258:THR:CG2  | 2.60                     | 0.74              |
| 6:AS:295:SER:HB2  | 11:A0:65:LEU:HB2  | 1.69                     | 0.74              |
| 10:A3:94:ALA:O    | 10:A3:98:GLU:HG3  | 1.88                     | 0.74              |
| 10:A4:7:ILE:HB    | 6:BX:278:THR:HG21 | 1.70                     | 0.74              |
| 6:UI:94:HIS:CB    | 6:UI:146:THR:HG21 | 2.17                     | 0.74              |
| 6:UO:94:HIS:CB    | 6:UO:146:THR:HG21 | 2.17                     | 0.74              |
| 6:WD:149:PRO:HG2  | 6:WD:190:GLN:HE22 | 1.52                     | 0.74              |
| 6:WH:199:SER:HA   | 6:WH:205:LEU:HD23 | 1.68                     | 0.74              |
| 6:WI:200:SER:O    | 6:WJ:158:ALA:HB3  | 1.87                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WP:181:GLU:HB2  | 6:WP:184:ARG:CG    | 2.07                     | 0.74              |
| 2:g:258:ARG:HH12  | 2:i:140:ASN:ND2    | 1.86                     | 0.73              |
| 3:6:242:ILE:HD12  | 3:ZC:1:MET:HE1     | 1.70                     | 0.73              |
| 4:ZS:182:GLY:HA2  | 4:Zd:131:GLY:HA3   | 1.70                     | 0.73              |
| 5:AB:70:GLN:HG2   | 3:AM:6:TRP:CD1     | 2.22                     | 0.73              |
| 3:AI:45:LEU:HD23  | 12:BD:76:LEU:CD1   | 2.17                     | 0.73              |
| 6:UK:94:HIS:CB    | 6:UK:146:THR:HG21  | 2.17                     | 0.73              |
| 6:UM:73:MET:HE1   | 6:UM:99:ARG:CD     | 2.17                     | 0.73              |
| 6:UM:139:GLU:OE1  | 6:UM:142:ARG:NH2   | 2.20                     | 0.73              |
| 2:k:258:ARG:HH12  | 2:m:140:ASN:ND2    | 1.86                     | 0.73              |
| 2:n:258:ARG:HH12  | 2:p:140:ASN:ND2    | 1.86                     | 0.73              |
| 2:r:258:ARG:HH12  | 2:t:140:ASN:ND2    | 1.86                     | 0.73              |
| 4:ZP:270:ASN:HD22 | 4:ZV:192:ASN:HA    | 1.51                     | 0.73              |
| 4:ZQ:369:SER:HA   | 4:Zb:399:LEU:HD12  | 1.70                     | 0.73              |
| 9:Ax:160:GLN:HA   | 6:WE:166:VAL:CG2   | 2.18                     | 0.73              |
| 6:UM:94:HIS:CB    | 6:UM:146:THR:HG21  | 2.17                     | 0.73              |
| 6:UN:94:HIS:CB    | 6:UN:146:THR:HG21  | 2.17                     | 0.73              |
| 6:UP:94:HIS:CB    | 6:UP:146:THR:HG21  | 2.17                     | 0.73              |
| 6:WJ:199:SER:HA   | 6:WJ:205:LEU:HD23  | 1.68                     | 0.73              |
| 2:u:258:ARG:HH12  | 2:w:140:ASN:ND2    | 1.86                     | 0.73              |
| 3:2:257:LEU:HG    | 3:AF:230:LEU:HD12  | 1.68                     | 0.73              |
| 4:ZI:373:VAL:HG21 | 4:ZO:10:LEU:HD22   | 1.70                     | 0.73              |
| 4:ZW:130:GLN:OE1  | 4:ZW:130:GLN:N     | 2.21                     | 0.73              |
| 3:AG:28:ASN:HD21  | 3:AL:43:ASP:HB3    | 1.53                     | 0.73              |
| 6:WI:199:SER:HA   | 6:WI:205:LEU:HD23  | 1.69                     | 0.73              |
| 6:WN:197:LEU:HD12 | 6:WO:175:SER:CB    | 2.17                     | 0.73              |
| 12:BE:6:ILE:HD13  | 12:BE:122:VAL:HG21 | 1.70                     | 0.73              |
| 2:i:258:ARG:HH12  | 2:k:140:ASN:ND2    | 1.86                     | 0.73              |
| 2:v:258:ARG:HH12  | 2:x:140:ASN:ND2    | 1.86                     | 0.73              |
| 3:8:57:SER:OG     | 3:AG:154:ASP:OD2   | 2.05                     | 0.73              |
| 4:ZU:372:LEU:HD12 | 4:Zf:396:LEU:CD2   | 2.19                     | 0.73              |
| 5:AA:48:GLY:HA3   | 11:A6:93:PRO:HB3   | 1.68                     | 0.73              |
| 3:AJ:100:GLN:NE2  | 3:AJ:181:ASP:OD2   | 2.21                     | 0.73              |
| 8:At:23:VAL:HA    | 8:At:150:LEU:HD21  | 1.69                     | 0.73              |
| 8:At:145:TRP:NE1  | 6:WJ:164:LEU:CB    | 2.48                     | 0.73              |
| 8:At:145:TRP:HE1  | 6:WJ:164:LEU:CB    | 2.01                     | 0.73              |
| 6:UM:73:MET:CE    | 6:UM:99:ARG:CD     | 2.67                     | 0.73              |
| 6:UN:73:MET:HE1   | 6:UN:99:ARG:CD     | 2.17                     | 0.73              |
| 6:UO:73:MET:HE1   | 6:UO:99:ARG:CD     | 2.17                     | 0.73              |
| 6:UP:73:MET:HE1   | 6:UP:99:ARG:CD     | 2.17                     | 0.73              |
| 6:WD:197:LEU:HA   | 6:WE:175:SER:OG    | 1.89                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WO:181:GLU:HB2  | 6:WO:184:ARG:CG   | 2.07                     | 0.73              |
| 3:7:226:VAL:HG11  | 3:ZC:242:ILE:HD13 | 1.70                     | 0.73              |
| 5:AD:214:VAL:HG11 | 3:AJ:12:LEU:HB2   | 1.71                     | 0.73              |
| 7:As:29:LEU:CD1   | 8:At:216:ILE:HG13 | 2.18                     | 0.73              |
| 10:A2:61:LEU:HD13 | 11:A7:50:LYS:HZ1  | 1.53                     | 0.73              |
| 6:UK:73:MET:CE    | 6:UK:99:ARG:CD    | 2.66                     | 0.73              |
| 6:UL:73:MET:CE    | 6:UL:99:ARG:CD    | 2.66                     | 0.73              |
| 6:UP:73:MET:CE    | 6:UP:99:ARG:CD    | 2.66                     | 0.73              |
| 6:WB:197:LEU:HD12 | 6:WC:175:SER:CB   | 2.18                     | 0.73              |
| 6:WC:197:LEU:HD12 | 6:WD:175:SER:OG   | 1.88                     | 0.73              |
| 6:WR:200:SER:OG   | 6:WS:175:SER:HB2  | 1.88                     | 0.73              |
| 2:b:258:ARG:HH12  | 2:d:140:ASN:ND2   | 1.86                     | 0.73              |
| 2:c:258:ARG:HH12  | 2:e:140:ASN:ND2   | 1.86                     | 0.73              |
| 3:ZB:122:VAL:CG2  | 4:ZG:321:ALA:O    | 2.36                     | 0.73              |
| 3:ZE:54:ALA:HB1   | 3:AM:150:THR:CG2  | 2.15                     | 0.73              |
| 4:ZW:379:GLN:NE2  | 4:Zb:394:GLN:OE1  | 2.21                     | 0.73              |
| 5:AD:16:LEU:HD23  | 3:AI:253:MET:HE2  | 1.57                     | 0.73              |
| 6:UI:73:MET:HE1   | 6:UI:99:ARG:CD    | 2.17                     | 0.73              |
| 6:WC:197:LEU:HD12 | 6:WD:175:SER:CB   | 2.18                     | 0.73              |
| 2:f:258:ARG:HH12  | 2:h:140:ASN:ND2   | 1.86                     | 0.73              |
| 3:1:6:TRP:HB2     | 5:AE:70:GLN:HB3   | 1.68                     | 0.73              |
| 3:ZE:31:THR:CG2   | 4:ZJ:39:PHE:HB2   | 2.18                     | 0.73              |
| 5:AB:53:THR:HG22  | 12:BC:23:VAL:HG23 | 1.69                     | 0.73              |
| 5:AB:70:GLN:HB3   | 3:AM:6:TRP:NE1    | 2.04                     | 0.73              |
| 2:a:258:ARG:HH12  | 2:c:140:ASN:ND2   | 1.86                     | 0.73              |
| 2:o:258:ARG:HH12  | 2:q:140:ASN:ND2   | 1.86                     | 0.73              |
| 2:w:258:ARG:HH12  | 2:y:140:ASN:ND2   | 1.86                     | 0.73              |
| 2:x:346:MET:HE3   | 2:z:142:LEU:HD11  | 1.71                     | 0.73              |
| 3:1:257:LEU:C     | 5:AE:217:MET:HE3  | 2.12                     | 0.73              |
| 3:2:244:SER:OG    | 3:7:256:LYS:NZ    | 2.21                     | 0.73              |
| 9:Av:158:PRO:HD3  | 6:WU:167:ARG:HH12 | 1.53                     | 0.73              |
| 6:WT:200:SER:OG   | 6:WU:175:SER:HB2  | 1.88                     | 0.73              |
| 2:t:258:ARG:HH12  | 2:v:140:ASN:ND2   | 1.86                     | 0.73              |
| 6:Aj:372:ILE:CB   | 10:A1:11:ILE:HG21 | 2.18                     | 0.73              |
| 9:Aw:152:ARG:CD   | 6:WB:166:VAL:O    | 2.37                     | 0.73              |
| 2:a:142:LEU:HD11  | 2:y:346:MET:HE3   | 1.71                     | 0.73              |
| 4:ZH:236:GLY:CA   | 4:ZN:190:GLN:HE22 | 2.01                     | 0.73              |
| 4:ZT:99:GLN:NE2   | 4:ZY:38:SER:OG    | 2.21                     | 0.73              |
| 5:AA:55:THR:OG1   | 12:BB:45:LYS:NZ   | 2.21                     | 0.73              |
| 5:AD:4:ALA:HB2    | 12:BE:22:ASN:OD1  | 1.88                     | 0.73              |
| 7:Ab:8:MET:CE     | 6:WS:124:SER:CB   | 2.67                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:d:258:ARG:HH12  | 2:f:140:ASN:ND2   | 1.86                     | 0.72              |
| 2:q:51:GLN:CG     | 3:AI:209:ASN:ND2  | 2.52                     | 0.72              |
| 3:8:56:SER:O      | 3:AG:152:GLY:HA3  | 1.89                     | 0.72              |
| 4:ZZ:269:GLN:CG   | 4:Zf:286:PRO:HG3  | 2.19                     | 0.72              |
| 5:AA:58:THR:HG22  | 3:AF:50:ARG:HH22  | 1.54                     | 0.72              |
| 5:AB:5:ILE:HD11   | 12:BB:106:MET:CE  | 2.18                     | 0.72              |
| 5:AB:217:MET:HE2  | 3:AG:245:LYS:HG2  | 1.72                     | 0.72              |
| 3:AK:260:LEU:HB3  | 12:BF:106:MET:CE  | 2.18                     | 0.72              |
| 6:UO:73:MET:CE    | 6:UO:99:ARG:CD    | 2.66                     | 0.72              |
| 12:BC:79:GLU:HG2  | 12:BC:82:ASN:HB2  | 1.70                     | 0.72              |
| 2:s:258:ARG:HH12  | 2:u:140:ASN:ND2   | 1.86                     | 0.72              |
| 2:w:346:MET:HE3   | 2:y:142:LEU:HD11  | 1.71                     | 0.72              |
| 4:ZM:319:ASN:ND2  | 4:ZM:352:ASN:OD1  | 2.18                     | 0.72              |
| 5:AA:241:GLU:OE2  | 11:A6:106:ARG:NH1 | 2.23                     | 0.72              |
| 5:AB:26:LEU:CD2   | 3:AG:242:ILE:HG21 | 2.12                     | 0.72              |
| 5:AC:240:ASN:HD21 | 12:BD:109:SER:HA  | 1.53                     | 0.72              |
| 6:UK:139:GLU:OE1  | 6:UK:142:ARG:NH2  | 2.20                     | 0.72              |
| 2:b:140:ASN:ND2   | 2:z:258:ARG:HH12  | 1.86                     | 0.72              |
| 2:b:142:LEU:HD11  | 2:z:346:MET:HE3   | 1.71                     | 0.72              |
| 3:1:238:ARG:NE    | 3:7:251:ASP:OD1   | 2.20                     | 0.72              |
| 4:ZS:77:ILE:HG22  | 4:ZS:356:LEU:HD22 | 1.71                     | 0.72              |
| 5:AA:26:LEU:HD13  | 3:AF:242:ILE:HG23 | 1.70                     | 0.72              |
| 5:AB:28:ASN:OD1   | 3:AG:72:VAL:CB    | 2.38                     | 0.72              |
| 6:Aj:372:ILE:HD13 | 10:A1:11:ILE:CG2  | 2.16                     | 0.72              |
| 6:UI:73:MET:CE    | 6:UI:99:ARG:CD    | 2.66                     | 0.72              |
| 6:UJ:139:GLU:OE1  | 6:UJ:142:ARG:NH2  | 2.20                     | 0.72              |
| 6:UL:139:GLU:OE1  | 6:UL:142:ARG:NH2  | 2.20                     | 0.72              |
| 4:ZL:331:ASP:HA   | 4:ZQ:40:ALA:HB1   | 1.72                     | 0.72              |
| 4:ZQ:22:ASN:ND2   | 4:ZV:49:GLY:O     | 2.23                     | 0.72              |
| 4:ZQ:181:LYS:NZ   | 4:Zb:129:GLN:HE21 | 1.86                     | 0.72              |
| 4:Zd:118:GLY:HA2  | 4:Zd:316:VAL:HG12 | 1.71                     | 0.72              |
| 5:AA:73:TYR:CZ    | 3:AL:74:PRO:HD2   | 2.24                     | 0.72              |
| 5:AB:70:GLN:HE21  | 3:AM:1:MET:H2     | 1.35                     | 0.72              |
| 3:AF:62:LEU:CG    | 12:BB:84:LEU:HD11 | 2.20                     | 0.72              |
| 6:Aj:372:ILE:CB   | 10:A1:11:ILE:CG2  | 2.67                     | 0.72              |
| 2:j:258:ARG:HH12  | 2:l:140:ASN:ND2   | 1.86                     | 0.72              |
| 2:x:258:ARG:HH12  | 2:z:140:ASN:ND2   | 1.86                     | 0.72              |
| 3:1:193:ILE:HG22  | 5:AE:152:PRO:HG3  | 1.48                     | 0.72              |
| 3:4:74:PRO:HB2    | 3:9:66:LEU:HD21   | 1.70                     | 0.72              |
| 3:ZC:31:THR:HG22  | 4:ZH:39:PHE:CB    | 2.19                     | 0.72              |
| 4:ZY:269:GLN:HG2  | 4:Ze:286:PRO:CG   | 2.19                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AA:9:MET:HB2    | 12:BA:103:VAL:HG21 | 1.71                     | 0.72              |
| 5:AD:27:ALA:O     | 3:AI:72:VAL:HG11   | 1.90                     | 0.72              |
| 5:AD:107:VAL:O    | 3:AI:180:ASN:ND2   | 2.21                     | 0.72              |
| 3:AG:257:LEU:CD1  | 12:BB:102:MET:SD   | 2.77                     | 0.72              |
| 3:AL:98:LYS:HD2   | 3:AL:213:LEU:HD12  | 1.69                     | 0.72              |
| 2:a:80:GLN:OE1    | 3:8:58:GLU:HG3     | 1.89                     | 0.72              |
| 3:8:42:GLU:HB2    | 3:8:75:VAL:HG23    | 1.72                     | 0.72              |
| 5:AA:229:MET:CG   | 3:AG:258:THR:HG22  | 2.15                     | 0.72              |
| 6:Ae:372:ILE:CG2  | 10:A2:4:ILE:HG13   | 2.20                     | 0.72              |
| 6:WM:197:LEU:HA   | 6:WN:175:SER:OG    | 1.89                     | 0.72              |
| 2:e:258:ARG:HH12  | 2:g:140:ASN:ND2    | 1.86                     | 0.72              |
| 2:e:346:MET:HE3   | 2:g:142:LEU:HD11   | 1.71                     | 0.72              |
| 2:i:208:ARG:NH2   | 2:i:238:ASP:OD2    | 2.23                     | 0.72              |
| 2:v:346:MET:HE3   | 2:x:142:LEU:HD11   | 1.71                     | 0.72              |
| 5:AB:49:LEU:CB    | 11:A7:90:PRO:HG2   | 2.19                     | 0.72              |
| 5:AE:173:ARG:NH1  | 3:AJ:46:TYR:OH     | 2.23                     | 0.72              |
| 6:WE:128:GLU:HB3  | 6:WF:126:PHE:CE2   | 2.25                     | 0.72              |
| 6:WV:197:LEU:HD12 | 6:WW:175:SER:HB3   | 1.71                     | 0.72              |
| 2:a:140:ASN:ND2   | 2:y:258:ARG:HH12   | 1.86                     | 0.72              |
| 2:h:208:ARG:NH2   | 2:h:238:ASP:OD2    | 2.23                     | 0.72              |
| 3:ZB:122:VAL:O    | 4:ZG:322:ASN:HB2   | 1.90                     | 0.72              |
| 2:a:346:MET:HE3   | 2:c:142:LEU:HD11   | 1.71                     | 0.72              |
| 2:d:346:MET:HE3   | 2:f:142:LEU:HD11   | 1.71                     | 0.72              |
| 2:g:208:ARG:NH2   | 2:g:238:ASP:OD2    | 2.23                     | 0.72              |
| 2:j:208:ARG:NH2   | 2:j:238:ASP:OD2    | 2.23                     | 0.72              |
| 3:1:6:TRP:CB      | 5:AE:70:GLN:CB     | 2.68                     | 0.72              |
| 3:7:241:GLU:HG2   | 3:ZC:256:LYS:HG3   | 1.72                     | 0.72              |
| 3:8:215:TYR:OH    | 3:ZE:189:GLU:OE2   | 2.07                     | 0.72              |
| 4:Zc:379:GLN:HE22 | 4:Zh:394:GLN:HE21  | 1.36                     | 0.72              |
| 5:AA:70:GLN:CG    | 3:AL:3:SER:CA      | 2.36                     | 0.72              |
| 11:A7:46:ALA:O    | 11:A7:50:LYS:HG3   | 1.90                     | 0.72              |
| 6:UN:73:MET:CE    | 6:UN:99:ARG:CD     | 2.66                     | 0.72              |
| 2:f:208:ARG:NH2   | 2:f:238:ASP:OD2    | 2.23                     | 0.72              |
| 2:f:346:MET:HE3   | 2:h:142:LEU:HD11   | 1.71                     | 0.72              |
| 2:k:208:ARG:NH2   | 2:k:238:ASP:OD2    | 2.23                     | 0.72              |
| 4:ZM:270:ASN:HD22 | 4:ZS:192:ASN:HA    | 1.54                     | 0.72              |
| 4:ZR:160:SER:HA   | 4:ZR:268:GLN:HE21  | 1.55                     | 0.72              |
| 5:AC:55:THR:OG1   | 12:BD:45:LYS:NZ    | 2.22                     | 0.72              |
| 9:Av:152:ARG:NH1  | 6:WV:164:LEU:HB3   | 2.05                     | 0.72              |
| 9:Ay:152:ARG:NH2  | 6:WJ:164:LEU:C     | 2.45                     | 0.72              |
| 6:WH:193:ALA:HB1  | 6:WI:213:VAL:CG1   | 2.18                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:r:346:MET:HE3   | 2:t:142:LEU:HD11   | 1.71                     | 0.71              |
| 4:ZS:77:ILE:HD11  | 4:ZS:96:ARG:HD3    | 1.70                     | 0.71              |
| 4:Za:234:GLU:HG3  | 4:Zg:253:GLY:O     | 1.90                     | 0.71              |
| 5:AB:72:ASP:HB2   | 3:AM:9:LYS:NZ      | 2.04                     | 0.71              |
| 3:AG:260:LEU:HD23 | 12:BB:106:MET:SD   | 2.30                     | 0.71              |
| 11:A8:42:ASP:OD2  | 11:A8:43:ILE:N     | 2.22                     | 0.71              |
| 6:WM:200:SER:O    | 6:WN:158:ALA:CB    | 2.37                     | 0.71              |
| 1:I:166:GLU:CB    | 1:J:35:THR:HG21    | 2.20                     | 0.71              |
| 2:e:208:ARG:NH2   | 2:e:238:ASP:OD2    | 2.23                     | 0.71              |
| 2:q:346:MET:HE3   | 2:s:142:LEU:HD11   | 1.71                     | 0.71              |
| 4:ZG:45:GLY:O     | 4:ZG:46:SER:HB3    | 1.90                     | 0.71              |
| 4:ZY:269:GLN:HG2  | 4:Ze:286:PRO:HG2   | 1.71                     | 0.71              |
| 3:AF:189:GLU:HB2  | 3:AK:42:GLU:OE2    | 1.90                     | 0.71              |
| 3:AH:50:ARG:HH11  | 6:BM:328:ILE:HG21  | 1.54                     | 0.71              |
| 6:UI:62:ASP:OD2   | 6:WA:184:ARG:NH2   | 2.24                     | 0.71              |
| 6:UJ:73:MET:CE    | 6:UJ:99:ARG:CD     | 2.67                     | 0.71              |
| 6:UJ:98:LEU:CD1   | 6:UJ:146:THR:OG1   | 2.38                     | 0.71              |
| 6:UN:98:LEU:CD1   | 6:UN:146:THR:OG1   | 2.39                     | 0.71              |
| 12:BB:6:ILE:HG21  | 12:BB:122:VAL:HG21 | 1.72                     | 0.71              |
| 3:l:83:GLN:NE2    | 3:ZC:45:LEU:HD12   | 2.04                     | 0.71              |
| 4:ZF:65:THR:HG23  | 4:ZQ:50:LEU:HD21   | 1.72                     | 0.71              |
| 5:AC:59:ALA:CB    | 3:AH:66:LEU:HD21   | 2.20                     | 0.71              |
| 3:AH:250:THR:HA   | 3:AH:253:MET:HE2   | 1.72                     | 0.71              |
| 6:AT:294:ARG:HG3  | 11:A0:72:HIS:CE1   | 2.25                     | 0.71              |
| 6:UL:98:LEU:CD1   | 6:UL:146:THR:OG1   | 2.38                     | 0.71              |
| 6:WD:190:GLN:HG3  | 6:WE:217:GLY:HA3   | 1.72                     | 0.71              |
| 2:l:208:ARG:NH2   | 2:l:238:ASP:OD2    | 2.23                     | 0.71              |
| 2:w:208:ARG:NH2   | 2:w:238:ASP:OD2    | 2.23                     | 0.71              |
| 3:3:189:GLU:HA    | 3:8:42:GLU:CD      | 2.15                     | 0.71              |
| 3:ZE:28:ASN:OD1   | 4:ZJ:52:VAL:CB     | 2.37                     | 0.71              |
| 4:ZG:45:GLY:O     | 4:ZG:46:SER:CB     | 2.38                     | 0.71              |
| 4:ZY:285:LYS:O    | 4:ZY:306:ASN:ND2   | 2.20                     | 0.71              |
| 5:AB:60:SER:HB2   | 3:AG:65:GLY:O      | 1.88                     | 0.71              |
| 5:AE:229:MET:HE2  | 3:AK:257:LEU:HD23  | 1.71                     | 0.71              |
| 10:A2:11:ILE:C    | 10:A2:11:ILE:CD1   | 2.57                     | 0.71              |
| 6:UI:98:LEU:CD1   | 6:UI:146:THR:OG1   | 2.39                     | 0.71              |
| 2:m:208:ARG:NH2   | 2:m:238:ASP:OD2    | 2.23                     | 0.71              |
| 2:v:208:ARG:NH2   | 2:v:238:ASP:OD2    | 2.23                     | 0.71              |
| 2:x:208:ARG:NH2   | 2:x:238:ASP:OD2    | 2.23                     | 0.71              |
| 2:y:208:ARG:NH2   | 2:y:238:ASP:OD2    | 2.23                     | 0.71              |
| 3:l:51:GLN:NE2    | 3:AK:75:VAL:O      | 2.22                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:8:208:LEU:O    | 3:8:210:GLY:N     | 2.23                     | 0.71              |
| 4:ZG:390:LYS:HB2 | 4:ZL:402:LEU:HD22 | 1.72                     | 0.71              |
| 5:AB:109:PRO:HG2 | 3:AG:197:SER:HA   | 1.72                     | 0.71              |
| 5:AB:228:GLU:OE1 | 3:AH:258:THR:OG1  | 2.04                     | 0.71              |
| 7:Ab:52:ILE:HD11 | 9:Au:206:ALA:HB1  | 1.70                     | 0.71              |
| 6:WK:143:THR:HG1 | 6:WL:156:HIS:CE1  | 2.04                     | 0.71              |
| 1:J:166:GLU:CB   | 1:K:35:THR:HG21   | 2.20                     | 0.71              |
| 2:d:208:ARG:NH2  | 2:d:238:ASP:OD2   | 2.23                     | 0.71              |
| 2:g:346:MET:HE3  | 2:i:142:LEU:HD11  | 1.71                     | 0.71              |
| 2:s:346:MET:HE3  | 2:u:142:LEU:HD11  | 1.71                     | 0.71              |
| 2:z:208:ARG:NH2  | 2:z:238:ASP:OD2   | 2.23                     | 0.71              |
| 7:Ab:8:MET:HE2   | 6:WS:124:SER:HA   | 1.70                     | 0.71              |
| 2:c:346:MET:HE3  | 2:e:142:LEU:HD11  | 1.71                     | 0.71              |
| 2:n:208:ARG:NH2  | 2:n:238:ASP:OD2   | 2.23                     | 0.71              |
| 2:u:208:ARG:NH2  | 2:u:238:ASP:OD2   | 2.23                     | 0.71              |
| 2:u:346:MET:HE3  | 2:w:142:LEU:HD11  | 1.71                     | 0.71              |
| 3:7:167:PRO:CG   | 4:ZI:338:GLN:OE1  | 2.39                     | 0.71              |
| 4:ZX:289:LEU:O   | 4:Zc:352:ASN:ND2  | 2.22                     | 0.71              |
| 5:AA:26:LEU:CD2  | 3:AF:242:ILE:HG21 | 2.21                     | 0.71              |
| 3:AM:4:SER:HB2   | 3:AM:250:THR:HG21 | 1.72                     | 0.71              |
| 10:A5:11:ILE:CG2 | 6:BR:372:ILE:HG21 | 2.21                     | 0.71              |
| 6:UP:98:LEU:CD1  | 6:UP:146:THR:OG1  | 2.38                     | 0.71              |
| 2:t:208:ARG:NH2  | 2:t:238:ASP:OD2   | 2.23                     | 0.71              |
| 3:6:76:ALA:HB1   | 3:ZB:64:SER:O     | 1.91                     | 0.71              |
| 3:7:79:ARG:NH2   | 3:7:184:LEU:O     | 2.23                     | 0.71              |
| 3:9:226:VAL:HG11 | 3:ZE:242:ILE:HD13 | 1.72                     | 0.71              |
| 3:ZC:240:TYR:CE2 | 4:ZH:395:ILE:CG2  | 2.73                     | 0.71              |
| 4:ZQ:380:ARG:HD2 | 4:ZW:396:LEU:HB3  | 1.71                     | 0.71              |
| 4:ZV:65:THR:HG21 | 4:Zg:4:SER:OG     | 1.90                     | 0.71              |
| 4:Zb:18:ASP:CG   | 4:Zg:5:GLN:HE22   | 1.98                     | 0.71              |
| 5:AB:26:LEU:HD13 | 3:AG:242:ILE:CG2  | 2.21                     | 0.71              |
| 5:AB:70:GLN:CG   | 3:AM:6:TRP:NE1    | 2.53                     | 0.71              |
| 3:AF:44:LEU:CD2  | 12:BA:78:TYR:CD1  | 2.74                     | 0.71              |
| 10:A5:7:ILE:HG22 | 6:BR:278:THR:HG21 | 1.73                     | 0.71              |
| 6:UO:98:LEU:CD1  | 6:UO:146:THR:OG1  | 2.38                     | 0.71              |
| 2:a:208:ARG:NH2  | 2:a:238:ASP:OD2   | 2.23                     | 0.71              |
| 2:c:208:ARG:NH2  | 2:c:238:ASP:OD2   | 2.23                     | 0.71              |
| 2:o:208:ARG:NH2  | 2:o:238:ASP:OD2   | 2.23                     | 0.71              |
| 2:p:208:ARG:NH2  | 2:p:238:ASP:OD2   | 2.23                     | 0.71              |
| 3:3:241:GLU:HG2  | 3:8:256:LYS:HG3   | 1.71                     | 0.71              |
| 3:ZD:76:ALA:HA   | 4:ZI:47:LYS:HE3   | 1.70                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Za:373:VAL:HG21 | 4:Zg:10:LEU:CD2   | 2.20                     | 0.71              |
| 5:AC:4:ALA:HB2    | 12:BD:22:ASN:OD1  | 1.91                     | 0.71              |
| 7:Aq:2:THR:CG2    | 6:WW:125:GLN:CD   | 2.64                     | 0.71              |
| 7:As:54:LYS:NZ    | 8:At:215:VAL:HA   | 2.06                     | 0.71              |
| 6:UO:126:PHE:CD1  | 6:UO:130:VAL:HG21 | 2.26                     | 0.71              |
| 2:b:346:MET:HE3   | 2:d:142:LEU:HD11  | 1.71                     | 0.71              |
| 3:3:56:SER:O      | 5:AB:138:ALA:HB1  | 1.91                     | 0.71              |
| 3:ZC:162:GLN:HG2  | 4:ZH:351:GLY:HA2  | 1.73                     | 0.71              |
| 5:AC:28:ASN:HD21  | 3:AH:43:ASP:HB3   | 1.53                     | 0.71              |
| 5:AE:180:ARG:HG3  | 5:AE:180:ARG:HH11 | 1.56                     | 0.71              |
| 3:AH:44:LEU:HD21  | 12:BC:78:TYR:HB2  | 1.69                     | 0.71              |
| 3:AH:208:LEU:H    | 3:AH:208:LEU:HD13 | 1.56                     | 0.71              |
| 7:Ab:8:MET:HE1    | 6:WS:123:ILE:C    | 2.16                     | 0.71              |
| 7:Ab:37:ILE:HD13  | 7:Aq:44:ILE:CD1   | 2.20                     | 0.71              |
| 6:UI:126:PHE:CD1  | 6:UI:130:VAL:HG21 | 2.26                     | 0.71              |
| 1:K:166:GLU:CB    | 1:L:35:THR:HG21   | 2.20                     | 0.70              |
| 1:R:166:GLU:CB    | 1:S:35:THR:HG21   | 2.20                     | 0.70              |
| 2:c:110:MET:O     | 2:d:84:VAL:HG23   | 1.92                     | 0.70              |
| 2:d:110:MET:O     | 2:e:84:VAL:HG23   | 1.92                     | 0.70              |
| 2:p:346:MET:HE3   | 2:r:142:LEU:HD11  | 1.71                     | 0.70              |
| 2:q:208:ARG:NH2   | 2:q:238:ASP:OD2   | 2.23                     | 0.70              |
| 2:r:208:ARG:NH2   | 2:r:238:ASP:OD2   | 2.23                     | 0.70              |
| 2:s:208:ARG:NH2   | 2:s:238:ASP:OD2   | 2.23                     | 0.70              |
| 3:2:230:LEU:HD12  | 3:ZD:257:LEU:HD23 | 1.72                     | 0.70              |
| 4:ZH:165:PRO:HG2  | 4:ZH:201:VAL:HG13 | 1.71                     | 0.70              |
| 4:ZI:24:ILE:HG22  | 4:ZN:385:ASN:OD1  | 1.91                     | 0.70              |
| 6:AS:294:ARG:HD2  | 11:A0:68:THR:HG21 | 1.71                     | 0.70              |
| 7:Aq:39:GLN:HE21  | 7:Aq:49:LEU:HD12  | 1.56                     | 0.70              |
| 6:UM:98:LEU:CD1   | 6:UM:146:THR:OG1  | 2.39                     | 0.70              |
| 12:BD:47:VAL:O    | 6:BN:313:PRO:HD2  | 1.91                     | 0.70              |
| 1:S:166:GLU:CB    | 1:T:35:THR:HG21   | 2.20                     | 0.70              |
| 1:T:166:GLU:CB    | 1:U:35:THR:HG21   | 2.20                     | 0.70              |
| 1:U:166:GLU:CB    | 1:V:35:THR:HG21   | 2.20                     | 0.70              |
| 2:b:208:ARG:NH2   | 2:b:238:ASP:OD2   | 2.23                     | 0.70              |
| 2:e:110:MET:O     | 2:f:84:VAL:HG23   | 1.92                     | 0.70              |
| 3:ZC:145:ASN:HA   | 4:ZH:352:ASN:HD22 | 1.55                     | 0.70              |
| 4:ZK:18:ASP:HB3   | 4:ZP:5:GLN:HE22   | 1.56                     | 0.70              |
| 5:AA:227:PHE:CE2  | 3:AF:253:MET:O    | 2.44                     | 0.70              |
| 5:AB:221:ILE:HG21 | 3:AH:251:ASP:CG   | 2.16                     | 0.70              |
| 5:AE:243:ARG:NH1  | 3:AF:259:GLN:OE1  | 2.23                     | 0.70              |
| 6:AS:297:GLN:HB2  | 11:A0:65:LEU:HD21 | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:At:149:LEU:CD1  | 6:WK:165:PHE:HA   | 2.21                     | 0.70              |
| 6:UJ:126:PHE:CD1  | 6:UJ:130:VAL:HG21 | 2.26                     | 0.70              |
| 6:UP:126:PHE:CD1  | 6:UP:130:VAL:HG21 | 2.26                     | 0.70              |
| 6:WE:197:LEU:HD12 | 6:WF:175:SER:CB   | 2.21                     | 0.70              |
| 12:BD:57:GLN:C    | 12:BD:59:THR:H    | 1.98                     | 0.70              |
| 1:V:166:GLU:CB    | 1:W:35:THR:HG21   | 2.20                     | 0.70              |
| 1:W:166:GLU:CB    | 1:X:35:THR:HG21   | 2.20                     | 0.70              |
| 1:Y:166:GLU:CB    | 1:Z:35:THR:HG21   | 2.20                     | 0.70              |
| 2:f:110:MET:O     | 2:g:84:VAL:HG23   | 1.91                     | 0.70              |
| 2:t:346:MET:HE3   | 2:v:142:LEU:HD11  | 1.71                     | 0.70              |
| 4:ZL:390:LYS:HB2  | 4:ZQ:402:LEU:HD22 | 1.74                     | 0.70              |
| 6:Ae:374:HIS:HB2  | 10:A2:4:ILE:CD1   | 2.20                     | 0.70              |
| 6:Ag:295:SER:HB3  | 11:A8:72:HIS:HB3  | 1.72                     | 0.70              |
| 6:UL:126:PHE:O    | 6:UL:130:VAL:CG2  | 2.40                     | 0.70              |
| 6:WS:121:PHE:CE1  | 6:WT:120:LYS:NZ   | 2.55                     | 0.70              |
| 1:Q:166:GLU:CB    | 1:R:35:THR:HG21   | 2.20                     | 0.70              |
| 2:a:110:MET:O     | 2:b:84:VAL:HG23   | 1.92                     | 0.70              |
| 2:b:110:MET:O     | 2:c:84:VAL:HG23   | 1.92                     | 0.70              |
| 3:4:55:GLN:O      | 5:AC:138:ALA:CB   | 2.31                     | 0.70              |
| 5:AD:16:LEU:HD21  | 3:AI:253:MET:CE   | 2.20                     | 0.70              |
| 9:Ax:160:GLN:H    | 6:WE:166:VAL:HG22 | 1.53                     | 0.70              |
| 6:UL:103:GLN:HG2  | 6:WH:182:PRO:HB3  | 1.71                     | 0.70              |
| 6:UL:126:PHE:CD1  | 6:UL:130:VAL:HG21 | 2.26                     | 0.70              |
| 6:WK:200:SER:HA   | 6:WL:173:SER:OG   | 1.91                     | 0.70              |
| 6:WR:200:SER:O    | 6:WS:158:ALA:HB3  | 1.91                     | 0.70              |
| 2:g:110:MET:O     | 2:h:84:VAL:HG23   | 1.91                     | 0.70              |
| 2:l:346:MET:HE3   | 2:n:142:LEU:HD11  | 1.71                     | 0.70              |
| 2:x:110:MET:O     | 2:y:84:VAL:HG23   | 1.91                     | 0.70              |
| 4:Zc:159:ASN:ND2  | 4:Zc:161:THR:OG1  | 2.25                     | 0.70              |
| 5:AE:245:ASN:ND2  | 12:BE:113:GLN:OE1 | 2.16                     | 0.70              |
| 6:UK:126:PHE:O    | 6:UK:130:VAL:CG2  | 2.40                     | 0.70              |
| 6:UM:126:PHE:CD1  | 6:UM:130:VAL:HG21 | 2.26                     | 0.70              |
| 1:L:166:GLU:CB    | 1:M:35:THR:HG21   | 2.20                     | 0.70              |
| 1:P:166:GLU:CB    | 1:Q:35:THR:HG21   | 2.20                     | 0.70              |
| 1:X:166:GLU:CB    | 1:Y:35:THR:HG21   | 2.20                     | 0.70              |
| 2:a:84:VAL:HG23   | 2:z:110:MET:O     | 1.92                     | 0.70              |
| 2:k:346:MET:HE3   | 2:m:142:LEU:HD11  | 1.71                     | 0.70              |
| 3:0:47:GLN:NE2    | 5:AD:67:THR:CG2   | 2.55                     | 0.70              |
| 3:6:137:GLN:HA    | 3:6:138:PRO:C     | 2.17                     | 0.70              |
| 3:9:70:THR:HG22   | 3:9:71:GLY:H      | 1.57                     | 0.70              |
| 4:ZP:324:GLU:OE1  | 4:ZP:324:GLU:N    | 2.23                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:Av:45:LEU:CD1   | 10:A2:86:ILE:HG12  | 2.22                     | 0.70              |
| 9:Ay:240:ALA:CB   | 6:WG:165:PHE:HE1   | 2.00                     | 0.70              |
| 6:UK:98:LEU:CD1   | 6:UK:146:THR:OG1   | 2.38                     | 0.70              |
| 6:UN:126:PHE:CD1  | 6:UN:130:VAL:HG21  | 2.26                     | 0.70              |
| 6:WA:200:SER:O    | 6:WB:158:ALA:CB    | 2.40                     | 0.70              |
| 1:O:166:GLU:CB    | 1:P:35:THR:HG21    | 2.20                     | 0.70              |
| 3:2:83:GLN:HG2    | 3:ZD:45:LEU:HD22   | 1.72                     | 0.70              |
| 4:ZH:157:ASN:HD21 | 4:ZN:143:LEU:HD13  | 1.53                     | 0.70              |
| 4:ZH:379:GLN:HE21 | 4:ZM:391:THR:HG23  | 1.57                     | 0.70              |
| 4:ZU:99:GLN:NE2   | 4:ZZ:38:SER:OG     | 2.24                     | 0.70              |
| 3:AF:189:GLU:HB2  | 3:AK:42:GLU:CD     | 2.16                     | 0.70              |
| 6:An:278:THR:HG21 | 10:Az:14:LEU:HB3   | 1.72                     | 0.70              |
| 6:AP:278:THR:HG21 | 10:A5:21:ALA:HB3   | 1.73                     | 0.70              |
| 8:At:252:ALA:CB   | 6:WK:163:SER:O     | 2.40                     | 0.70              |
| 6:UJ:126:PHE:O    | 6:UJ:130:VAL:CG2   | 2.39                     | 0.70              |
| 6:WM:139:GLU:HB3  | 6:WN:154:ARG:NH2   | 2.06                     | 0.70              |
| 1:N:166:GLU:CB    | 1:O:35:THR:HG21    | 2.20                     | 0.70              |
| 2:o:346:MET:HE3   | 2:q:142:LEU:HD11   | 1.71                     | 0.70              |
| 3:O:195:THR:HG23  | 5:AD:152:PRO:HB2   | 1.72                     | 0.70              |
| 3:3:17:THR:HG23   | 3:8:68:ILE:HD11    | 1.74                     | 0.70              |
| 3:5:187:ILE:O     | 3:AN:98:LYS:NZ     | 2.18                     | 0.70              |
| 4:ZZ:157:ASN:HB3  | 4:ZZ:271:THR:HG21  | 1.72                     | 0.70              |
| 5:AB:26:LEU:HD13  | 3:AG:242:ILE:HG22  | 1.72                     | 0.70              |
| 9:Aw:132:GLN:HA   | 9:Aw:135:ARG:HD2   | 1.73                     | 0.70              |
| 6:UI:167:ARG:HH22 | 6:WW:188:GLU:HB3   | 1.57                     | 0.70              |
| 6:UM:126:PHE:O    | 6:UM:130:VAL:CG2   | 2.39                     | 0.70              |
| 2:h:346:MET:HE3   | 2:j:142:LEU:HD11   | 1.71                     | 0.70              |
| 2:i:346:MET:HE3   | 2:k:142:LEU:HD11   | 1.71                     | 0.70              |
| 2:n:346:MET:HE3   | 2:p:142:LEU:HD11   | 1.71                     | 0.70              |
| 2:y:110:MET:O     | 2:z:84:VAL:HG23    | 1.92                     | 0.70              |
| 3:O:242:ILE:HD12  | 3:AJ:230:LEU:HD11  | 1.72                     | 0.70              |
| 3:ZE:85:ASN:CG    | 4:ZP:50:LEU:CD2    | 2.65                     | 0.70              |
| 4:ZZ:369:SER:HB3  | 4:Zf:382:TYR:OH    | 1.92                     | 0.70              |
| 5:AE:9:MET:HB2    | 12:BE:103:VAL:HG21 | 1.73                     | 0.70              |
| 6:Am:294:ARG:HG2  | 11:A7:71:HIS:HB2   | 1.74                     | 0.70              |
| 9:Aw:190:PHE:CD1  | 9:Ax:220:PRO:HG3   | 2.26                     | 0.70              |
| 10:Az:77:LYS:HG3  | 11:A6:5:LEU:HD21   | 1.73                     | 0.70              |
| 6:WA:128:GLU:HG3  | 6:WB:126:PHE:HE2   | 1.54                     | 0.70              |
| 6:WB:200:SER:O    | 6:WC:158:ALA:HB2   | 1.91                     | 0.70              |
| 2:h:110:MET:O     | 2:i:84:VAL:HG23    | 1.92                     | 0.70              |
| 4:ZJ:349:GLY:O    | 4:ZP:89:ASN:ND2    | 2.25                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AD:109:PRO:HG3  | 3:AI:197:SER:C    | 2.17                     | 0.70              |
| 6:AW:299:ASN:HD22 | 11:A9:55:ARG:NH2  | 1.90                     | 0.70              |
| 8:At:145:TRP:CD1  | 6:WJ:164:LEU:CB   | 2.75                     | 0.70              |
| 8:At:156:THR:HG22 | 6:WK:167:ARG:CG   | 2.18                     | 0.70              |
| 6:UI:126:PHE:O    | 6:UI:130:VAL:CG2  | 2.40                     | 0.70              |
| 6:UL:62:ASP:OD2   | 6:WG:184:ARG:NH2  | 2.25                     | 0.70              |
| 2:j:346:MET:HE3   | 2:l:142:LEU:HD11  | 1.71                     | 0.69              |
| 2:m:346:MET:HE3   | 2:o:142:LEU:HD11  | 1.71                     | 0.69              |
| 2:s:110:MET:O     | 2:t:84:VAL:HG23   | 1.91                     | 0.69              |
| 3:6:17:THR:HG23   | 3:ZB:68:ILE:HD11  | 1.72                     | 0.69              |
| 3:ZA:42:GLU:HG2   | 3:ZA:75:VAL:HG23  | 1.73                     | 0.69              |
| 4:ZV:102:LEU:HD21 | 4:ZV:106:ARG:HD3  | 1.74                     | 0.69              |
| 5:AA:49:LEU:HD21  | 11:A6:90:PRO:HD2  | 1.72                     | 0.69              |
| 7:Aq:2:THR:HG21   | 6:WW:125:GLN:OE1  | 1.89                     | 0.69              |
| 1:M:166:GLU:CB    | 1:N:35:THR:HG21   | 2.20                     | 0.69              |
| 2:o:110:MET:O     | 2:p:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:p:110:MET:O     | 2:q:84:VAL:HG23   | 1.92                     | 0.69              |
| 3:6:56:SER:HA     | 5:AE:138:ALA:HB1  | 0.71                     | 0.69              |
| 4:ZJ:370:LYS:HE2  | 4:ZP:11:ASN:HD21  | 1.53                     | 0.69              |
| 4:Zg:110:ASN:HB2  | 4:Zg:114:MET:HB2  | 1.73                     | 0.69              |
| 5:AD:229:MET:HG2  | 12:BE:102:MET:SD  | 2.33                     | 0.69              |
| 5:AD:237:VAL:HG22 | 12:BE:21:LEU:HD21 | 1.74                     | 0.69              |
| 5:AE:109:PRO:HG3  | 3:AJ:197:SER:CA   | 2.16                     | 0.69              |
| 6:UM:139:GLU:CD   | 6:UM:142:ARG:HH21 | 2.00                     | 0.69              |
| 6:UO:126:PHE:O    | 6:UO:130:VAL:CG2  | 2.40                     | 0.69              |
| 6:WN:196:HIS:CB   | 6:WO:211:THR:HG21 | 2.19                     | 0.69              |
| 2:q:110:MET:O     | 2:r:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:r:110:MET:O     | 2:s:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:x:54:GLN:OE1    | 3:AM:200:ALA:HB2  | 1.92                     | 0.69              |
| 3:5:124:GLN:HB2   | 3:ZA:199:GLY:HA2  | 1.74                     | 0.69              |
| 4:ZQ:373:VAL:HG11 | 4:ZW:7:VAL:HG22   | 1.74                     | 0.69              |
| 4:ZZ:269:GLN:HG2  | 4:Zf:286:PRO:HG3  | 1.73                     | 0.69              |
| 5:AB:211:VAL:O    | 3:AM:1:MET:CA     | 2.39                     | 0.69              |
| 5:AC:34:PHE:CE1   | 3:AH:46:TYR:OH    | 2.45                     | 0.69              |
| 6:AX:361:ASN:ND2  | 11:A9:78:VAL:HG12 | 2.06                     | 0.69              |
| 6:UJ:126:PHE:O    | 6:UJ:130:VAL:CB   | 2.41                     | 0.69              |
| 6:UK:126:PHE:CD1  | 6:UK:130:VAL:HG21 | 2.26                     | 0.69              |
| 6:UN:139:GLU:CD   | 6:UN:142:ARG:HH21 | 2.00                     | 0.69              |
| 3:5:240:TYR:HE1   | 3:ZA:257:LEU:HB2  | 1.56                     | 0.69              |
| 3:ZD:27:ALA:C     | 4:ZI:52:VAL:CG2   | 2.64                     | 0.69              |
| 4:ZY:382:TYR:CE1  | 4:Zd:395:ILE:HG23 | 2.28                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AE:45:PRO:CD    | 12:BF:37:PRO:HG3  | 2.22                     | 0.69              |
| 3:AJ:127:GLN:HE22 | 3:AJ:139:ALA:HB1  | 1.55                     | 0.69              |
| 3:AL:89:THR:O     | 3:AL:91:ASN:N     | 2.25                     | 0.69              |
| 9:Ax:162:PRO:CD   | 6:WE:167:ARG:NH2  | 2.54                     | 0.69              |
| 11:A8:128:LYS:HE2 | 12:BC:134:GLN:HG2 | 1.75                     | 0.69              |
| 11:A9:91:ASP:OD2  | 11:A9:104:ARG:NH1 | 2.25                     | 0.69              |
| 6:UJ:139:GLU:CD   | 6:UJ:142:ARG:HH21 | 2.00                     | 0.69              |
| 6:UL:139:GLU:CD   | 6:UL:142:ARG:HH21 | 2.00                     | 0.69              |
| 6:WE:134:ARG:HB3  | 6:WE:134:ARG:HH21 | 1.57                     | 0.69              |
| 6:WP:193:ALA:HB1  | 6:WQ:213:VAL:HG11 | 1.74                     | 0.69              |
| 1:J:144:PHE:CE2   | 1:K:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:O:144:PHE:CE2   | 1:P:171:ILE:HD11  | 2.28                     | 0.69              |
| 2:c:78:ASN:ND2    | 3:AG:145:ASN:HD21 | 1.91                     | 0.69              |
| 2:t:110:MET:O     | 2:u:84:VAL:HG23   | 1.92                     | 0.69              |
| 3:1:251:ASP:OD1   | 3:AJ:238:ARG:NE   | 2.25                     | 0.69              |
| 3:ZE:167:PRO:HG2  | 4:ZP:338:GLN:NE2  | 2.07                     | 0.69              |
| 4:Zd:2:SER:OG     | 4:Zd:3:PHE:N      | 2.25                     | 0.69              |
| 5:AD:59:ALA:O     | 3:AI:66:LEU:CD1   | 2.41                     | 0.69              |
| 6:Ad:372:ILE:HB   | 10:A2:11:ILE:HG22 | 1.74                     | 0.69              |
| 6:Al:294:ARG:HD3  | 11:A7:68:THR:CG2  | 2.23                     | 0.69              |
| 9:Av:116:PHE:CE2  | 11:A7:4:ARG:NH2   | 2.61                     | 0.69              |
| 10:A4:21:ALA:HB1  | 6:BV:278:THR:CG2  | 2.21                     | 0.69              |
| 6:UK:139:GLU:CD   | 6:UK:142:ARG:HH21 | 2.00                     | 0.69              |
| 6:UN:126:PHE:O    | 6:UN:130:VAL:CB   | 2.41                     | 0.69              |
| 6:UO:139:GLU:CD   | 6:UO:142:ARG:HH21 | 2.00                     | 0.69              |
| 1:R:144:PHE:CE2   | 1:S:171:ILE:HD11  | 2.28                     | 0.69              |
| 2:n:110:MET:O     | 2:o:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:w:110:MET:O     | 2:x:84:VAL:HG23   | 1.92                     | 0.69              |
| 3:9:85:ASN:HD22   | 4:ZK:4:SER:HB2    | 0.60                     | 0.69              |
| 3:ZA:111:THR:CG2  | 3:AN:163:GLY:HA2  | 2.19                     | 0.69              |
| 4:ZK:380:ARG:NH2  | 4:ZQ:393:ASP:OD1  | 2.25                     | 0.69              |
| 4:ZQ:183:THR:HG21 | 4:Zb:132:ALA:HA   | 1.75                     | 0.69              |
| 4:ZV:269:GLN:OE1  | 4:Zb:190:GLN:HA   | 1.91                     | 0.69              |
| 4:ZY:42:MET:HG2   | 4:ZY:53:LYS:HG2   | 1.73                     | 0.69              |
| 5:AA:48:GLY:CA    | 11:A6:93:PRO:HB3  | 2.22                     | 0.69              |
| 6:UI:126:PHE:O    | 6:UI:130:VAL:CB   | 2.41                     | 0.69              |
| 6:WA:175:SER:OG   | 6:WW:197:LEU:HA   | 1.93                     | 0.69              |
| 1:G:144:PHE:CE2   | 1:H:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:T:144:PHE:CE2   | 1:U:171:ILE:HD11  | 2.28                     | 0.69              |
| 2:i:110:MET:O     | 2:j:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:u:110:MET:O     | 2:v:84:VAL:HG23   | 1.92                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:128:LEU:HD12  | 3:2:140:ILE:HG13  | 1.75                     | 0.69              |
| 3:7:98:LYS:NZ     | 3:ZD:187:ILE:O    | 2.25                     | 0.69              |
| 4:ZS:390:LYS:HE2  | 4:ZS:394:GLN:HE22 | 1.57                     | 0.69              |
| 4:Zb:349:GLY:O    | 4:Zh:89:ASN:ND2   | 2.26                     | 0.69              |
| 5:AA:175:ASP:HA   | 3:AF:46:TYR:HB2   | 1.75                     | 0.69              |
| 5:AB:132:GLY:HA3  | 3:AG:179:MET:SD   | 2.32                     | 0.69              |
| 5:AB:224:ALA:N    | 3:AG:253:MET:CE   | 2.56                     | 0.69              |
| 5:AD:234:ILE:HG21 | 3:AI:260:LEU:HD21 | 1.75                     | 0.69              |
| 3:AJ:62:LEU:HD23  | 12:BF:83:PRO:HG2  | 1.74                     | 0.69              |
| 6:UN:126:PHE:O    | 6:UN:130:VAL:CG2  | 2.39                     | 0.69              |
| 6:WM:193:ALA:HB1  | 6:WN:213:VAL:CG1  | 2.22                     | 0.69              |
| 1:L:144:PHE:CE2   | 1:M:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:M:144:PHE:CE2   | 1:N:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:Q:144:PHE:CE2   | 1:R:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:S:144:PHE:CE2   | 1:T:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:U:144:PHE:CE2   | 1:V:171:ILE:HD11  | 2.28                     | 0.69              |
| 2:m:110:MET:O     | 2:n:84:VAL:HG23   | 1.92                     | 0.69              |
| 4:ZU:309:GLU:OE1  | 4:Zf:338:GLN:NE2  | 2.25                     | 0.69              |
| 5:AD:1:MET:HG2    | 5:AD:241:GLU:CD   | 2.18                     | 0.69              |
| 5:AD:200:ARG:HH12 | 3:AJ:189:GLU:H    | 1.38                     | 0.69              |
| 3:AH:44:LEU:HB3   | 12:BC:90:TYR:CZ   | 2.25                     | 0.69              |
| 6:UL:126:PHE:O    | 6:UL:130:VAL:CB   | 2.41                     | 0.69              |
| 6:UM:126:PHE:O    | 6:UM:130:VAL:CB   | 2.41                     | 0.69              |
| 6:UP:126:PHE:O    | 6:UP:130:VAL:CG2  | 2.40                     | 0.69              |
| 6:UP:139:GLU:CD   | 6:UP:142:ARG:HH21 | 2.00                     | 0.69              |
| 6:WL:197:LEU:HD13 | 6:WM:175:SER:OG   | 1.91                     | 0.69              |
| 1:V:144:PHE:CE2   | 1:W:171:ILE:HD11  | 2.28                     | 0.69              |
| 3:0:193:ILE:HD12  | 5:AD:152:PRO:HD2  | 1.73                     | 0.69              |
| 3:4:51:GLN:NE2    | 5:AC:146:LEU:CD1  | 2.56                     | 0.69              |
| 3:ZD:218:TYR:OH   | 4:ZO:53:LYS:HD2   | 1.93                     | 0.69              |
| 5:AE:229:MET:HE1  | 3:AK:254:LEU:HD22 | 1.75                     | 0.69              |
| 9:Au:60:MET:HE1   | 9:Av:91:GLY:HA3   | 1.74                     | 0.69              |
| 9:Av:45:LEU:HD13  | 10:A2:86:ILE:HG12 | 1.73                     | 0.69              |
| 1:D:144:PHE:CE2   | 1:E:171:ILE:HD11  | 2.28                     | 0.69              |
| 1:I:144:PHE:CE2   | 1:J:171:ILE:HD11  | 2.28                     | 0.69              |
| 2:j:110:MET:O     | 2:k:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:k:110:MET:O     | 2:l:84:VAL:HG23   | 1.92                     | 0.69              |
| 2:v:110:MET:O     | 2:w:84:VAL:HG23   | 1.92                     | 0.69              |
| 4:ZO:111:MET:HA   | 4:ZO:111:MET:HE3  | 1.75                     | 0.69              |
| 4:ZR:165:PRO:HG2  | 4:ZR:201:VAL:HG13 | 1.73                     | 0.69              |
| 4:ZU:159:ASN:ND2  | 4:ZU:161:THR:OG1  | 2.26                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zb:238:LEU:HD21 | 4:Zb:242:GLY:HA3  | 1.75                     | 0.69              |
| 4:Ze:84:ARG:NH1   | 4:Ze:134:PRO:HB2  | 2.08                     | 0.69              |
| 3:AL:52:PRO:CD    | 12:BB:80:PRO:CB   | 2.70                     | 0.69              |
| 6:AS:294:ARG:HD3  | 11:A0:68:THR:HG22 | 1.73                     | 0.69              |
| 9:Ay:143:ARG:HH22 | 9:Ay:177:SER:HA   | 1.58                     | 0.69              |
| 9:Ay:241:GLN:CG   | 6:WG:164:LEU:O    | 2.31                     | 0.69              |
| 6:UN:103:GLN:HG2  | 6:WS:182:PRO:HB3  | 1.75                     | 0.69              |
| 6:UO:126:PHE:O    | 6:UO:130:VAL:CB   | 2.41                     | 0.69              |
| 6:WA:213:VAL:HG11 | 6:WW:193:ALA:HB1  | 1.73                     | 0.69              |
| 6:WD:193:ALA:HB1  | 6:WE:213:VAL:CG1  | 2.23                     | 0.69              |
| 6:WR:112:GLY:HA2  | 6:WR:135:ALA:CA   | 2.16                     | 0.69              |
| 1:C:228:ASN:ND2   | 1:E:24:TRP:CE2    | 2.61                     | 0.68              |
| 1:K:144:PHE:CE2   | 1:L:171:ILE:HD11  | 2.28                     | 0.68              |
| 2:I:110:MET:O     | 2:m:84:VAL:HG23   | 1.92                     | 0.68              |
| 3:0:238:ARG:HH21  | 3:6:255:GLN:HB2   | 1.58                     | 0.68              |
| 3:3:257:LEU:HG    | 3:AG:230:LEU:HD12 | 1.74                     | 0.68              |
| 3:5:5:LEU:HD23    | 3:AN:235:GLN:HG3  | 1.76                     | 0.68              |
| 3:ZE:85:ASN:CG    | 4:ZP:50:LEU:HD22  | 2.18                     | 0.68              |
| 4:ZT:349:GLY:O    | 4:ZZ:89:ASN:ND2   | 2.27                     | 0.68              |
| 4:Zc:238:LEU:HD21 | 4:Zc:242:GLY:HA3  | 1.73                     | 0.68              |
| 6:WE:112:GLY:HA2  | 6:WE:135:ALA:CA   | 2.18                     | 0.68              |
| 1:L:228:ASN:ND2   | 1:N:24:TRP:CE2    | 2.61                     | 0.68              |
| 1:N:228:ASN:ND2   | 1:P:24:TRP:CE2    | 2.62                     | 0.68              |
| 1:Q:228:ASN:ND2   | 1:S:24:TRP:CE2    | 2.62                     | 0.68              |
| 1:W:144:PHE:CE2   | 1:X:171:ILE:HD11  | 2.28                     | 0.68              |
| 3:5:73:ARG:HB2    | 3:AI:218:TYR:OH   | 1.92                     | 0.68              |
| 4:ZF:65:THR:HB    | 4:ZF:363:ALA:HB3  | 1.75                     | 0.68              |
| 4:ZH:208:TRP:NE1  | 4:ZH:268:GLN:OE1  | 2.25                     | 0.68              |
| 4:ZK:107:ASN:ND2  | 4:ZK:138:THR:OG1  | 2.26                     | 0.68              |
| 6:AS:297:GLN:HE22 | 11:A0:76:GLN:N    | 1.91                     | 0.68              |
| 7:As:54:LYS:HZ2   | 8:At:215:VAL:HA   | 1.58                     | 0.68              |
| 9:Ay:38:TRP:HA    | 10:A5:46:SER:OG   | 1.93                     | 0.68              |
| 6:WB:193:ALA:HB1  | 6:WC:213:VAL:HG11 | 1.76                     | 0.68              |
| 6:WK:197:LEU:HA   | 6:WL:175:SER:HB2  | 1.74                     | 0.68              |
| 12:BE:68:ILE:HD11 | 6:BP:312:VAL:CG2  | 2.24                     | 0.68              |
| 1:B:24:TRP:CE2    | 1:Z:228:ASN:ND2   | 2.62                     | 0.68              |
| 1:E:144:PHE:CE2   | 1:F:171:ILE:HD11  | 2.28                     | 0.68              |
| 1:F:144:PHE:CE2   | 1:G:171:ILE:HD11  | 2.28                     | 0.68              |
| 1:H:144:PHE:CE2   | 1:I:171:ILE:HD11  | 2.28                     | 0.68              |
| 1:N:144:PHE:CE2   | 1:O:171:ILE:HD11  | 2.28                     | 0.68              |
| 1:P:144:PHE:CE2   | 1:Q:171:ILE:HD11  | 2.28                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:228:ASN:ND2   | 1:U:24:TRP:CE2    | 2.61                     | 0.68              |
| 1:X:228:ASN:ND2   | 1:Z:24:TRP:CE2    | 2.62                     | 0.68              |
| 2:b:80:GLN:OE1    | 3:AG:170:VAL:O    | 2.12                     | 0.68              |
| 3:0:51:GLN:O      | 3:0:52:PRO:C      | 2.35                     | 0.68              |
| 3:0:52:PRO:HB3    | 12:BE:87:ALA:O    | 1.94                     | 0.68              |
| 3:6:1:MET:HB2     | 3:AJ:29:VAL:HG11  | 1.75                     | 0.68              |
| 10:A2:48:ARG:NH2  | 11:A8:6:ASP:OD2   | 2.26                     | 0.68              |
| 6:UP:126:PHE:O    | 6:UP:130:VAL:CB   | 2.41                     | 0.68              |
| 6:WC:197:LEU:HD12 | 6:WD:175:SER:HB3  | 1.76                     | 0.68              |
| 6:WP:190:GLN:HG2  | 6:WQ:217:GLY:HA3  | 1.75                     | 0.68              |
| 1:A:228:ASN:ND2   | 1:C:24:TRP:CE2    | 2.62                     | 0.68              |
| 1:E:228:ASN:ND2   | 1:G:24:TRP:CE2    | 2.62                     | 0.68              |
| 1:P:228:ASN:ND2   | 1:R:24:TRP:CE2    | 2.61                     | 0.68              |
| 1:X:144:PHE:CE2   | 1:Y:171:ILE:HD11  | 2.28                     | 0.68              |
| 3:2:58:GLU:CG     | 5:AA:140:ASP:OD2  | 2.40                     | 0.68              |
| 4:ZF:5:GLN:NE2    | 4:ZF:49:GLY:O     | 2.26                     | 0.68              |
| 4:ZL:10:LEU:HD21  | 4:ZQ:399:LEU:HD11 | 1.76                     | 0.68              |
| 4:ZQ:27:SER:OG    | 4:ZV:381:ASN:ND2  | 2.27                     | 0.68              |
| 4:ZT:331:ASP:HA   | 4:ZY:40:ALA:HB1   | 1.75                     | 0.68              |
| 4:Zc:210:VAL:O    | 4:Zc:227:SER:N    | 2.26                     | 0.68              |
| 5:AB:70:GLN:CG    | 3:AM:6:TRP:CD1    | 2.76                     | 0.68              |
| 5:AB:217:MET:SD   | 3:AM:257:LEU:O    | 2.50                     | 0.68              |
| 5:AB:220:MET:SD   | 3:AG:246:ALA:HA   | 2.34                     | 0.68              |
| 6:Ae:372:ILE:CG2  | 10:A2:4:ILE:CG1   | 2.70                     | 0.68              |
| 6:Am:278:THR:HG21 | 10:Az:21:ALA:HB3  | 1.71                     | 0.68              |
| 7:Aq:14:MET:HG3   | 7:Ar:59:PHE:HE1   | 1.56                     | 0.68              |
| 7:As:78:ARG:HE    | 9:Ay:229:VAL:HG12 | 1.58                     | 0.68              |
| 9:Au:109:TYR:HA   | 9:Au:113:TYR:HB2  | 1.74                     | 0.68              |
| 10:A4:7:ILE:HG21  | 6:BX:278:THR:HG21 | 1.31                     | 0.68              |
| 6:UI:139:GLU:CD   | 6:UI:142:ARG:HH21 | 2.00                     | 0.68              |
| 6:UK:126:PHE:O    | 6:UK:130:VAL:CB   | 2.41                     | 0.68              |
| 6:WS:197:LEU:HD12 | 6:WT:175:SER:OG   | 1.94                     | 0.68              |
| 1:A:144:PHE:CE2   | 1:B:171:ILE:HD11  | 2.28                     | 0.68              |
| 1:O:228:ASN:ND2   | 1:Q:24:TRP:CE2    | 2.62                     | 0.68              |
| 1:V:228:ASN:ND2   | 1:X:24:TRP:CE2    | 2.61                     | 0.68              |
| 2:p:53:THR:HG21   | 5:AD:154:THR:CG2  | 2.23                     | 0.68              |
| 5:AA:202:MET:CE   | 3:AL:73:ARG:NH2   | 2.57                     | 0.68              |
| 6:AV:355:PRO:HB2  | 6:BO:319:GLN:CD   | 2.19                     | 0.68              |
| 7:Ar:40:ALA:HB2   | 7:As:44:ILE:CD1   | 2.24                     | 0.68              |
| 10:A2:80:VAL:HG22 | 11:A8:131:MET:HG2 | 1.75                     | 0.68              |
| 6:WA:197:LEU:HD12 | 6:WB:175:SER:HB3  | 1.75                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C:144:PHE:CE2   | 1:D:171:ILE:HD11   | 2.28                     | 0.68              |
| 4:ZT:18:ASP:HB3   | 4:ZY:5:GLN:HE22    | 1.59                     | 0.68              |
| 5:AA:28:ASN:OD1   | 3:AF:72:VAL:HB     | 1.94                     | 0.68              |
| 9:Ay:68:ILE:HD11  | 10:A4:104:VAL:HG12 | 1.75                     | 0.68              |
| 6:BG:320:PRO:O    | 6:BG:322:PRO:HD3   | 1.93                     | 0.68              |
| 1:B:144:PHE:CE2   | 1:C:171:ILE:HD11   | 2.28                     | 0.68              |
| 1:B:228:ASN:ND2   | 1:D:24:TRP:CE2     | 2.61                     | 0.68              |
| 1:Y:144:PHE:CE2   | 1:Z:171:ILE:HD11   | 2.28                     | 0.68              |
| 3:4:17:THR:HG23   | 3:9:68:ILE:HD11    | 1.76                     | 0.68              |
| 3:6:218:TYR:OH    | 4:ZH:53:LYS:CG     | 2.41                     | 0.68              |
| 3:ZB:240:TYR:OH   | 4:ZG:399:LEU:HD11  | 1.93                     | 0.68              |
| 4:ZU:17:LEU:CD1   | 4:ZZ:395:ILE:HD11  | 2.24                     | 0.68              |
| 5:AA:231:MET:HE2  | 3:AF:257:LEU:HA    | 1.74                     | 0.68              |
| 3:AG:194:GLU:HG3  | 3:AG:199:GLY:HA2   | 1.76                     | 0.68              |
| 9:Ay:116:PHE:CE1  | 11:A0:4:ARG:NH2    | 2.61                     | 0.68              |
| 1:A:171:ILE:HD11  | 1:Z:144:PHE:CE2    | 2.28                     | 0.68              |
| 1:G:228:ASN:ND2   | 1:I:24:TRP:CE2     | 2.62                     | 0.68              |
| 1:U:228:ASN:ND2   | 1:W:24:TRP:CE2     | 2.61                     | 0.68              |
| 3:ZE:42:GLU:OE2   | 3:ZE:73:ARG:NH1    | 2.24                     | 0.68              |
| 4:ZJ:180:LYS:HD3  | 4:ZJ:274:ASN:HD22  | 1.57                     | 0.68              |
| 4:ZM:156:ILE:HD12 | 4:ZM:276:ILE:HG12  | 1.75                     | 0.68              |
| 4:ZQ:178:TYR:HA   | 4:ZQ:201:VAL:HG12  | 1.74                     | 0.68              |
| 4:ZW:269:GLN:OE1  | 4:Zc:286:PRO:HG3   | 1.94                     | 0.68              |
| 6:AX:278:THR:HG21 | 10:A3:7:ILE:HG21   | 1.76                     | 0.68              |
| 7:Aq:59:PHE:CZ    | 9:Av:198:LEU:HD21  | 2.25                     | 0.68              |
| 9:Ay:144:GLU:O    | 9:Ay:147:LEU:N     | 2.26                     | 0.68              |
| 11:A9:32:ASN:HD22 | 12:BD:62:VAL:HG12  | 1.59                     | 0.68              |
| 6:WR:113:PHE:HA   | 6:WS:134:ARG:HH12  | 1.58                     | 0.68              |
| 3:7:218:TYR:OH    | 4:ZI:53:LYS:HG3    | 1.93                     | 0.68              |
| 4:ZJ:382:TYR:CE1  | 4:ZO:395:ILE:HG23  | 2.29                     | 0.68              |
| 4:ZT:208:TRP:NE1  | 4:ZT:268:GLN:OE1   | 2.26                     | 0.68              |
| 4:ZU:379:GLN:HG2  | 4:ZU:380:ARG:HH21  | 1.58                     | 0.68              |
| 5:AD:48:GLY:HA3   | 11:A9:93:PRO:HB3   | 1.75                     | 0.68              |
| 3:AF:44:LEU:HD23  | 12:BA:78:TYR:CD1   | 2.28                     | 0.68              |
| 8:At:166:SER:O    | 8:At:168:ALA:N     | 2.26                     | 0.68              |
| 3:ZD:77:THR:H     | 4:ZI:47:LYS:CD     | 2.05                     | 0.68              |
| 4:ZS:379:GLN:NE2  | 4:ZX:394:GLN:OE1   | 2.25                     | 0.68              |
| 4:ZT:375:MET:HE1  | 4:ZY:388:THR:OG1   | 1.94                     | 0.68              |
| 4:ZY:2:SER:OG     | 4:ZY:3:PHE:N       | 2.24                     | 0.68              |
| 4:Za:309:GLU:OE1  | 4:Za:309:GLU:N     | 2.27                     | 0.68              |
| 5:AA:235:THR:OG1  | 3:AF:260:LEU:HD12  | 1.93                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:109:PRO:HG3  | 3:AG:198:SER:H    | 1.59                     | 0.68              |
| 6:AS:370:ARG:HE   | 10:A4:7:ILE:HD11  | 1.58                     | 0.68              |
| 9:Ay:86:ASN:O     | 9:Ay:88:VAL:N     | 2.27                     | 0.68              |
| 9:Ay:147:LEU:HD12 | 6:WH:166:VAL:HG12 | 1.76                     | 0.68              |
| 6:UK:125:GLN:HA   | 6:UK:128:GLU:HB2  | 1.76                     | 0.68              |
| 6:UM:98:LEU:HD12  | 6:UM:146:THR:OG1  | 1.94                     | 0.68              |
| 6:WN:200:SER:CA   | 6:WO:173:SER:OG   | 2.41                     | 0.68              |
| 6:WS:197:LEU:HD12 | 6:WT:175:SER:CB   | 2.24                     | 0.68              |
| 1:A:24:TRP:CE2    | 1:Y:228:ASN:ND2   | 2.62                     | 0.67              |
| 1:T:228:ASN:ND2   | 1:V:24:TRP:CE2    | 2.61                     | 0.67              |
| 3:7:73:ARG:HB2    | 3:AK:218:TYR:OH   | 1.94                     | 0.67              |
| 4:ZP:349:GLY:O    | 4:ZV:89:ASN:ND2   | 2.27                     | 0.67              |
| 4:ZR:331:ASP:HA   | 4:ZW:40:ALA:HB1   | 1.75                     | 0.67              |
| 5:AA:50:SER:HB3   | 11:A6:91:ASP:O    | 1.94                     | 0.67              |
| 6:UJ:125:GLN:HA   | 6:UJ:128:GLU:HB2  | 1.76                     | 0.67              |
| 6:UM:125:GLN:HA   | 6:UM:128:GLU:HB2  | 1.76                     | 0.67              |
| 6:WB:190:GLN:HG2  | 6:WC:216:SER:O    | 1.94                     | 0.67              |
| 1:I:228:ASN:ND2   | 1:K:24:TRP:CE2    | 2.61                     | 0.67              |
| 3:0:85:ASN:OD1    | 3:ZB:70:THR:HG22  | 1.94                     | 0.67              |
| 3:7:257:LEU:CG    | 3:AK:230:LEU:HD12 | 2.24                     | 0.67              |
| 4:ZH:285:LYS:HG2  | 4:ZH:286:PRO:HD2  | 1.76                     | 0.67              |
| 4:ZT:210:VAL:O    | 4:ZT:227:SER:N    | 2.27                     | 0.67              |
| 4:ZU:379:GLN:HE22 | 4:ZZ:391:THR:HA   | 1.60                     | 0.67              |
| 7:Aq:89:GLY:HA2   | 6:WW:165:PHE:HE1  | 0.69                     | 0.67              |
| 6:WD:196:HIS:HB3  | 6:WE:211:THR:HG21 | 1.76                     | 0.67              |
| 6:WD:197:LEU:HD12 | 6:WE:175:SER:CB   | 2.23                     | 0.67              |
| 6:WQ:197:LEU:HD12 | 6:WR:175:SER:CB   | 2.23                     | 0.67              |
| 1:W:228:ASN:ND2   | 1:Y:24:TRP:CE2    | 2.61                     | 0.67              |
| 3:1:22:ILE:HG21   | 3:1:233:MET:HG3   | 1.77                     | 0.67              |
| 3:ZA:122:VAL:O    | 4:ZF:322:ASN:OD1  | 2.13                     | 0.67              |
| 3:ZD:137:GLN:HA   | 3:ZD:139:ALA:H    | 1.60                     | 0.67              |
| 4:ZX:17:LEU:HD13  | 4:Zc:395:ILE:HD11 | 1.77                     | 0.67              |
| 5:AB:229:MET:HE3  | 3:AH:258:THR:CG2  | 2.25                     | 0.67              |
| 5:AD:27:ALA:HB1   | 3:AI:72:VAL:HG12  | 1.76                     | 0.67              |
| 5:AE:231:MET:CE   | 3:AJ:257:LEU:CD1  | 2.67                     | 0.67              |
| 3:AI:62:LEU:HG    | 12:BE:84:LEU:CD2  | 2.24                     | 0.67              |
| 6:UO:98:LEU:HD12  | 6:UO:146:THR:OG1  | 1.94                     | 0.67              |
| 6:WN:200:SER:O    | 6:WO:173:SER:OG   | 2.12                     | 0.67              |
| 1:H:88:ALA:CB     | 1:J:171:ILE:HD12  | 2.25                     | 0.67              |
| 1:I:88:ALA:CB     | 1:K:171:ILE:HD12  | 2.25                     | 0.67              |
| 1:K:228:ASN:ND2   | 1:M:24:TRP:CE2    | 2.61                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZL:294:ILE:O    | 4:ZL:358:ASN:ND2   | 2.27                     | 0.67              |
| 4:ZM:373:VAL:HG21 | 4:ZS:10:LEU:HD23   | 1.77                     | 0.67              |
| 4:ZW:102:LEU:O    | 4:Zb:322:ASN:ND2   | 2.28                     | 0.67              |
| 5:AA:200:ARG:NH2  | 3:AG:189:GLU:HB2   | 2.05                     | 0.67              |
| 5:AD:228:GLU:HG2  | 3:AI:256:LYS:CD    | 2.24                     | 0.67              |
| 3:AG:73:ARG:HD2   | 12:BB:78:TYR:CZ    | 2.28                     | 0.67              |
| 3:AJ:62:LEU:HD23  | 12:BF:83:PRO:HD2   | 1.74                     | 0.67              |
| 6:Am:295:SER:HB2  | 11:A7:73:ILE:CG1   | 2.22                     | 0.67              |
| 6:WH:203:ALA:CB   | 6:WI:160:PRO:HB3   | 2.19                     | 0.67              |
| 6:WO:167:ARG:O    | 6:WO:168:GLU:HB2   | 1.93                     | 0.67              |
| 1:D:88:ALA:CB     | 1:F:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:H:166:GLU:CB    | 1:I:35:THR:HG21    | 2.20                     | 0.67              |
| 1:J:88:ALA:CB     | 1:L:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:R:228:ASN:ND2   | 1:T:24:TRP:CE2     | 2.62                     | 0.67              |
| 3:1:257:LEU:HD23  | 5:AE:213:PRO:HB2   | 1.77                     | 0.67              |
| 3:2:56:SER:HA     | 5:AA:138:ALA:CB    | 2.24                     | 0.67              |
| 3:ZD:31:THR:HG22  | 4:ZI:39:PHE:CB     | 2.25                     | 0.67              |
| 4:ZH:349:GLY:O    | 4:ZN:89:ASN:ND2    | 2.26                     | 0.67              |
| 5:AB:70:GLN:NE2   | 3:AM:1:MET:H1      | 1.85                     | 0.67              |
| 6:UK:98:LEU:HD12  | 6:UK:146:THR:OG1   | 1.94                     | 0.67              |
| 6:UL:98:LEU:HD12  | 6:UL:146:THR:OG1   | 1.94                     | 0.67              |
| 6:UN:125:GLN:HA   | 6:UN:128:GLU:HB2   | 1.76                     | 0.67              |
| 6:WG:200:SER:O    | 6:WH:158:ALA:CB    | 2.42                     | 0.67              |
| 1:B:88:ALA:CB     | 1:D:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:C:88:ALA:CB     | 1:E:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:E:88:ALA:CB     | 1:G:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:G:88:ALA:CB     | 1:I:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:L:88:ALA:CB     | 1:N:171:ILE:HD12   | 2.25                     | 0.67              |
| 3:4:226:VAL:HG11  | 3:9:242:ILE:HD13   | 1.75                     | 0.67              |
| 4:ZG:160:SER:OG   | 4:ZM:192:ASN:OD1   | 2.13                     | 0.67              |
| 5:AA:220:MET:CE   | 3:AF:246:ALA:CB    | 2.71                     | 0.67              |
| 5:AB:9:MET:HG3    | 12:BB:103:VAL:HG21 | 1.76                     | 0.67              |
| 5:AC:9:MET:HB2    | 12:BC:103:VAL:HG21 | 1.77                     | 0.67              |
| 12:BA:6:ILE:HG21  | 12:BA:122:VAL:HG21 | 1.76                     | 0.67              |
| 6:WD:168:GLU:OE2  | 6:WD:170:LYS:HE3   | 1.94                     | 0.67              |
| 1:D:228:ASN:ND2   | 1:F:24:TRP:CE2     | 2.62                     | 0.67              |
| 1:F:88:ALA:CB     | 1:H:171:ILE:HD12   | 2.25                     | 0.67              |
| 1:K:88:ALA:CB     | 1:M:171:ILE:HD12   | 2.25                     | 0.67              |
| 3:4:70:THR:HG22   | 3:4:71:GLY:H       | 1.60                     | 0.67              |
| 3:ZB:205:THR:HB   | 3:ZB:208:LEU:HG    | 1.75                     | 0.67              |
| 4:ZF:331:ASP:HA   | 4:ZK:40:ALA:HB1    | 1.75                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZO:317:LEU:HD11 | 4:ZO:356:LEU:HD21  | 1.76                     | 0.67              |
| 5:AA:220:MET:CE   | 3:AF:246:ALA:CA    | 2.73                     | 0.67              |
| 5:AB:152:PRO:HD2  | 3:AM:193:ILE:HG21  | 1.76                     | 0.67              |
| 5:AB:213:PRO:CD   | 3:AM:2:ILE:HD11    | 2.24                     | 0.67              |
| 10:Az:73:ALA:HB1  | 10:Az:77:LYS:HZ3   | 1.60                     | 0.67              |
| 11:A0:36:PRO:HB3  | 11:A0:96:ASP:HB2   | 1.77                     | 0.67              |
| 6:UJ:98:LEU:HD12  | 6:UJ:146:THR:OG1   | 1.94                     | 0.67              |
| 1:A:88:ALA:CB     | 1:C:171:ILE:HD12   | 2.25                     | 0.67              |
| 2:m:54:GLN:OE1    | 3:AJ:137:GLN:HG2   | 1.95                     | 0.67              |
| 3:0:42:GLU:HG3    | 3:AJ:190:ASN:HB2   | 1.76                     | 0.67              |
| 3:0:99:GLY:O      | 3:0:116:ARG:NH2    | 2.28                     | 0.67              |
| 3:2:230:LEU:HD21  | 3:7:242:ILE:HG23   | 1.75                     | 0.67              |
| 3:ZC:115:THR:HB   | 3:ZC:191:LEU:HD23  | 1.77                     | 0.67              |
| 4:ZK:374:ASN:O    | 4:ZK:377:VAL:N     | 2.26                     | 0.67              |
| 4:Zh:3:PHE:HE2    | 4:Zh:396:LEU:HD12  | 1.60                     | 0.67              |
| 6:AQ:374:HIS:CD2  | 10:A5:15:GLN:HB2   | 2.30                     | 0.67              |
| 10:A3:75:MET:SD   | 11:A8:122:VAL:HG22 | 2.35                     | 0.67              |
| 6:UI:125:GLN:HA   | 6:UI:128:GLU:HB2   | 1.76                     | 0.67              |
| 1:B:171:ILE:HD12  | 1:Z:88:ALA:CB      | 2.25                     | 0.67              |
| 1:M:88:ALA:CB     | 1:O:171:ILE:HD12   | 2.25                     | 0.67              |
| 2:g:78:ASN:HD22   | 3:AF:168:VAL:HG22  | 1.59                     | 0.67              |
| 3:1:70:THR:CG2    | 5:AE:71:LEU:HG     | 2.22                     | 0.67              |
| 3:8:111:THR:CG2   | 3:AL:163:GLY:HA2   | 2.22                     | 0.67              |
| 3:ZB:28:ASN:HD21  | 4:ZG:52:VAL:HG23   | 1.57                     | 0.67              |
| 4:ZY:27:SER:OG    | 4:Zd:381:ASN:ND2   | 2.28                     | 0.67              |
| 4:Zc:379:GLN:HE22 | 4:Zh:394:GLN:NE2   | 1.93                     | 0.67              |
| 5:AB:35:ARG:HA    | 5:AB:210:ASN:HD21  | 1.60                     | 0.67              |
| 5:AB:104:ASN:ND2  | 3:AG:40:VAL:HG11   | 2.10                     | 0.67              |
| 5:AB:152:PRO:HG3  | 3:AM:185:GLU:OE1   | 1.94                     | 0.67              |
| 5:AD:221:ILE:HG21 | 3:AJ:251:ASP:OD2   | 1.95                     | 0.67              |
| 3:AG:158:SER:HA   | 3:AG:169:GLN:HA    | 1.77                     | 0.67              |
| 11:A8:31:ALA:HB1  | 12:BC:13:ALA:HB2   | 1.75                     | 0.67              |
| 6:WT:128:GLU:HG2  | 6:WU:126:PHE:HD2   | 1.60                     | 0.67              |
| 1:M:228:ASN:ND2   | 1:O:24:TRP:CE2     | 2.61                     | 0.67              |
| 2:j:51:GLN:HG3    | 3:6:59:GLN:HE21    | 1.58                     | 0.67              |
| 2:r:56:PRO:HD2    | 2:s:79:MET:HG2     | 1.77                     | 0.67              |
| 3:4:98:LYS:NZ     | 3:ZA:187:ILE:O     | 2.19                     | 0.67              |
| 3:ZA:22:ILE:HG21  | 3:ZA:233:MET:HG3   | 1.76                     | 0.67              |
| 4:ZI:373:VAL:HG23 | 4:ZT:399:LEU:HD21  | 1.77                     | 0.67              |
| 3:AM:52:PRO:HG2   | 12:BC:89:GLY:N     | 2.10                     | 0.67              |
| 6:Ao:278:THR:HG21 | 10:Az:7:ILE:CB     | 2.24                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Ay:147:LEU:HD11 | 6:WH:166:VAL:HG11 | 1.77                     | 0.67              |
| 6:UP:125:GLN:HA   | 6:UP:128:GLU:HB2  | 1.77                     | 0.67              |
| 6:WA:200:SER:O    | 6:WB:158:ALA:HB3  | 1.95                     | 0.67              |
| 6:WP:197:LEU:HD12 | 6:WQ:175:SER:CB   | 2.25                     | 0.67              |
| 1:G:166:GLU:CB    | 1:H:35:THR:HG21   | 2.20                     | 0.66              |
| 1:N:88:ALA:CB     | 1:P:171:ILE:HD12  | 2.25                     | 0.66              |
| 2:q:56:PRO:HD2    | 2:r:79:MET:HG2    | 1.78                     | 0.66              |
| 4:ZM:380:ARG:HB3  | 4:ZS:396:LEU:HD13 | 1.77                     | 0.66              |
| 5:AE:116:GLN:HG3  | 5:AE:118:HIS:CD2  | 2.30                     | 0.66              |
| 7:Aq:21:ALA:HB2   | 9:Aw:199:VAL:HG23 | 1.77                     | 0.66              |
| 1:A:171:ILE:HD12  | 1:Y:88:ALA:CB     | 2.25                     | 0.66              |
| 1:Q:219:MET:SD    | 1:R:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:R:219:MET:SD    | 1:S:212:TYR:HB2   | 2.36                     | 0.66              |
| 2:n:56:PRO:HD2    | 2:o:79:MET:HG2    | 1.77                     | 0.66              |
| 2:o:56:PRO:HD2    | 2:p:79:MET:HG2    | 1.77                     | 0.66              |
| 2:p:56:PRO:HD2    | 2:q:79:MET:HG2    | 1.78                     | 0.66              |
| 2:s:56:PRO:HD2    | 2:t:79:MET:HG2    | 1.77                     | 0.66              |
| 3:3:230:LEU:HD12  | 3:ZE:257:LEU:HD13 | 1.77                     | 0.66              |
| 3:5:259:GLN:O     | 3:5:260:LEU:C     | 2.37                     | 0.66              |
| 3:9:73:ARG:HG3    | 3:AM:218:TYR:OH   | 1.95                     | 0.66              |
| 3:ZA:235:GLN:NE2  | 4:ZG:3:PHE:HB3    | 2.10                     | 0.66              |
| 3:ZE:240:TYR:CE2  | 4:ZJ:395:ILE:HG23 | 2.30                     | 0.66              |
| 4:ZX:269:GLN:OE1  | 4:Zd:286:PRO:HG3  | 1.94                     | 0.66              |
| 4:Zc:29:THR:HG23  | 4:Zh:39:PHE:HB2   | 1.78                     | 0.66              |
| 5:AB:202:MET:HE2  | 3:AM:73:ARG:CZ    | 2.23                     | 0.66              |
| 5:AB:224:ALA:CA   | 3:AG:253:MET:HE3  | 2.25                     | 0.66              |
| 5:AC:26:LEU:HD13  | 3:AH:242:ILE:HG22 | 1.75                     | 0.66              |
| 5:AE:173:ARG:NH1  | 3:AJ:46:TYR:CE1   | 2.62                     | 0.66              |
| 6:UI:98:LEU:HD12  | 6:UI:146:THR:OG1  | 1.94                     | 0.66              |
| 12:BA:68:ILE:HD11 | 6:BH:312:VAL:CG2  | 2.26                     | 0.66              |
| 6:WW:186:LEU:HA   | 6:WW:190:GLN:OE1  | 1.95                     | 0.66              |
| 1:J:219:MET:SD    | 1:K:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:O:88:ALA:CB     | 1:Q:171:ILE:HD12  | 2.25                     | 0.66              |
| 1:S:219:MET:SD    | 1:T:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:V:219:MET:SD    | 1:W:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:X:219:MET:SD    | 1:Y:212:TYR:HB2   | 2.36                     | 0.66              |
| 2:c:56:PRO:HD2    | 2:d:79:MET:HG2    | 1.77                     | 0.66              |
| 2:d:56:PRO:HD2    | 2:e:79:MET:HG2    | 1.77                     | 0.66              |
| 4:Za:102:LEU:O    | 4:Zf:322:ASN:HB2  | 1.95                     | 0.66              |
| 5:AB:224:ALA:HA   | 3:AG:253:MET:CE   | 2.25                     | 0.66              |
| 3:AH:238:ARG:NH2  | 3:AN:251:ASP:OD1  | 2.23                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:Ab:4:GLU:HB2    | 6:WS:125:GLN:HB2   | 1.76                     | 0.66              |
| 10:Az:75:MET:HE1  | 10:A5:88:VAL:HG22  | 1.76                     | 0.66              |
| 6:WE:112:GLY:HA3  | 6:WE:139:GLU:OE1   | 1.95                     | 0.66              |
| 1:K:219:MET:SD    | 1:L:212:TYR:HB2    | 2.36                     | 0.66              |
| 1:X:88:ALA:CB     | 1:Z:171:ILE:HD12   | 2.25                     | 0.66              |
| 1:Y:219:MET:SD    | 1:Z:212:TYR:HB2    | 2.36                     | 0.66              |
| 3:8:75:VAL:O      | 3:ZD:50:ARG:NH1    | 2.27                     | 0.66              |
| 4:ZZ:210:VAL:O    | 4:ZZ:227:SER:N     | 2.28                     | 0.66              |
| 3:AM:22:ILE:HD11  | 3:AM:232:ASN:HB3   | 1.76                     | 0.66              |
| 7:Ab:48:THR:CG2   | 9:Au:208:GLY:HA2   | 2.25                     | 0.66              |
| 6:An:278:THR:CG2  | 10:Az:14:LEU:CD2   | 2.62                     | 0.66              |
| 6:UL:125:GLN:HA   | 6:UL:128:GLU:HB2   | 1.76                     | 0.66              |
| 12:BB:122:VAL:O   | 12:BB:126:MET:HG2  | 1.96                     | 0.66              |
| 1:P:219:MET:SD    | 1:Q:212:TYR:HB2    | 2.36                     | 0.66              |
| 2:a:56:PRO:HD2    | 2:b:79:MET:HG2     | 1.77                     | 0.66              |
| 2:b:56:PRO:HD2    | 2:c:79:MET:HG2     | 1.78                     | 0.66              |
| 2:e:56:PRO:HD2    | 2:f:79:MET:HG2     | 1.77                     | 0.66              |
| 2:m:56:PRO:HD2    | 2:n:79:MET:HG2     | 1.77                     | 0.66              |
| 2:x:33:GLU:HG3    | 2:x:95:PRO:HD3     | 1.78                     | 0.66              |
| 2:y:33:GLU:HG3    | 2:y:95:PRO:HD3     | 1.78                     | 0.66              |
| 3:9:175:LEU:HD11  | 3:9:214:LEU:HD21   | 1.77                     | 0.66              |
| 4:ZL:165:PRO:HG3  | 4:ZL:179:ASN:HD21  | 1.60                     | 0.66              |
| 4:ZQ:390:LYS:HB2  | 4:ZV:402:LEU:HD22  | 1.76                     | 0.66              |
| 3:AF:229:GLU:O    | 3:AF:233:MET:HG3   | 1.95                     | 0.66              |
| 3:AG:73:ARG:HG3   | 12:BB:78:TYR:CE2   | 2.30                     | 0.66              |
| 3:AJ:260:LEU:HD11 | 12:BE:106:MET:SD   | 2.35                     | 0.66              |
| 10:A2:75:MET:HE1  | 11:A7:122:VAL:HG13 | 1.77                     | 0.66              |
| 6:UO:62:ASP:OD2   | 6:WT:184:ARG:NH2   | 2.28                     | 0.66              |
| 1:I:219:MET:SD    | 1:J:212:TYR:HB2    | 2.36                     | 0.66              |
| 1:W:219:MET:SD    | 1:X:212:TYR:HB2    | 2.36                     | 0.66              |
| 2:t:56:PRO:HD2    | 2:u:79:MET:HG2     | 1.78                     | 0.66              |
| 4:ZM:204:LYS:HD2  | 4:ZM:205:ASP:H     | 1.59                     | 0.66              |
| 4:Zd:154:MET:HE2  | 4:Zd:263:PHE:HE1   | 1.60                     | 0.66              |
| 5:AB:12:ALA:HB3   | 12:BB:99:VAL:HG11  | 1.78                     | 0.66              |
| 5:AB:223:ASN:CB   | 3:AG:253:MET:HE1   | 2.25                     | 0.66              |
| 5:AD:26:LEU:CD1   | 3:AI:242:ILE:HG22  | 2.13                     | 0.66              |
| 5:AD:217:MET:CE   | 3:AI:242:ILE:HD13  | 2.24                     | 0.66              |
| 3:AL:195:THR:HG22 | 3:AL:197:SER:H     | 1.59                     | 0.66              |
| 3:AM:128:LEU:HD12 | 3:AM:140:ILE:HD12  | 1.77                     | 0.66              |
| 6:WA:112:GLY:HA3  | 6:WA:139:GLU:OE1   | 1.95                     | 0.66              |
| 6:WF:128:GLU:HG2  | 6:WG:126:PHE:CD2   | 2.29                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:BT:391:VAL:HG21 | 6:BT:409:MET:HE1  | 1.78                     | 0.66              |
| 1:M:219:MET:SD    | 1:N:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:N:219:MET:SD    | 1:O:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:O:219:MET:SD    | 1:P:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:P:88:ALA:CB     | 1:R:171:ILE:HD12  | 2.25                     | 0.66              |
| 1:W:88:ALA:CB     | 1:Y:171:ILE:HD12  | 2.25                     | 0.66              |
| 2:m:80:GLN:NE2    | 3:AJ:204:SER:N    | 2.43                     | 0.66              |
| 2:t:33:GLU:HG3    | 2:t:95:PRO:HD3    | 1.78                     | 0.66              |
| 2:u:33:GLU:HG3    | 2:u:95:PRO:HD3    | 1.78                     | 0.66              |
| 3:8:36:ARG:CZ     | 3:8:38:ARG:HH22   | 2.08                     | 0.66              |
| 4:ZI:156:ILE:HG13 | 4:ZI:276:ILE:HA   | 1.77                     | 0.66              |
| 3:AH:229:GLU:O    | 3:AH:233:MET:HG3  | 1.96                     | 0.66              |
| 6:AS:294:ARG:HD2  | 11:A0:68:THR:CG2  | 2.25                     | 0.66              |
| 6:UK:207:PRO:CG   | 6:WE:187:ASP:CG   | 2.68                     | 0.66              |
| 6:BU:391:VAL:HG21 | 6:BU:409:MET:HE1  | 1.78                     | 0.66              |
| 1:A:212:TYR:HB2   | 1:Z:219:MET:SD    | 2.36                     | 0.66              |
| 1:D:219:MET:SD    | 1:E:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:E:219:MET:SD    | 1:F:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:G:219:MET:SD    | 1:H:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:L:219:MET:SD    | 1:M:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:T:219:MET:SD    | 1:U:212:TYR:HB2   | 2.36                     | 0.66              |
| 2:l:56:PRO:HD2    | 2:m:79:MET:HG2    | 1.77                     | 0.66              |
| 2:o:319:LEU:HD21  | 2:p:264:MET:CE    | 2.26                     | 0.66              |
| 2:r:319:LEU:HD21  | 2:s:264:MET:CE    | 2.26                     | 0.66              |
| 2:u:319:LEU:HD21  | 2:v:264:MET:CE    | 2.26                     | 0.66              |
| 3:2:238:ARG:O     | 3:2:239:ALA:C     | 2.39                     | 0.66              |
| 3:ZE:50:ARG:HB3   | 3:ZE:66:LEU:H     | 1.61                     | 0.66              |
| 4:ZF:157:ASN:ND2  | 4:ZL:143:LEU:HD13 | 2.10                     | 0.66              |
| 4:ZZ:104:GLU:OE1  | 4:Ze:338:GLN:NE2  | 2.29                     | 0.66              |
| 5:AB:211:VAL:O    | 3:AM:1:MET:CB     | 2.43                     | 0.66              |
| 3:AG:82:SER:HB3   | 3:AG:223:ASN:HD21 | 1.61                     | 0.66              |
| 3:AJ:3:SER:CB     | 12:BE:75:LYS:HZ3  | 2.07                     | 0.66              |
| 9:Av:116:PHE:HE2  | 11:A7:4:ARG:CZ    | 2.08                     | 0.66              |
| 6:BV:391:VAL:HG21 | 6:BV:409:MET:HE1  | 1.78                     | 0.66              |
| 1:C:219:MET:SD    | 1:D:212:TYR:HB2   | 2.36                     | 0.66              |
| 1:F:228:ASN:ND2   | 1:H:24:TRP:CE2    | 2.61                     | 0.66              |
| 1:Q:88:ALA:CB     | 1:S:171:ILE:HD12  | 2.25                     | 0.66              |
| 1:T:47:ALA:HB3    | 2:q:178:GLN:CG    | 2.26                     | 0.66              |
| 1:U:50:SER:HB3    | 2:r:32:ARG:NH1    | 2.11                     | 0.66              |
| 2:a:79:MET:HG2    | 2:z:56:PRO:HD2    | 1.78                     | 0.66              |
| 2:a:80:GLN:HE22   | 3:8:58:GLU:HG2    | 1.59                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:b:80:GLN:OE1    | 3:AG:170:VAL:HA    | 1.96                     | 0.66              |
| 2:f:56:PRO:HD2    | 2:g:79:MET:HG2     | 1.77                     | 0.66              |
| 2:m:319:LEU:HD21  | 2:n:264:MET:CE     | 2.26                     | 0.66              |
| 2:n:319:LEU:HD21  | 2:o:264:MET:CE     | 2.26                     | 0.66              |
| 2:w:33:GLU:HG3    | 2:w:95:PRO:HD3     | 1.78                     | 0.66              |
| 3:7:257:LEU:HG    | 3:AK:230:LEU:CD1   | 2.25                     | 0.66              |
| 5:AA:35:ARG:O     | 5:AA:173:ARG:NH2   | 2.28                     | 0.66              |
| 5:AC:208:GLY:HA3  | 3:AN:6:TRP:HZ3     | 1.61                     | 0.66              |
| 3:AK:130:THR:HG23 | 3:AK:132:GLY:H     | 1.61                     | 0.66              |
| 6:Ac:391:VAL:HG21 | 6:Ac:409:MET:HE1   | 1.78                     | 0.66              |
| 6:Af:391:VAL:HG21 | 6:Af:409:MET:HE1   | 1.78                     | 0.66              |
| 9:Ay:152:ARG:HH21 | 6:WJ:165:PHE:HA    | 1.60                     | 0.66              |
| 6:WF:197:LEU:HD12 | 6:WG:175:SER:HB3   | 1.74                     | 0.66              |
| 6:BS:391:VAL:HG21 | 6:BS:409:MET:HE1   | 1.78                     | 0.66              |
| 1:B:47:ALA:HB3    | 2:y:178:GLN:CG     | 2.26                     | 0.66              |
| 1:U:47:ALA:HB3    | 2:r:178:GLN:CG     | 2.26                     | 0.66              |
| 2:k:56:PRO:HD2    | 2:l:79:MET:HG2     | 1.77                     | 0.66              |
| 2:l:319:LEU:HD21  | 2:m:264:MET:CE     | 2.26                     | 0.66              |
| 2:u:56:PRO:HD2    | 2:v:79:MET:HG2     | 1.77                     | 0.66              |
| 2:v:33:GLU:HG3    | 2:v:95:PRO:HD3     | 1.78                     | 0.66              |
| 2:z:33:GLU:HG3    | 2:z:95:PRO:HD3     | 1.78                     | 0.66              |
| 3:2:196:GLN:HE22  | 3:7:55:GLN:HE21    | 1.44                     | 0.66              |
| 3:8:17:THR:HG23   | 3:ZD:68:ILE:HD11   | 1.76                     | 0.66              |
| 4:ZM:33:LYS:HD2   | 4:ZM:61:PHE:HA     | 1.77                     | 0.66              |
| 4:ZR:337:THR:HG22 | 4:ZR:339:ALA:H     | 1.61                     | 0.66              |
| 4:ZT:17:LEU:CD1   | 4:ZY:395:ILE:HD11  | 2.22                     | 0.66              |
| 4:ZX:380:ARG:HE   | 4:Zd:393:ASP:CG    | 2.03                     | 0.66              |
| 5:AB:240:ASN:ND2  | 12:BC:113:GLN:HE21 | 1.94                     | 0.66              |
| 6:AT:294:ARG:HE   | 11:A0:72:HIS:HE1   | 1.43                     | 0.66              |
| 6:Ae:391:VAL:HG21 | 6:Ae:409:MET:HE1   | 1.78                     | 0.66              |
| 6:Ag:391:VAL:HG21 | 6:Ag:409:MET:HE1   | 1.78                     | 0.66              |
| 6:Ai:391:VAL:HG21 | 6:Ai:409:MET:HE1   | 1.78                     | 0.66              |
| 6:Ak:391:VAL:HG21 | 6:Ak:409:MET:HE1   | 1.78                     | 0.66              |
| 9:Ay:143:ARG:NH2  | 9:Ay:177:SER:HA    | 2.10                     | 0.66              |
| 6:UP:98:LEU:HD12  | 6:UP:146:THR:OG1   | 1.94                     | 0.66              |
| 6:BR:391:VAL:HG21 | 6:BR:409:MET:HE1   | 1.78                     | 0.66              |
| 1:F:50:SER:HB3    | 2:c:32:ARG:NH1     | 2.11                     | 0.65              |
| 1:G:50:SER:HB3    | 2:d:32:ARG:NH1     | 2.12                     | 0.65              |
| 1:S:47:ALA:HB3    | 2:p:178:GLN:CG     | 2.26                     | 0.65              |
| 1:V:88:ALA:CB     | 1:X:171:ILE:HD12   | 2.25                     | 0.65              |
| 2:b:33:GLU:HG3    | 2:b:95:PRO:HD3     | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:k:319:LEU:HD21  | 2:l:264:MET:CE    | 2.26                     | 0.65              |
| 2:p:319:LEU:HD21  | 2:q:264:MET:CE    | 2.26                     | 0.65              |
| 3:2:51:GLN:NE2    | 5:AA:134:GLU:OE2  | 2.29                     | 0.65              |
| 3:4:86:LEU:HD12   | 4:ZF:42:MET:HE1   | 1.78                     | 0.65              |
| 3:ZA:42:GLU:OE2   | 3:ZA:73:ARG:NH1   | 2.28                     | 0.65              |
| 4:ZS:196:MET:HA   | 4:ZS:196:MET:HE3  | 1.78                     | 0.65              |
| 4:ZX:285:LYS:O    | 4:ZX:306:ASN:ND2  | 2.23                     | 0.65              |
| 5:AA:48:GLY:N     | 11:A6:93:PRO:HB3  | 2.11                     | 0.65              |
| 5:AB:206:LEU:HD22 | 3:AG:38:ARG:NH2   | 2.11                     | 0.65              |
| 3:AI:73:ARG:HD3   | 12:BD:78:TYR:CZ   | 2.31                     | 0.65              |
| 6:Ad:391:VAL:HG21 | 6:Ad:409:MET:HE1  | 1.78                     | 0.65              |
| 6:Ah:391:VAL:HG21 | 6:Ah:409:MET:HE1  | 1.78                     | 0.65              |
| 9:Ay:68:ILE:O     | 9:Ay:71:PHE:N     | 2.29                     | 0.65              |
| 6:UN:98:LEU:HD12  | 6:UN:146:THR:OG1  | 1.94                     | 0.65              |
| 6:UO:125:GLN:HA   | 6:UO:128:GLU:HB2  | 1.77                     | 0.65              |
| 6:WR:122:GLY:O    | 6:WR:123:ILE:C    | 2.39                     | 0.65              |
| 1:A:47:ALA:HB3    | 2:x:178:GLN:CG    | 2.26                     | 0.65              |
| 1:C:50:SER:HB3    | 2:z:32:ARG:NH1    | 2.11                     | 0.65              |
| 1:H:219:MET:SD    | 1:I:212:TYR:HB2   | 2.36                     | 0.65              |
| 1:R:88:ALA:CB     | 1:T:171:ILE:HD12  | 2.25                     | 0.65              |
| 1:U:219:MET:SD    | 1:V:212:TYR:HB2   | 2.36                     | 0.65              |
| 1:V:47:ALA:HB3    | 2:s:178:GLN:CG    | 2.26                     | 0.65              |
| 2:a:33:GLU:HG3    | 2:a:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:g:56:PRO:HD2    | 2:h:79:MET:HG2    | 1.77                     | 0.65              |
| 2:j:319:LEU:HD21  | 2:k:264:MET:CE    | 2.26                     | 0.65              |
| 2:k:33:GLU:HG3    | 2:k:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:s:33:GLU:HG3    | 2:s:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:y:56:PRO:HD2    | 2:z:79:MET:HG2    | 1.77                     | 0.65              |
| 3:ZD:205:THR:HB   | 3:ZD:208:LEU:HD23 | 1.77                     | 0.65              |
| 4:ZK:331:ASP:HA   | 4:ZP:40:ALA:HB1   | 1.78                     | 0.65              |
| 5:AE:131:GLU:HG2  | 3:AJ:179:MET:HE3  | 1.78                     | 0.65              |
| 6:Aa:391:VAL:HG21 | 6:Aa:409:MET:HE1  | 1.78                     | 0.65              |
| 6:Aj:391:VAL:HG21 | 6:Aj:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AP:391:VAL:HG21 | 6:AP:409:MET:HE1  | 1.78                     | 0.65              |
| 6:BP:312:VAL:O    | 6:BP:317:SER:OG   | 2.11                     | 0.65              |
| 6:BW:391:VAL:HG21 | 6:BW:409:MET:HE1  | 1.78                     | 0.65              |
| 1:A:50:SER:HB3    | 2:x:32:ARG:NH1    | 2.11                     | 0.65              |
| 1:B:50:SER:HB3    | 2:y:32:ARG:NH1    | 2.12                     | 0.65              |
| 1:D:50:SER:HB3    | 2:a:32:ARG:NH1    | 2.12                     | 0.65              |
| 1:E:50:SER:HB3    | 2:b:32:ARG:NH1    | 2.11                     | 0.65              |
| 1:F:219:MET:SD    | 1:G:212:TYR:HB2   | 2.36                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:T:50:SER:HB3    | 2:q:32:ARG:NH1    | 2.12                     | 0.65              |
| 1:V:50:SER:HB3    | 2:s:32:ARG:NH1    | 2.11                     | 0.65              |
| 2:c:33:GLU:HG3    | 2:c:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:l:33:GLU:HG3    | 2:l:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:q:319:LEU:HD21  | 2:r:264:MET:CE    | 2.26                     | 0.65              |
| 2:w:319:LEU:HD21  | 2:x:264:MET:CE    | 2.26                     | 0.65              |
| 2:x:319:LEU:HD21  | 2:y:264:MET:CE    | 2.26                     | 0.65              |
| 3:ZA:208:LEU:O    | 3:ZA:210:GLY:N    | 2.30                     | 0.65              |
| 3:ZC:99:GLY:HA3   | 3:ZC:212:GLY:HA3  | 1.79                     | 0.65              |
| 4:ZX:2:SER:OG     | 4:ZX:3:PHE:N      | 2.27                     | 0.65              |
| 3:AI:52:PRO:HA    | 3:AI:64:SER:O     | 1.96                     | 0.65              |
| 6:AR:391:VAL:HG21 | 6:AR:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AI:391:VAL:HG21 | 6:AI:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AQ:391:VAL:HG21 | 6:AQ:409:MET:HE1  | 1.78                     | 0.65              |
| 6:BX:391:VAL:HG21 | 6:BX:409:MET:HE1  | 1.78                     | 0.65              |
| 1:B:219:MET:SD    | 1:C:212:TYR:HB2   | 2.36                     | 0.65              |
| 1:C:47:ALA:HB3    | 2:z:178:GLN:CG    | 2.27                     | 0.65              |
| 1:J:228:ASN:ND2   | 1:L:24:TRP:CE2    | 2.61                     | 0.65              |
| 1:N:47:ALA:HB3    | 2:k:178:GLN:CG    | 2.26                     | 0.65              |
| 1:O:47:ALA:HB3    | 2:l:178:GLN:CG    | 2.26                     | 0.65              |
| 2:h:33:GLU:HG3    | 2:h:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:i:319:LEU:HD21  | 2:j:264:MET:CE    | 2.26                     | 0.65              |
| 2:y:319:LEU:HD21  | 2:z:264:MET:CE    | 2.26                     | 0.65              |
| 3:0:6:TRP:HB2     | 5:AD:70:GLN:HB3   | 1.77                     | 0.65              |
| 3:ZB:28:ASN:HD22  | 4:ZG:52:VAL:HG23  | 1.61                     | 0.65              |
| 4:ZK:270:ASN:ND2  | 4:ZQ:192:ASN:HA   | 2.12                     | 0.65              |
| 4:ZL:373:VAL:O    | 4:ZL:376:ILE:N    | 2.27                     | 0.65              |
| 3:AF:17:THR:HG23  | 3:AK:68:ILE:HD11  | 1.78                     | 0.65              |
| 3:AK:6:TRP:NE1    | 12:BF:77:VAL:HG11 | 2.12                     | 0.65              |
| 6:AZ:391:VAL:HG21 | 6:AZ:409:MET:HE1  | 1.78                     | 0.65              |
| 7:Ab:83:ASN:O     | 7:Ab:87:ILE:HG23  | 1.97                     | 0.65              |
| 6:AI:389:VAL:HG21 | 6:AI:416:THR:HG21 | 1.79                     | 0.65              |
| 6:Am:391:VAL:HG21 | 6:Am:409:MET:HE1  | 1.78                     | 0.65              |
| 6:An:391:VAL:HG21 | 6:An:409:MET:HE1  | 1.78                     | 0.65              |
| 6:Ap:391:VAL:HG21 | 6:Ap:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AO:391:VAL:HG21 | 6:AO:409:MET:HE1  | 1.78                     | 0.65              |
| 8:At:193:LEU:HD22 | 8:At:228:LEU:HD11 | 1.77                     | 0.65              |
| 9:Aw:66:ARG:NH2   | 9:Aw:242:SER:OG   | 2.30                     | 0.65              |
| 6:WO:197:LEU:HD12 | 6:WP:175:SER:CB   | 2.26                     | 0.65              |
| 1:A:219:MET:SD    | 1:B:212:TYR:HB2   | 2.36                     | 0.65              |
| 1:M:47:ALA:HB3    | 2:j:178:GLN:CG    | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:T:88:ALA:CB     | 1:V:171:ILE:HD12  | 2.25                     | 0.65              |
| 1:U:88:ALA:CB     | 1:W:171:ILE:HD12  | 2.25                     | 0.65              |
| 1:Z:50:SER:HB3    | 2:w:32:ARG:NH1    | 2.11                     | 0.65              |
| 2:a:319:LEU:HD21  | 2:b:264:MET:CE    | 2.26                     | 0.65              |
| 2:j:56:PRO:HD2    | 2:k:79:MET:HG2    | 1.78                     | 0.65              |
| 2:s:80:GLN:NE2    | 3:Al:141:THR:HG23 | 2.01                     | 0.65              |
| 2:t:319:LEU:HD21  | 2:u:264:MET:CE    | 2.26                     | 0.65              |
| 2:v:56:PRO:HD2    | 2:w:79:MET:HG2    | 1.77                     | 0.65              |
| 4:ZK:112:GLN:HE21 | 4:ZK:331:ASP:HB3  | 1.61                     | 0.65              |
| 5:AD:51:LEU:O     | 11:A9:93:PRO:HD3  | 1.96                     | 0.65              |
| 3:AK:153:ARG:HG2  | 3:AK:213:LEU:HD12 | 1.78                     | 0.65              |
| 6:AY:391:VAL:HG21 | 6:AY:409:MET:HE1  | 1.78                     | 0.65              |
| 7:Ab:75:ASP:OD1   | 6:WQ:124:SER:CB   | 2.45                     | 0.65              |
| 6:Al:389:VAL:HG21 | 6:Al:416:THR:HG21 | 1.79                     | 0.65              |
| 6:Ao:391:VAL:HG21 | 6:Ao:409:MET:HE1  | 1.78                     | 0.65              |
| 6:WD:115:LEU:CD2  | 6:WD:134:ARG:HD2  | 2.24                     | 0.65              |
| 1:P:50:SER:HB3    | 2:m:32:ARG:NH1    | 2.11                     | 0.65              |
| 1:S:88:ALA:CB     | 1:U:171:ILE:HD12  | 2.25                     | 0.65              |
| 1:W:47:ALA:HB3    | 2:t:178:GLN:CG    | 2.27                     | 0.65              |
| 1:Z:47:ALA:HB3    | 2:w:178:GLN:CG    | 2.26                     | 0.65              |
| 2:a:264:MET:CE    | 2:z:319:LEU:HD21  | 2.26                     | 0.65              |
| 2:g:33:GLU:HG3    | 2:g:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:h:319:LEU:HD21  | 2:i:264:MET:CE    | 2.26                     | 0.65              |
| 2:j:33:GLU:HG3    | 2:j:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:m:33:GLU:HG3    | 2:m:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:r:33:GLU:HG3    | 2:r:95:PRO:HD3    | 1.78                     | 0.65              |
| 3:ZA:37:GLN:HG2   | 3:ZA:79:ARG:HD3   | 1.77                     | 0.65              |
| 3:ZB:28:ASN:HD22  | 3:ZB:31:THR:HG21  | 1.62                     | 0.65              |
| 4:ZL:144:MET:HE3  | 4:ZL:306:ASN:HD21 | 1.61                     | 0.65              |
| 6:AU:391:VAL:HG21 | 6:AU:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AW:278:THR:HG21 | 10:A3:14:LEU:HB3  | 1.77                     | 0.65              |
| 6:AW:391:VAL:HG21 | 6:AW:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AX:391:VAL:HG21 | 6:AX:409:MET:HE1  | 1.78                     | 0.65              |
| 7:Ab:67:PRO:HB3   | 6:WP:123:ILE:HG23 | 1.78                     | 0.65              |
| 9:Au:58:LEU:O     | 9:Au:62:THR:OG1   | 2.14                     | 0.65              |
| 9:Ax:204:LEU:HD22 | 9:Ax:212:VAL:HG11 | 1.78                     | 0.65              |
| 10:A4:11:ILE:HG22 | 6:BX:372:ILE:HB   | 1.77                     | 0.65              |
| 6:WH:197:LEU:HA   | 6:WI:175:SER:OG   | 1.97                     | 0.65              |
| 6:WJ:128:GLU:HG2  | 6:WK:126:PHE:CD2  | 2.15                     | 0.65              |
| 6:BX:389:VAL:HG21 | 6:BX:416:THR:HG21 | 1.79                     | 0.65              |
| 1:D:47:ALA:HB3    | 2:a:178:GLN:CG    | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:50:SER:HB3    | 2:e:32:ARG:NH1    | 2.12                     | 0.65              |
| 1:K:50:SER:HB3    | 2:h:32:ARG:NH1    | 2.11                     | 0.65              |
| 1:N:57:PRO:HB2    | 2:l:132:GLN:OE1   | 1.97                     | 0.65              |
| 1:P:57:PRO:HB2    | 2:n:132:GLN:OE1   | 1.97                     | 0.65              |
| 1:Q:57:PRO:HB2    | 2:o:132:GLN:OE1   | 1.97                     | 0.65              |
| 1:R:47:ALA:HB3    | 2:o:178:GLN:CG    | 2.27                     | 0.65              |
| 2:b:319:LEU:HD21  | 2:c:264:MET:CE    | 2.26                     | 0.65              |
| 2:c:319:LEU:HD21  | 2:d:264:MET:CE    | 2.26                     | 0.65              |
| 2:h:56:PRO:HD2    | 2:i:79:MET:HG2    | 1.77                     | 0.65              |
| 2:i:56:PRO:HD2    | 2:j:79:MET:HG2    | 1.77                     | 0.65              |
| 2:q:33:GLU:HG3    | 2:q:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:x:56:PRO:HD2    | 2:y:79:MET:HG2    | 1.78                     | 0.65              |
| 3:2:55:GLN:HG2    | 5:AA:142:THR:HG21 | 1.78                     | 0.65              |
| 3:2:122:VAL:O     | 3:7:180:ASN:ND2   | 2.29                     | 0.65              |
| 3:ZE:205:THR:HB   | 3:ZE:208:LEU:HD22 | 1.77                     | 0.65              |
| 4:ZF:379:GLN:HG3  | 4:ZK:391:THR:HG23 | 1.79                     | 0.65              |
| 4:ZK:18:ASP:HB3   | 4:ZP:5:GLN:NE2    | 2.11                     | 0.65              |
| 4:ZL:269:GLN:HG3  | 4:ZL:270:ASN:H    | 1.61                     | 0.65              |
| 4:ZQ:288:ASP:H    | 4:ZQ:305:SER:HB3  | 1.61                     | 0.65              |
| 4:ZV:234:GLU:HB3  | 4:Zb:255:THR:HG22 | 1.78                     | 0.65              |
| 4:Za:104:GLU:CD   | 4:Zf:341:GLY:HA2  | 2.21                     | 0.65              |
| 3:AH:6:TRP:NE1    | 12:BC:77:VAL:HB   | 2.11                     | 0.65              |
| 3:AI:50:ARG:CB    | 6:BN:322:PRO:HG3  | 2.26                     | 0.65              |
| 6:AS:389:VAL:HG21 | 6:AS:416:THR:HG21 | 1.79                     | 0.65              |
| 6:Ag:295:SER:CB   | 11:A8:72:HIS:HA   | 2.27                     | 0.65              |
| 6:WM:143:THR:OG1  | 6:WN:154:ARG:CG   | 2.42                     | 0.65              |
| 6:BW:389:VAL:HG21 | 6:BW:416:THR:HG21 | 1.79                     | 0.65              |
| 1:H:47:ALA:HB3    | 2:e:178:GLN:CG    | 2.26                     | 0.65              |
| 1:H:228:ASN:ND2   | 1:J:24:TRP:CE2    | 2.61                     | 0.65              |
| 1:O:57:PRO:HB2    | 2:m:132:GLN:OE1   | 1.97                     | 0.65              |
| 2:e:319:LEU:HD21  | 2:f:264:MET:CE    | 2.26                     | 0.65              |
| 2:f:319:LEU:HD21  | 2:g:264:MET:CE    | 2.26                     | 0.65              |
| 2:g:319:LEU:HD21  | 2:h:264:MET:CE    | 2.26                     | 0.65              |
| 2:i:33:GLU:HG3    | 2:i:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:s:319:LEU:HD21  | 2:t:264:MET:CE    | 2.26                     | 0.65              |
| 2:v:319:LEU:HD21  | 2:w:264:MET:CE    | 2.26                     | 0.65              |
| 3:1:43:ASP:HA     | 3:1:72:VAL:HA     | 1.78                     | 0.65              |
| 3:5:70:THR:HG23   | 3:AI:85:ASN:CG    | 2.21                     | 0.65              |
| 3:ZE:85:ASN:HD22  | 4:ZP:4:SER:CB     | 2.10                     | 0.65              |
| 4:ZI:375:MET:SD   | 4:ZN:388:THR:OG1  | 2.51                     | 0.65              |
| 4:Zc:390:LYS:HB2  | 4:Zh:402:LEU:HD22 | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:70:GLN:CB    | 3:AM:6:TRP:NE1    | 2.59                     | 0.65              |
| 5:AC:104:ASN:ND2  | 3:AH:38:ARG:NH2   | 2.44                     | 0.65              |
| 3:AH:153:ARG:HH21 | 3:AN:108:PRO:HG2  | 1.61                     | 0.65              |
| 6:AT:389:VAL:HG21 | 6:AT:416:THR:HG21 | 1.79                     | 0.65              |
| 6:AT:391:VAL:HG21 | 6:AT:409:MET:HE1  | 1.78                     | 0.65              |
| 6:AV:391:VAL:HG21 | 6:AV:409:MET:HE1  | 1.78                     | 0.65              |
| 6:Ak:389:VAL:HG21 | 6:Ak:416:THR:HG21 | 1.79                     | 0.65              |
| 6:An:389:VAL:HG21 | 6:An:416:THR:HG21 | 1.79                     | 0.65              |
| 1:F:166:GLU:CB    | 1:G:35:THR:HG21   | 2.20                     | 0.65              |
| 1:I:47:ALA:HB3    | 2:f:178:GLN:CG    | 2.26                     | 0.65              |
| 1:L:50:SER:HB3    | 2:i:32:ARG:NH1    | 2.11                     | 0.65              |
| 1:Q:50:SER:HB3    | 2:n:32:ARG:NH1    | 2.12                     | 0.65              |
| 1:R:57:PRO:HB2    | 2:p:132:GLN:OE1   | 1.97                     | 0.65              |
| 2:d:33:GLU:HG3    | 2:d:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:d:319:LEU:HD21  | 2:e:264:MET:CE    | 2.26                     | 0.65              |
| 3:1:42:GLU:OE1    | 3:AK:189:GLU:HA   | 1.96                     | 0.65              |
| 3:ZE:31:THR:CG2   | 4:ZJ:39:PHE:CB    | 2.72                     | 0.65              |
| 3:ZE:85:ASN:ND2   | 4:ZP:50:LEU:CD2   | 2.60                     | 0.65              |
| 5:AB:70:GLN:CD    | 3:AM:6:TRP:HE1    | 2.04                     | 0.65              |
| 3:AI:50:ARG:HG3   | 6:BN:322:PRO:HG3  | 1.77                     | 0.65              |
| 3:AJ:257:LEU:HD11 | 12:BE:102:MET:HG3 | 1.79                     | 0.65              |
| 3:AK:44:LEU:CD2   | 12:BF:78:TYR:HB2  | 2.27                     | 0.65              |
| 6:Ag:389:VAL:HG21 | 6:Ag:416:THR:HG21 | 1.79                     | 0.65              |
| 6:Aj:389:VAL:HG21 | 6:Aj:416:THR:HG21 | 1.79                     | 0.65              |
| 6:UK:103:GLN:CD   | 6:WF:182:PRO:HB3  | 2.21                     | 0.65              |
| 6:BU:389:VAL:HG21 | 6:BU:416:THR:HG21 | 1.79                     | 0.65              |
| 6:BV:389:VAL:HG21 | 6:BV:416:THR:HG21 | 1.79                     | 0.65              |
| 1:X:47:ALA:HB3    | 2:u:178:GLN:CG    | 2.26                     | 0.65              |
| 2:l:35:SER:HB3    | 2:m:123:MET:HE1   | 1.79                     | 0.65              |
| 2:n:33:GLU:HG3    | 2:n:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:p:33:GLU:HG3    | 2:p:95:PRO:HD3    | 1.78                     | 0.65              |
| 2:p:80:GLN:CD     | 5:AD:154:THR:HA   | 2.17                     | 0.65              |
| 3:8:46:TYR:HA     | 3:8:69:GLY:HA2    | 1.79                     | 0.65              |
| 4:ZI:294:ILE:O    | 4:ZI:358:ASN:ND2  | 2.29                     | 0.65              |
| 4:ZN:269:GLN:NE2  | 4:ZT:146:ALA:HB3  | 2.12                     | 0.65              |
| 4:ZO:235:ASN:HD22 | 4:ZU:189:SER:HB2  | 1.61                     | 0.65              |
| 4:ZW:380:ARG:CZ   | 4:Zc:393:ASP:OD2  | 2.45                     | 0.65              |
| 5:AC:220:MET:HE3  | 3:AH:245:LYS:HD3  | 1.77                     | 0.65              |
| 3:AF:62:LEU:HD11  | 12:BB:84:LEU:HD11 | 1.77                     | 0.65              |
| 3:AF:238:ARG:NH2  | 3:AL:251:ASP:OD1  | 2.26                     | 0.65              |
| 3:AG:73:ARG:HD2   | 12:BB:78:TYR:OH   | 1.97                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AS:391:VAL:HG21 | 6:AS:409:MET:HE1  | 1.78                     | 0.65              |
| 10:A4:76:GLN:NE2  | 12:BE:132:LEU:O   | 2.29                     | 0.65              |
| 6:WB:200:SER:O    | 6:WC:158:ALA:CB   | 2.45                     | 0.65              |
| 6:WE:123:ILE:HB   | 6:WE:128:GLU:OE1  | 1.96                     | 0.65              |
| 6:WH:197:LEU:HD12 | 6:WI:175:SER:OG   | 1.97                     | 0.65              |
| 6:WW:134:ARG:HB3  | 6:WW:134:ARG:HH21 | 1.61                     | 0.65              |
| 1:M:57:PRO:HB2    | 2:k:132:GLN:OE1   | 1.97                     | 0.64              |
| 1:P:47:ALA:HB3    | 2:m:178:GLN:CG    | 2.27                     | 0.64              |
| 1:S:50:SER:HB3    | 2:p:32:ARG:NH1    | 2.11                     | 0.64              |
| 1:S:57:PRO:HB2    | 2:q:132:GLN:OE1   | 1.97                     | 0.64              |
| 1:W:50:SER:HB3    | 2:t:32:ARG:NH1    | 2.11                     | 0.64              |
| 1:Y:50:SER:HB3    | 2:v:32:ARG:NH1    | 2.12                     | 0.64              |
| 2:f:33:GLU:HG3    | 2:f:95:PRO:HD3    | 1.78                     | 0.64              |
| 2:j:35:SER:HB3    | 2:k:123:MET:HE1   | 1.79                     | 0.64              |
| 2:k:35:SER:HB3    | 2:l:123:MET:HE1   | 1.79                     | 0.64              |
| 3:0:115:THR:HB    | 3:0:191:LEU:HD23  | 1.79                     | 0.64              |
| 3:4:56:SER:O      | 5:AC:138:ALA:CB   | 2.32                     | 0.64              |
| 3:8:1:MET:HB3     | 3:AL:29:VAL:HB    | 1.79                     | 0.64              |
| 3:ZA:76:ALA:HA    | 4:ZF:47:LYS:CD    | 2.27                     | 0.64              |
| 4:ZJ:57:ILE:HG13  | 4:ZO:47:LYS:HB2   | 1.78                     | 0.64              |
| 4:ZM:223:PRO:HD2  | 4:ZM:223:PRO:O    | 1.97                     | 0.64              |
| 5:AE:228:GLU:HB2  | 3:AK:258:THR:CG2  | 2.06                     | 0.64              |
| 3:AG:73:ARG:HG3   | 12:BB:78:TYR:HE2  | 1.62                     | 0.64              |
| 1:A:166:GLU:CB    | 1:B:35:THR:HG21   | 2.20                     | 0.64              |
| 1:B:166:GLU:CB    | 1:C:35:THR:HG21   | 2.20                     | 0.64              |
| 1:E:166:GLU:CB    | 1:F:35:THR:HG21   | 2.20                     | 0.64              |
| 1:L:57:PRO:HB2    | 2:j:132:GLN:OE1   | 1.97                     | 0.64              |
| 1:O:50:SER:HB3    | 2:l:32:ARG:NH1    | 2.11                     | 0.64              |
| 1:Y:47:ALA:HB3    | 2:v:178:GLN:CG    | 2.27                     | 0.64              |
| 2:l:258:ARG:NH1   | 2:n:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:o:33:GLU:HG3    | 2:o:95:PRO:HD3    | 1.78                     | 0.64              |
| 2:w:56:PRO:HD2    | 2:x:79:MET:HG2    | 1.78                     | 0.64              |
| 3:0:2:ILE:HG23    | 5:AD:212:LYS:HA   | 1.79                     | 0.64              |
| 3:8:151:ILE:HG23  | 3:8:157:VAL:HG22  | 1.79                     | 0.64              |
| 3:ZA:145:ASN:HA   | 4:ZF:352:ASN:ND2  | 2.10                     | 0.64              |
| 4:ZG:118:GLY:HA2  | 4:ZG:316:VAL:HG12 | 1.77                     | 0.64              |
| 4:ZQ:18:ASP:O     | 4:ZV:5:GLN:NE2    | 2.27                     | 0.64              |
| 4:ZQ:331:ASP:HA   | 4:ZV:40:ALA:HB1   | 1.79                     | 0.64              |
| 4:ZV:267:MET:HE3  | 4:ZV:269:GLN:HE21 | 1.61                     | 0.64              |
| 4:ZZ:269:GLN:CD   | 4:Zf:286:PRO:HG3  | 2.22                     | 0.64              |
| 5:AA:72:ASP:CB    | 3:AL:9:LYS:HZ1    | 2.06                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AB:9:MET:HE3    | 12:BB:103:VAL:HG11 | 1.79                     | 0.64              |
| 5:AE:133:SER:HA   | 5:AE:148:PRO:HD3   | 1.77                     | 0.64              |
| 6:AU:389:VAL:HG21 | 6:AU:416:THR:HG21  | 1.79                     | 0.64              |
| 6:AV:389:VAL:HG21 | 6:AV:416:THR:HG21  | 1.79                     | 0.64              |
| 6:Ah:389:VAL:HG21 | 6:Ah:416:THR:HG21  | 1.79                     | 0.64              |
| 9:Au:160:GLN:O    | 6:WP:165:PHE:CB    | 2.45                     | 0.64              |
| 9:Ay:85:PRO:O     | 9:Ay:86:ASN:C      | 2.40                     | 0.64              |
| 6:BS:389:VAL:HG21 | 6:BS:416:THR:HG21  | 1.79                     | 0.64              |
| 1:C:166:GLU:CB    | 1:D:35:THR:HG21    | 2.20                     | 0.64              |
| 1:T:57:PRO:HB2    | 2:r:132:GLN:OE1    | 1.97                     | 0.64              |
| 2:m:35:SER:HB3    | 2:n:123:MET:HE1    | 1.80                     | 0.64              |
| 2:n:35:SER:HB3    | 2:o:123:MET:HE1    | 1.80                     | 0.64              |
| 2:r:258:ARG:NH1   | 2:t:140:ASN:ND2    | 2.46                     | 0.64              |
| 2:s:258:ARG:NH1   | 2:u:140:ASN:ND2    | 2.46                     | 0.64              |
| 3:1:73:ARG:NH1    | 5:AE:202:MET:CE    | 2.59                     | 0.64              |
| 3:3:50:ARG:HH21   | 3:AM:73:ARG:NH2    | 1.96                     | 0.64              |
| 3:7:70:THR:HG22   | 3:7:71:GLY:H       | 1.62                     | 0.64              |
| 4:ZN:269:GLN:HG2  | 4:ZT:190:GLN:O     | 1.96                     | 0.64              |
| 4:ZS:65:THR:HG21  | 4:Zd:4:SER:HG      | 1.62                     | 0.64              |
| 4:ZU:155:GLN:HG3  | 4:ZU:277:VAL:HB    | 1.79                     | 0.64              |
| 4:ZV:77:ILE:HD12  | 4:ZV:96:ARG:HD3    | 1.77                     | 0.64              |
| 5:AA:220:MET:HE3  | 3:AF:246:ALA:HB2   | 1.79                     | 0.64              |
| 6:AT:236:LYS:HZ3  | 6:UJ:167:ARG:HH11  | 1.44                     | 0.64              |
| 6:Am:389:VAL:HG21 | 6:Am:416:THR:HG21  | 1.79                     | 0.64              |
| 6:Ao:389:VAL:HG21 | 6:Ao:416:THR:HG21  | 1.79                     | 0.64              |
| 6:Ap:389:VAL:HG21 | 6:Ap:416:THR:HG21  | 1.79                     | 0.64              |
| 7:Aq:58:VAL:HG21  | 9:Aw:207:LEU:HD11  | 1.79                     | 0.64              |
| 9:Ay:86:ASN:O     | 9:Ay:89:LEU:N      | 2.29                     | 0.64              |
| 11:A7:36:PRO:HB3  | 11:A7:96:ASP:HB2   | 1.79                     | 0.64              |
| 1:X:50:SER:HB3    | 2:u:32:ARG:NH1     | 2.12                     | 0.64              |
| 2:k:258:ARG:NH1   | 2:m:140:ASN:ND2    | 2.46                     | 0.64              |
| 2:k:319:LEU:HD21  | 2:l:264:MET:HE2    | 1.80                     | 0.64              |
| 3:7:254:LEU:O     | 3:7:258:THR:HG23   | 1.97                     | 0.64              |
| 4:ZJ:65:THR:HG22  | 4:ZU:50:LEU:HD12   | 1.79                     | 0.64              |
| 5:AB:224:ALA:HA   | 3:AG:253:MET:HE3   | 1.79                     | 0.64              |
| 5:AD:16:LEU:HD21  | 3:AI:253:MET:HE2   | 1.76                     | 0.64              |
| 3:AF:259:GLN:O    | 3:AF:260:LEU:C     | 2.39                     | 0.64              |
| 6:AX:372:ILE:HG21 | 10:A3:11:ILE:CG2   | 2.28                     | 0.64              |
| 9:Au:52:THR:OG1   | 10:Az:91:LYS:NZ    | 2.31                     | 0.64              |
| 9:Av:116:PHE:CE2  | 11:A7:4:ARG:NH1    | 2.66                     | 0.64              |
| 9:Ax:141:GLN:HA   | 6:WD:165:PHE:HE2   | 1.62                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Ay:82:SER:O     | 9:Ay:83:ALA:C     | 2.41                     | 0.64              |
| 6:WA:154:ARG:HG2  | 6:WW:143:THR:OG1  | 1.97                     | 0.64              |
| 6:BT:389:VAL:HG21 | 6:BT:416:THR:HG21 | 1.79                     | 0.64              |
| 1:D:166:GLU:CB    | 1:E:35:THR:HG21   | 2.20                     | 0.64              |
| 1:I:50:SER:HB3    | 2:f:32:ARG:NH1    | 2.12                     | 0.64              |
| 1:J:50:SER:HB3    | 2:g:32:ARG:NH1    | 2.12                     | 0.64              |
| 1:K:57:PRO:HB2    | 2:i:132:GLN:OE1   | 1.97                     | 0.64              |
| 2:c:319:LEU:HD21  | 2:d:264:MET:HE2   | 1.79                     | 0.64              |
| 2:d:319:LEU:HD21  | 2:e:264:MET:HE2   | 1.80                     | 0.64              |
| 2:j:319:LEU:HD21  | 2:k:264:MET:HE2   | 1.79                     | 0.64              |
| 2:m:258:ARG:NH1   | 2:o:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:o:35:SER:HB3    | 2:p:123:MET:HE1   | 1.80                     | 0.64              |
| 3:0:2:ILE:CG2     | 5:AD:211:VAL:C    | 2.68                     | 0.64              |
| 3:3:240:TYR:CD2   | 3:8:253:MET:HE3   | 2.32                     | 0.64              |
| 3:5:219:VAL:HG11  | 3:ZA:38:ARG:NH2   | 2.12                     | 0.64              |
| 4:ZR:71:ARG:NH1   | 4:ZR:74:ASP:OD1   | 2.30                     | 0.64              |
| 4:ZY:159:ASN:ND2  | 4:ZY:161:THR:OG1  | 2.30                     | 0.64              |
| 4:Zc:2:SER:OG     | 4:Zc:3:PHE:N      | 2.21                     | 0.64              |
| 5:AB:231:MET:SD   | 3:AG:260:LEU:HD13 | 2.38                     | 0.64              |
| 5:AD:59:ALA:C     | 3:AI:66:LEU:CD1   | 2.71                     | 0.64              |
| 3:AM:109:ASP:OD2  | 3:AM:111:THR:OG1  | 2.15                     | 0.64              |
| 7:Ab:8:MET:CE     | 6:WS:123:ILE:C    | 2.70                     | 0.64              |
| 6:Ac:394:LYS:HA   | 6:Ac:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:Ae:372:ILE:CD1  | 10:A2:3:ALA:C     | 2.70                     | 0.64              |
| 6:Ae:389:VAL:HG21 | 6:Ae:416:THR:HG21 | 1.79                     | 0.64              |
| 6:AP:389:VAL:HG21 | 6:AP:416:THR:HG21 | 1.79                     | 0.64              |
| 6:AQ:389:VAL:HG21 | 6:AQ:416:THR:HG21 | 1.79                     | 0.64              |
| 11:A8:95:LEU:HD23 | 6:BL:318:ASN:C    | 2.21                     | 0.64              |
| 1:A:35:THR:HG21   | 1:Z:166:GLU:CB    | 2.20                     | 0.64              |
| 1:J:47:ALA:HB3    | 2:g:178:GLN:CG    | 2.26                     | 0.64              |
| 1:R:50:SER:HB3    | 2:o:32:ARG:NH1    | 2.12                     | 0.64              |
| 2:e:319:LEU:HD21  | 2:f:264:MET:HE2   | 1.80                     | 0.64              |
| 2:i:35:SER:HB3    | 2:j:123:MET:HE1   | 1.80                     | 0.64              |
| 2:l:319:LEU:HD21  | 2:m:264:MET:HE2   | 1.79                     | 0.64              |
| 2:q:258:ARG:NH1   | 2:s:140:ASN:ND2   | 2.46                     | 0.64              |
| 3:1:1:MET:HA      | 5:AE:211:VAL:O    | 1.97                     | 0.64              |
| 4:ZK:248:THR:OG1  | 4:ZK:257:ALA:N    | 2.31                     | 0.64              |
| 4:ZX:71:ARG:HD3   | 4:ZX:74:ASP:OD1   | 1.98                     | 0.64              |
| 4:Za:146:ALA:HB2  | 4:Za:286:PRO:HD3  | 1.80                     | 0.64              |
| 5:AB:224:ALA:HB2  | 3:AG:249:THR:HG23 | 1.79                     | 0.64              |
| 5:AE:26:LEU:CD2   | 3:AJ:242:ILE:HG12 | 2.27                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AE:54:ARG:NH1   | 12:BF:22:ASN:OD1  | 2.30                     | 0.64              |
| 5:AE:231:MET:HE3  | 3:AJ:257:LEU:HA   | 0.69                     | 0.64              |
| 5:AE:240:ASN:OD1  | 12:BF:109:SER:OG  | 2.16                     | 0.64              |
| 6:AX:394:LYS:HA   | 6:AX:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:AO:389:VAL:HG21 | 6:AO:416:THR:HG21 | 1.79                     | 0.64              |
| 6:BR:389:VAL:HG21 | 6:BR:416:THR:HG21 | 1.79                     | 0.64              |
| 1:M:50:SER:HB3    | 2:j:32:ARG:NH1    | 2.11                     | 0.64              |
| 1:Q:47:ALA:HB3    | 2:n:178:GLN:CG    | 2.26                     | 0.64              |
| 1:U:57:PRO:HB2    | 2:s:132:GLN:OE1   | 1.97                     | 0.64              |
| 2:h:35:SER:HB3    | 2:i:123:MET:HE1   | 1.79                     | 0.64              |
| 2:w:258:ARG:NH1   | 2:y:140:ASN:ND2   | 2.46                     | 0.64              |
| 3:0:89:THR:C      | 3:0:91:ASN:H      | 2.06                     | 0.64              |
| 3:1:239:ALA:HB2   | 3:7:1:MET:HE1     | 1.78                     | 0.64              |
| 3:ZB:244:SER:CB   | 4:ZG:399:LEU:HD23 | 2.27                     | 0.64              |
| 5:AA:4:ALA:HB2    | 12:BB:22:ASN:OD1  | 1.98                     | 0.64              |
| 5:AA:29:ALA:HB1   | 3:AL:1:MET:SD     | 2.38                     | 0.64              |
| 3:AH:126:GLY:HA2  | 3:AM:179:MET:HE3  | 1.79                     | 0.64              |
| 6:AT:394:LYS:HA   | 6:AT:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:AX:389:VAL:HG21 | 6:AX:416:THR:HG21 | 1.79                     | 0.64              |
| 6:AY:370:ARG:HE   | 10:A3:7:ILE:HD11  | 1.62                     | 0.64              |
| 6:AZ:394:LYS:HE3  | 6:AZ:394:LYS:HA   | 1.80                     | 0.64              |
| 6:Aa:394:LYS:HA   | 6:Aa:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:Ac:389:VAL:HG21 | 6:Ac:416:THR:HG21 | 1.79                     | 0.64              |
| 6:Af:389:VAL:HG21 | 6:Af:416:THR:HG21 | 1.79                     | 0.64              |
| 6:Ai:235:LEU:HD22 | 6:Aj:244:ARG:HH12 | 1.63                     | 0.64              |
| 6:Aj:372:ILE:HG21 | 10:A1:11:ILE:HG23 | 1.76                     | 0.64              |
| 7:Ar:8:MET:HG2    | 6:WD:124:SER:OG   | 1.98                     | 0.64              |
| 8:At:149:LEU:HD13 | 6:WK:165:PHE:HA   | 1.80                     | 0.64              |
| 9:Au:139:LEU:O    | 6:WO:166:VAL:CG2  | 2.46                     | 0.64              |
| 1:D:57:PRO:HB2    | 2:b:132:GLN:OE1   | 1.97                     | 0.64              |
| 1:E:47:ALA:HB3    | 2:b:178:GLN:CG    | 2.27                     | 0.64              |
| 1:E:57:PRO:HB2    | 2:c:132:GLN:OE1   | 1.97                     | 0.64              |
| 2:e:33:GLU:HG3    | 2:e:95:PRO:HD3    | 1.78                     | 0.64              |
| 2:g:258:ARG:NH1   | 2:i:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:p:35:SER:HB3    | 2:q:123:MET:HE1   | 1.80                     | 0.64              |
| 2:x:258:ARG:NH1   | 2:z:140:ASN:ND2   | 2.46                     | 0.64              |
| 3:ZB:240:TYR:CE2  | 4:ZG:395:ILE:HG23 | 2.32                     | 0.64              |
| 3:ZC:259:GLN:O    | 3:ZC:260:LEU:C    | 2.40                     | 0.64              |
| 4:ZI:159:ASN:ND2  | 4:ZI:271:THR:O    | 2.31                     | 0.64              |
| 4:ZU:382:TYR:CE1  | 4:ZZ:395:ILE:HG23 | 2.32                     | 0.64              |
| 4:ZW:373:VAL:HG21 | 4:Zc:10:LEU:HD23  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:116:GLN:NE2  | 3:AG:42:GLU:HG3   | 2.13                     | 0.64              |
| 6:AS:297:GLN:NE2  | 11:A0:76:GLN:H    | 1.95                     | 0.64              |
| 6:AU:394:LYS:HA   | 6:AU:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:AV:394:LYS:HA   | 6:AV:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:AW:389:VAL:HG21 | 6:AW:416:THR:HG21 | 1.79                     | 0.64              |
| 6:AY:389:VAL:HG21 | 6:AY:416:THR:HG21 | 1.79                     | 0.64              |
| 6:Ad:389:VAL:HG21 | 6:Ad:416:THR:HG21 | 1.79                     | 0.64              |
| 6:Ae:394:LYS:HA   | 6:Ae:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:Ag:235:LEU:HD22 | 6:Ah:244:ARG:HH12 | 1.63                     | 0.64              |
| 9:Ax:162:PRO:HD2  | 6:WE:167:ARG:HH21 | 1.63                     | 0.64              |
| 6:WH:197:LEU:HD12 | 6:WI:175:SER:CB   | 2.28                     | 0.64              |
| 6:WM:200:SER:O    | 6:WN:158:ALA:HB2  | 1.97                     | 0.64              |
| 1:C:57:PRO:HB2    | 2:a:132:GLN:OE1   | 1.97                     | 0.64              |
| 1:J:57:PRO:HB2    | 2:h:132:GLN:OE1   | 1.97                     | 0.64              |
| 1:V:57:PRO:HB2    | 2:t:132:GLN:OE1   | 1.97                     | 0.64              |
| 2:d:54:GLN:OE1    | 3:AL:106:MET:HE1  | 1.98                     | 0.64              |
| 2:f:258:ARG:NH1   | 2:h:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:i:319:LEU:HD21  | 2:j:264:MET:HE2   | 1.79                     | 0.64              |
| 2:j:258:ARG:NH1   | 2:l:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:p:258:ARG:NH1   | 2:r:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:t:258:ARG:NH1   | 2:v:140:ASN:ND2   | 2.46                     | 0.64              |
| 3:9:45:LEU:HD21   | 3:AM:215:TYR:CE2  | 2.32                     | 0.64              |
| 4:ZR:18:ASP:HB3   | 4:ZW:5:GLN:HE22   | 1.61                     | 0.64              |
| 4:ZW:281:GLN:NE2  | 4:ZW:283:GLY:O    | 2.29                     | 0.64              |
| 5:AC:26:LEU:HD13  | 3:AH:242:ILE:CG2  | 2.28                     | 0.64              |
| 5:AD:34:PHE:HE1   | 3:AI:46:TYR:OH    | 1.80                     | 0.64              |
| 5:AE:58:THR:OG1   | 3:AJ:50:ARG:NH2   | 2.31                     | 0.64              |
| 3:AL:52:PRO:CG    | 12:BB:80:PRO:CB   | 2.61                     | 0.64              |
| 6:AR:394:LYS:HE3  | 6:AR:394:LYS:HA   | 1.80                     | 0.64              |
| 6:AS:394:LYS:HA   | 6:AS:394:LYS:HE3  | 1.80                     | 0.64              |
| 6:AV:235:LEU:HD22 | 6:AW:244:ARG:HH12 | 1.63                     | 0.64              |
| 6:AW:287:ASP:HB3  | 6:AW:290:LYS:HE2  | 1.80                     | 0.64              |
| 7:Ab:17:ALA:HB2   | 9:Av:195:ILE:CD1  | 2.28                     | 0.64              |
| 7:Ab:85:PRO:HD3   | 9:Av:238:SER:OG   | 1.98                     | 0.64              |
| 6:Ae:372:ILE:HG21 | 10:A2:4:ILE:HG13  | 1.79                     | 0.64              |
| 9:Av:148:ALA:HB1  | 6:WU:165:PHE:HA   | 1.79                     | 0.64              |
| 9:Ay:139:LEU:HA   | 9:Ay:142:THR:HG22 | 1.78                     | 0.64              |
| 6:WR:143:THR:OG1  | 6:WS:154:ARG:HG2  | 1.97                     | 0.64              |
| 6:BV:235:LEU:HD22 | 6:BW:244:ARG:HH12 | 1.63                     | 0.64              |
| 1:F:57:PRO:HB2    | 2:d:132:GLN:OE1   | 1.97                     | 0.64              |
| 2:f:319:LEU:HD21  | 2:g:264:MET:HE2   | 1.80                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:35:SER:HB3    | 2:h:123:MET:HE1   | 1.79                     | 0.64              |
| 2:n:258:ARG:NH1   | 2:p:140:ASN:ND2   | 2.46                     | 0.64              |
| 2:v:258:ARG:NH1   | 2:x:140:ASN:ND2   | 2.46                     | 0.64              |
| 4:ZP:17:LEU:HD13  | 4:ZU:395:ILE:HD11 | 1.80                     | 0.64              |
| 4:ZT:87:ASP:HB3   | 4:ZT:114:MET:HE2  | 1.80                     | 0.64              |
| 4:ZY:128:ILE:HD13 | 4:ZY:314:GLN:HB2  | 1.78                     | 0.64              |
| 5:AC:152:PRO:CD   | 3:AN:193:ILE:HD12 | 2.28                     | 0.64              |
| 3:AF:47:GLN:NE2   | 12:BA:73:PRO:HB2  | 2.13                     | 0.64              |
| 6:AS:244:ARG:HH12 | 6:BX:235:LEU:HD22 | 1.63                     | 0.64              |
| 6:AT:235:LEU:HD22 | 6:AU:244:ARG:HH12 | 1.63                     | 0.64              |
| 6:AV:287:ASP:HB3  | 6:AV:290:LYS:HE2  | 1.80                     | 0.64              |
| 6:AZ:389:VAL:HG21 | 6:AZ:416:THR:HG21 | 1.79                     | 0.64              |
| 6:Aa:389:VAL:HG21 | 6:Aa:416:THR:HG21 | 1.79                     | 0.64              |
| 6:Ae:235:LEU:HD22 | 6:Af:244:ARG:HH12 | 1.63                     | 0.64              |
| 6:Aj:287:ASP:HB3  | 6:Aj:290:LYS:HE2  | 1.80                     | 0.64              |
| 6:Ak:235:LEU:HD22 | 6:Al:244:ARG:HH12 | 1.63                     | 0.64              |
| 6:Ao:287:ASP:HB3  | 6:Ao:290:LYS:HE2  | 1.80                     | 0.64              |
| 7:Ar:36:SER:HG    | 7:As:44:ILE:HG23  | 1.62                     | 0.64              |
| 8:At:144:LEU:HB3  | 9:Ay:149:LEU:HD22 | 1.79                     | 0.64              |
| 6:WG:139:GLU:HB3  | 6:WH:154:ARG:HH21 | 1.63                     | 0.64              |
| 1:B:57:PRO:HB2    | 2:z:132:GLN:OE1   | 1.97                     | 0.63              |
| 1:N:50:SER:HB3    | 2:k:32:ARG:NH1    | 2.11                     | 0.63              |
| 1:W:57:PRO:HB2    | 2:u:132:GLN:OE1   | 1.97                     | 0.63              |
| 2:h:258:ARG:NH1   | 2:j:140:ASN:ND2   | 2.46                     | 0.63              |
| 3:ZC:106:MET:HE2  | 3:ZC:137:GLN:HE21 | 1.62                     | 0.63              |
| 4:ZH:269:GLN:HB2  | 4:ZN:286:PRO:HG2  | 1.80                     | 0.63              |
| 4:ZJ:2:SER:HB3    | 4:ZJ:392:GLN:HG3  | 1.78                     | 0.63              |
| 4:ZT:379:GLN:HE22 | 4:ZY:394:GLN:CD   | 2.04                     | 0.63              |
| 5:AA:231:MET:HE3  | 3:AF:260:LEU:HD13 | 1.80                     | 0.63              |
| 6:AX:235:LEU:HD22 | 6:AY:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:AY:294:ARG:HG2  | 11:A9:66:THR:OG1  | 1.98                     | 0.63              |
| 6:AZ:235:LEU:HD22 | 6:Aa:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ag:394:LYS:HA   | 6:Ag:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:Am:235:LEU:HD22 | 6:An:244:ARG:HH12 | 1.63                     | 0.63              |
| 9:Ax:152:ARG:HD3  | 6:WG:165:PHE:HD2  | 1.61                     | 0.63              |
| 10:A5:7:ILE:HD12  | 6:BS:372:ILE:HD12 | 1.80                     | 0.63              |
| 1:G:57:PRO:HB2    | 2:e:132:GLN:OE1   | 1.97                     | 0.63              |
| 1:P:66:PHE:HE1    | 2:o:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:U:66:PHE:HE1    | 2:t:41:LEU:HD12   | 1.63                     | 0.63              |
| 1:V:66:PHE:HE1    | 2:u:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:W:66:PHE:HE1    | 2:v:41:LEU:HD12   | 1.64                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:319:LEU:HD21  | 2:c:264:MET:HE2   | 1.80                     | 0.63              |
| 3:4:86:LEU:CD1    | 4:ZF:42:MET:CE    | 2.71                     | 0.63              |
| 4:ZR:375:MET:HE1  | 4:ZW:388:THR:CG2  | 2.25                     | 0.63              |
| 6:AW:394:LYS:HA   | 6:AW:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:Ad:394:LYS:HA   | 6:Ad:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:Af:394:LYS:HA   | 6:Af:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:AQ:235:LEU:HD22 | 6:BR:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:BR:235:LEU:HD22 | 6:BS:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:I:57:PRO:HB2    | 2:g:132:GLN:OE1   | 1.97                     | 0.63              |
| 1:R:66:PHE:HE1    | 2:q:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:S:66:PHE:HE1    | 2:r:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:X:57:PRO:HB2    | 2:v:132:GLN:OE1   | 1.97                     | 0.63              |
| 2:b:258:ARG:NH1   | 2:d:140:ASN:ND2   | 2.46                     | 0.63              |
| 2:m:319:LEU:HD21  | 2:n:264:MET:HE2   | 1.80                     | 0.63              |
| 2:q:35:SER:HB3    | 2:r:123:MET:HE1   | 1.79                     | 0.63              |
| 3:1:127:GLN:HA    | 3:1:140:ILE:O     | 1.98                     | 0.63              |
| 4:ZS:382:TYR:CE1  | 4:ZX:395:ILE:HG23 | 2.33                     | 0.63              |
| 5:AC:221:ILE:HG23 | 3:AI:251:ASP:OD2  | 1.99                     | 0.63              |
| 5:AD:106:GLN:NE2  | 3:AI:78:GLU:OE1   | 2.31                     | 0.63              |
| 6:AR:235:LEU:HD22 | 6:Ac:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:AR:389:VAL:HG21 | 6:AR:416:THR:HG21 | 1.79                     | 0.63              |
| 6:AU:287:ASP:HB3  | 6:AU:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:AX:287:ASP:HB3  | 6:AX:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:Ai:287:ASP:HB3  | 6:Ai:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:An:235:LEU:HD22 | 6:Ao:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ap:287:ASP:HB3  | 6:Ap:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:AO:235:LEU:HD22 | 6:AP:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:AP:235:LEU:HD22 | 6:AQ:244:ARG:HH12 | 1.63                     | 0.63              |
| 7:Aq:89:GLY:O     | 6:WW:164:LEU:CG   | 2.46                     | 0.63              |
| 10:A4:11:ILE:CG2  | 6:BX:372:ILE:HG21 | 2.28                     | 0.63              |
| 6:WG:193:ALA:HB1  | 6:WH:213:VAL:HG11 | 1.81                     | 0.63              |
| 6:BT:235:LEU:HD22 | 6:BU:244:ARG:HH12 | 1.63                     | 0.63              |
| 1:A:57:PRO:HB2    | 2:y:132:GLN:OE1   | 1.97                     | 0.63              |
| 1:O:66:PHE:HE1    | 2:n:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:Q:66:PHE:HE1    | 2:p:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:Y:57:PRO:HB2    | 2:w:132:GLN:OE1   | 1.97                     | 0.63              |
| 4:ZJ:17:LEU:HD13  | 4:ZO:395:ILE:HD11 | 1.81                     | 0.63              |
| 4:ZX:27:SER:HB3   | 4:ZX:368:LEU:HD21 | 1.78                     | 0.63              |
| 3:AM:187:ILE:HD12 | 3:AM:193:ILE:HD11 | 1.79                     | 0.63              |
| 6:AR:244:ARG:HH12 | 6:Aa:235:LEU:HD22 | 1.63                     | 0.63              |
| 6:AY:235:LEU:HD22 | 6:AZ:244:ARG:HH12 | 1.63                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AY:365:ASN:CB   | 11:A9:72:HIS:CD2  | 2.66                     | 0.63              |
| 6:AY:394:LYS:HA   | 6:AY:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:Ac:235:LEU:HD22 | 6:Ad:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ah:394:LYS:HE3  | 6:Ah:394:LYS:HA   | 1.80                     | 0.63              |
| 7:Ar:36:SER:OG    | 7:As:44:ILE:CG2   | 2.35                     | 0.63              |
| 9:Ay:229:VAL:O    | 9:Ay:230:ASP:C    | 2.41                     | 0.63              |
| 6:BS:235:LEU:HD22 | 6:BT:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:BW:394:LYS:HA   | 6:BW:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:H:57:PRO:HB2    | 2:f:132:GLN:OE1   | 1.97                     | 0.63              |
| 2:a:140:ASN:ND2   | 2:y:258:ARG:NH1   | 2.46                     | 0.63              |
| 2:a:258:ARG:NH1   | 2:c:140:ASN:ND2   | 2.46                     | 0.63              |
| 2:e:258:ARG:NH1   | 2:g:140:ASN:ND2   | 2.46                     | 0.63              |
| 2:u:319:LEU:HD21  | 2:v:264:MET:HE2   | 1.79                     | 0.63              |
| 3:ZD:27:ALA:HB1   | 4:ZI:52:VAL:CG2   | 2.28                     | 0.63              |
| 4:ZP:217:ASP:HB3  | 4:ZP:220:ALA:HB2  | 1.80                     | 0.63              |
| 4:ZY:281:GLN:NE2  | 4:ZY:283:GLY:O    | 2.32                     | 0.63              |
| 4:Zb:199:TYR:HB2  | 4:Zb:211:TYR:HB2  | 1.80                     | 0.63              |
| 5:AB:48:GLY:HA3   | 11:A7:93:PRO:HB3  | 1.81                     | 0.63              |
| 5:AD:214:VAL:HG13 | 3:AJ:12:LEU:CD1   | 2.29                     | 0.63              |
| 6:AY:370:ARG:HH21 | 10:A3:7:ILE:HD11  | 1.61                     | 0.63              |
| 7:Ab:84:LEU:HB3   | 7:Ab:85:PRO:CD    | 2.28                     | 0.63              |
| 6:Ad:235:LEU:HD22 | 6:Ae:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ak:287:ASP:HB3  | 6:Ak:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:An:287:ASP:HB3  | 6:An:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:AO:287:ASP:HB3  | 6:AO:290:LYS:HE2  | 1.80                     | 0.63              |
| 7:Aq:14:MET:HG3   | 7:Ar:59:PHE:CE1   | 2.33                     | 0.63              |
| 7:Aq:89:GLY:CA    | 6:WW:165:PHE:CE1  | 2.53                     | 0.63              |
| 7:As:20:LEU:HD23  | 9:Ay:199:VAL:HG21 | 1.80                     | 0.63              |
| 10:A5:55:GLN:NE2  | 10:A5:74:ASP:OD2  | 2.31                     | 0.63              |
| 6:WU:128:GLU:HG2  | 6:WV:126:PHE:HD2  | 1.64                     | 0.63              |
| 12:BE:47:VAL:O    | 6:BP:313:PRO:CD   | 2.46                     | 0.63              |
| 6:BV:287:ASP:HB3  | 6:BV:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:BW:287:ASP:HB3  | 6:BW:290:LYS:HE2  | 1.80                     | 0.63              |
| 6:BX:394:LYS:HA   | 6:BX:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:K:47:ALA:HB3    | 2:h:178:GLN:CG    | 2.26                     | 0.63              |
| 1:L:47:ALA:HB3    | 2:i:178:GLN:CG    | 2.26                     | 0.63              |
| 1:N:66:PHE:HE1    | 2:m:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:T:66:PHE:HE1    | 2:s:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:X:66:PHE:HE1    | 2:w:41:LEU:HD12   | 1.64                     | 0.63              |
| 2:c:258:ARG:NH1   | 2:e:140:ASN:ND2   | 2.46                     | 0.63              |
| 2:t:319:LEU:HD21  | 2:u:264:MET:HE2   | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:v:319:LEU:HD21  | 2:w:264:MET:HE2   | 1.79                     | 0.63              |
| 4:ZQ:112:GLN:OE1  | 4:ZQ:112:GLN:N    | 2.31                     | 0.63              |
| 5:AC:215:GLU:CG   | 3:AI:9:LYS:HE3    | 2.28                     | 0.63              |
| 3:AL:52:PRO:HD3   | 12:BB:80:PRO:HB2  | 1.79                     | 0.63              |
| 7:As:13:ALA:HB1   | 9:Ay:195:ILE:HD11 | 1.81                     | 0.63              |
| 11:A7:74:PRO:O    | 11:A7:75:ALA:C    | 2.40                     | 0.63              |
| 6:WG:139:GLU:HB3  | 6:WH:154:ARG:NH2  | 2.14                     | 0.63              |
| 1:K:62:TYR:HD1    | 2:i:129:VAL:HG11  | 1.62                     | 0.63              |
| 1:M:66:PHE:HE1    | 2:l:41:LEU:HD12   | 1.64                     | 0.63              |
| 1:Z:57:PRO:HB2    | 2:x:132:GLN:OE1   | 1.97                     | 0.63              |
| 2:f:35:SER:HB3    | 2:g:123:MET:HE1   | 1.79                     | 0.63              |
| 2:u:258:ARG:NH1   | 2:w:140:ASN:ND2   | 2.46                     | 0.63              |
| 3:ZB:28:ASN:ND2   | 4:ZG:52:VAL:HB    | 2.13                     | 0.63              |
| 4:ZI:374:ASN:O    | 4:ZI:377:VAL:N    | 2.31                     | 0.63              |
| 5:AE:48:GLY:HA3   | 6:BQ:324:ASN:HD21 | 1.64                     | 0.63              |
| 3:AJ:127:GLN:NE2  | 3:AJ:139:ALA:HB1  | 2.13                     | 0.63              |
| 6:AW:235:LEU:HD22 | 6:AX:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ae:372:ILE:HG22 | 10:A2:4:ILE:CG1   | 2.29                     | 0.63              |
| 6:Ai:394:LYS:HA   | 6:Ai:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:Al:235:LEU:HD22 | 6:Am:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ao:235:LEU:HD22 | 6:Ap:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:Ap:235:LEU:HD22 | 6:AO:244:ARG:HH12 | 1.63                     | 0.63              |
| 7:Ar:14:MET:CE    | 7:As:63:ILE:HD13  | 2.29                     | 0.63              |
| 7:Ar:23:PRO:O     | 7:Ar:27:VAL:HG12  | 1.99                     | 0.63              |
| 6:UP:103:GLN:HG2  | 6:WW:182:PRO:HB3  | 0.71                     | 0.63              |
| 6:WO:197:LEU:CD1  | 6:WP:175:SER:OG   | 2.42                     | 0.63              |
| 6:BU:287:ASP:HB3  | 6:BU:290:LYS:HE2  | 1.80                     | 0.63              |
| 2:g:319:LEU:HD21  | 2:h:264:MET:HE2   | 1.80                     | 0.63              |
| 2:i:258:ARG:NH1   | 2:k:140:ASN:ND2   | 2.46                     | 0.63              |
| 2:o:220:THR:OG1   | 2:p:98:ARG:HD2    | 1.99                     | 0.63              |
| 2:s:319:LEU:HD21  | 2:t:264:MET:HE2   | 1.80                     | 0.63              |
| 2:x:35:SER:HB3    | 2:y:123:MET:HE1   | 1.79                     | 0.63              |
| 3:7:45:LEU:HD22   | 3:AK:98:LYS:HG3   | 1.80                     | 0.63              |
| 3:ZB:244:SER:CB   | 4:ZG:399:LEU:CD2  | 2.77                     | 0.63              |
| 4:ZH:162:ASP:OD1  | 4:ZH:274:ASN:ND2  | 2.30                     | 0.63              |
| 4:ZR:181:LYS:HD2  | 4:Zc:129:GLN:NE2  | 2.14                     | 0.63              |
| 6:Ap:394:LYS:HA   | 6:Ap:394:LYS:HE3  | 1.80                     | 0.63              |
| 6:AQ:394:LYS:HA   | 6:AQ:394:LYS:HE3  | 1.80                     | 0.63              |
| 7:Ar:36:SER:O     | 7:As:44:ILE:HD12  | 1.99                     | 0.63              |
| 7:Ar:75:ASP:O     | 7:Ar:79:THR:HG23  | 1.98                     | 0.63              |
| 9:Ax:162:PRO:HD2  | 6:WE:167:ARG:NH2  | 2.13                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WE:197:LEU:CD1  | 6:WF:175:SER:OG   | 2.44                     | 0.63              |
| 6:WP:128:GLU:HG3  | 6:WQ:126:PHE:HE2  | 1.62                     | 0.63              |
| 6:BU:235:LEU:HD22 | 6:BV:244:ARG:HH12 | 1.63                     | 0.63              |
| 6:BV:394:LYS:HA   | 6:BV:394:LYS:HE3  | 1.80                     | 0.63              |
| 2:h:319:LEU:HD21  | 2:i:264:MET:HE2   | 1.80                     | 0.63              |
| 2:o:258:ARG:NH1   | 2:q:140:ASN:ND2   | 2.46                     | 0.63              |
| 2:p:220:THR:OG1   | 2:q:98:ARG:HD2    | 1.99                     | 0.63              |
| 2:r:35:SER:HB3    | 2:s:123:MET:HE1   | 1.79                     | 0.63              |
| 2:v:35:SER:HB3    | 2:w:123:MET:HE1   | 1.79                     | 0.63              |
| 3:4:56:SER:CA     | 5:AC:138:ALA:HB1  | 2.29                     | 0.63              |
| 3:6:2:ILE:HD13    | 3:AJ:226:VAL:CG2  | 2.29                     | 0.63              |
| 3:ZC:54:ALA:HB1   | 3:AK:150:THR:CG2  | 2.25                     | 0.63              |
| 5:AB:214:VAL:HG22 | 3:AM:257:LEU:HD22 | 1.79                     | 0.63              |
| 5:AD:175:ASP:O    | 3:AI:45:LEU:HD12  | 1.98                     | 0.63              |
| 9:Ax:143:ARG:CA   | 6:WD:165:PHE:HB2  | 2.23                     | 0.63              |
| 11:A8:22:ARG:NH2  | 11:A8:108:GLN:OE1 | 2.31                     | 0.63              |
| 6:WP:214:ASP:OD1  | 6:WP:218:HIS:HB2  | 1.99                     | 0.63              |
| 6:BU:394:LYS:HA   | 6:BU:394:LYS:HE3  | 1.80                     | 0.63              |
| 1:F:47:ALA:HB3    | 2:c:178:GLN:CG    | 2.26                     | 0.62              |
| 1:L:66:PHE:HE1    | 2:k:41:LEU:HD12   | 1.64                     | 0.62              |
| 2:n:220:THR:OG1   | 2:o:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:q:319:LEU:HD21  | 2:r:264:MET:HE2   | 1.79                     | 0.62              |
| 2:w:319:LEU:HD21  | 2:x:264:MET:HE2   | 1.80                     | 0.62              |
| 2:y:35:SER:HB3    | 2:z:123:MET:HE1   | 1.79                     | 0.62              |
| 3:7:22:ILE:HG21   | 3:7:233:MET:HG3   | 1.81                     | 0.62              |
| 4:ZH:78:SER:O     | 4:ZH:354:GLY:HA3  | 1.99                     | 0.62              |
| 4:ZI:17:LEU:HD13  | 4:ZN:395:ILE:HD11 | 1.81                     | 0.62              |
| 6:AZ:236:LYS:HE2  | 6:UP:167:ARG:HH11 | 1.63                     | 0.62              |
| 6:Aa:287:ASP:HB3  | 6:Aa:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:WS:168:GLU:HB3  | 6:WS:170:LYS:HE3  | 1.81                     | 0.62              |
| 6:BX:287:ASP:HB3  | 6:BX:290:LYS:HE2  | 1.80                     | 0.62              |
| 1:Y:66:PHE:HE1    | 2:x:41:LEU:HD12   | 1.64                     | 0.62              |
| 2:a:319:LEU:HD21  | 2:b:264:MET:HE2   | 1.79                     | 0.62              |
| 2:r:319:LEU:HD21  | 2:s:264:MET:HE2   | 1.79                     | 0.62              |
| 2:u:35:SER:HB3    | 2:v:123:MET:HE1   | 1.79                     | 0.62              |
| 2:w:220:THR:OG1   | 2:x:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:x:220:THR:OG1   | 2:y:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:y:220:THR:OG1   | 2:z:98:ARG:HD2    | 1.99                     | 0.62              |
| 3:4:231:VAL:HG11  | 3:ZA:9:LYS:HG3    | 1.81                     | 0.62              |
| 3:5:76:ALA:HB1    | 3:ZA:64:SER:O     | 2.00                     | 0.62              |
| 4:ZR:180:LYS:HB3  | 4:ZR:200:PHE:CD1  | 2.34                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zc:154:MET:HE1  | 4:Zc:198:VAL:HG21 | 1.79                     | 0.62              |
| 5:AB:234:ILE:HG23 | 12:BB:106:MET:HE1 | 1.81                     | 0.62              |
| 5:AC:184:GLU:OE2  | 3:AH:55:GLN:C     | 2.43                     | 0.62              |
| 5:AE:165:LYS:HB2  | 5:AE:199:ILE:HD11 | 1.81                     | 0.62              |
| 3:AI:47:GLN:N     | 3:AI:68:ILE:O     | 2.31                     | 0.62              |
| 3:AM:37:GLN:NE2   | 3:AM:77:THR:OG1   | 2.32                     | 0.62              |
| 6:AR:287:ASP:HB3  | 6:AR:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Af:287:ASP:HB3  | 6:Af:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Ah:287:ASP:HB3  | 6:Ah:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Aj:394:LYS:HA   | 6:Aj:394:LYS:HE3  | 1.80                     | 0.62              |
| 6:Ao:394:LYS:HA   | 6:Ao:394:LYS:HE3  | 1.80                     | 0.62              |
| 7:Aq:73:LEU:HD21  | 9:Aw:225:LEU:HD13 | 1.80                     | 0.62              |
| 8:At:185:MET:HA   | 8:At:188:LEU:HD23 | 1.80                     | 0.62              |
| 9:Ay:66:ARG:HB3   | 9:Ay:178:GLU:OE1  | 2.00                     | 0.62              |
| 12:BD:68:ILE:CD1  | 6:BN:312:VAL:CG2  | 2.75                     | 0.62              |
| 2:a:35:SER:HB3    | 2:b:123:MET:HE1   | 1.80                     | 0.62              |
| 2:a:123:MET:HE1   | 2:z:35:SER:HB3    | 1.80                     | 0.62              |
| 2:b:35:SER:HB3    | 2:c:123:MET:HE1   | 1.79                     | 0.62              |
| 2:d:258:ARG:NH1   | 2:f:140:ASN:ND2   | 2.46                     | 0.62              |
| 2:m:220:THR:OG1   | 2:n:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:n:319:LEU:HD21  | 2:o:264:MET:HE2   | 1.79                     | 0.62              |
| 2:u:220:THR:OG1   | 2:v:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:v:220:THR:OG1   | 2:w:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:w:35:SER:HB3    | 2:x:123:MET:HE1   | 1.80                     | 0.62              |
| 2:x:319:LEU:HD21  | 2:y:264:MET:HE2   | 1.80                     | 0.62              |
| 3:9:16:GLN:NE2    | 3:9:20:ASP:OD1    | 2.32                     | 0.62              |
| 3:ZC:70:THR:HG22  | 3:ZC:71:GLY:H     | 1.62                     | 0.62              |
| 4:ZK:167:LYS:NZ   | 4:ZK:168:THR:O    | 2.31                     | 0.62              |
| 4:Zh:112:GLN:OE1  | 4:Zh:112:GLN:N    | 2.32                     | 0.62              |
| 6:AW:299:ASN:ND2  | 11:A9:55:ARG:CZ   | 2.62                     | 0.62              |
| 6:Af:235:LEU:HD22 | 6:Ag:244:ARG:HH12 | 1.63                     | 0.62              |
| 6:Ah:235:LEU:HD22 | 6:Ai:244:ARG:HH12 | 1.63                     | 0.62              |
| 6:Al:287:ASP:HB3  | 6:Al:290:LYS:HE2  | 1.80                     | 0.62              |
| 11:A9:32:ASN:HD22 | 12:BD:62:VAL:CG1  | 2.12                     | 0.62              |
| 6:UI:167:ARG:NH2  | 6:WW:188:GLU:HB3  | 2.13                     | 0.62              |
| 6:WA:187:ASP:CG   | 6:WA:190:GLN:HG3  | 2.24                     | 0.62              |
| 6:WH:197:LEU:HD11 | 6:WI:156:HIS:HD2  | 1.63                     | 0.62              |
| 6:WQ:128:GLU:HG2  | 6:WR:126:PHE:HD2  | 1.65                     | 0.62              |
| 1:K:66:PHE:HE1    | 2:j:41:LEU:HD12   | 1.64                     | 0.62              |
| 2:a:220:THR:OG1   | 2:b:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:b:140:ASN:ND2   | 2:z:258:ARG:NH1   | 2.46                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:220:THR:OG1   | 2:c:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:c:35:SER:HB3    | 2:d:123:MET:HE1   | 1.79                     | 0.62              |
| 2:c:220:THR:OG1   | 2:d:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:f:220:THR:OG1   | 2:g:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:q:220:THR:OG1   | 2:r:98:ARG:HD2    | 1.99                     | 0.62              |
| 3:0:44:LEU:HD22   | 5:AD:71:LEU:HD23  | 1.80                     | 0.62              |
| 3:0:130:THR:HG23  | 3:0:132:GLY:H     | 1.63                     | 0.62              |
| 3:2:114:TYR:CG    | 3:2:178:PHE:HZ    | 2.17                     | 0.62              |
| 3:ZA:50:ARG:HB2   | 3:ZA:66:LEU:H     | 1.62                     | 0.62              |
| 3:ZA:70:THR:HG22  | 3:ZA:71:GLY:H     | 1.64                     | 0.62              |
| 4:ZP:146:ALA:HB2  | 4:ZP:286:PRO:HD3  | 1.81                     | 0.62              |
| 4:ZP:373:VAL:O    | 4:ZP:376:ILE:N    | 2.30                     | 0.62              |
| 5:AE:248:LEU:HB2  | 12:BE:117:GLU:HB3 | 1.82                     | 0.62              |
| 3:AI:50:ARG:HB2   | 6:BN:322:PRO:HG3  | 1.79                     | 0.62              |
| 6:AY:287:ASP:HB3  | 6:AY:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:AZ:287:ASP:HB3  | 6:AZ:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Am:287:ASP:HB3  | 6:Am:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Am:394:LYS:HA   | 6:Am:394:LYS:HE3  | 1.80                     | 0.62              |
| 6:AP:287:ASP:HB3  | 6:AP:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:AP:394:LYS:HA   | 6:AP:394:LYS:HE3  | 1.80                     | 0.62              |
| 9:Ax:161:GLY:N    | 6:WE:167:ARG:CD   | 2.61                     | 0.62              |
| 6:WT:128:GLU:HG2  | 6:WU:126:PHE:CD2  | 2.35                     | 0.62              |
| 6:BT:287:ASP:HB3  | 6:BT:290:LYS:HE2  | 1.81                     | 0.62              |
| 1:J:66:PHE:HE1    | 2:i:41:LEU:HD12   | 1.64                     | 0.62              |
| 2:a:98:ARG:HD2    | 2:z:220:THR:OG1   | 1.99                     | 0.62              |
| 2:d:220:THR:OG1   | 2:e:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:e:35:SER:HB3    | 2:f:123:MET:HE1   | 1.79                     | 0.62              |
| 2:e:220:THR:OG1   | 2:f:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:g:220:THR:OG1   | 2:h:98:ARG:HD2    | 1.99                     | 0.62              |
| 3:4:253:MET:HE2   | 3:AN:240:TYR:CD1  | 2.34                     | 0.62              |
| 3:5:237:GLN:HE21  | 3:ZA:252:GLN:HB3  | 1.65                     | 0.62              |
| 4:ZG:185:THR:OG1  | 4:ZR:133:ASN:OD1  | 2.17                     | 0.62              |
| 4:Zb:84:ARG:NH1   | 4:Zb:134:PRO:HB2  | 2.14                     | 0.62              |
| 5:AB:231:MET:SD   | 3:AG:257:LEU:HA   | 2.40                     | 0.62              |
| 5:AE:214:VAL:HG11 | 3:AK:12:LEU:HB2   | 1.81                     | 0.62              |
| 5:AE:228:GLU:CA   | 3:AK:258:THR:HG21 | 2.22                     | 0.62              |
| 3:AG:62:LEU:HD23  | 12:BC:83:PRO:HG2  | 1.80                     | 0.62              |
| 3:AG:80:LEU:C     | 3:AG:82:SER:H     | 2.07                     | 0.62              |
| 3:AL:104:GLN:NE2  | 3:AL:203:GLU:OE2  | 2.33                     | 0.62              |
| 6:AT:287:ASP:HB3  | 6:AT:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:AU:235:LEU:HD22 | 6:AV:244:ARG:HH12 | 1.63                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Ae:287:ASP:HB3  | 6:Ae:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:WK:197:LEU:HD11 | 6:WL:156:HIS:HD2  | 1.63                     | 0.62              |
| 6:BW:235:LEU:HD22 | 6:BX:244:ARG:HH12 | 1.63                     | 0.62              |
| 1:D:66:PHE:HE1    | 2:c:41:LEU:HD12   | 1.63                     | 0.62              |
| 1:I:66:PHE:HE1    | 2:h:41:LEU:HD12   | 1.64                     | 0.62              |
| 2:d:35:SER:HB3    | 2:e:123:MET:HE1   | 1.79                     | 0.62              |
| 2:h:220:THR:OG1   | 2:i:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:j:364:ILE:HD13  | 2:l:142:LEU:HB2   | 1.82                     | 0.62              |
| 2:p:319:LEU:HD21  | 2:q:264:MET:HE2   | 1.80                     | 0.62              |
| 2:s:220:THR:OG1   | 2:t:98:ARG:HD2    | 1.99                     | 0.62              |
| 3:6:57:SER:CB     | 3:AK:108:PRO:CG   | 2.73                     | 0.62              |
| 3:8:36:ARG:HH21   | 3:8:38:ARG:HH12   | 1.46                     | 0.62              |
| 3:9:45:LEU:HD12   | 3:AM:86:LEU:HD21  | 1.80                     | 0.62              |
| 3:ZA:231:VAL:HG11 | 4:ZG:7:VAL:HG22   | 1.80                     | 0.62              |
| 3:ZD:31:THR:HG22  | 4:ZI:39:PHE:C     | 2.23                     | 0.62              |
| 4:ZH:238:LEU:HD21 | 4:ZH:242:GLY:HA3  | 1.81                     | 0.62              |
| 4:ZX:380:ARG:NE   | 4:Zd:393:ASP:OD1  | 2.29                     | 0.62              |
| 4:Zc:396:LEU:O    | 4:Zc:400:VAL:HG23 | 2.00                     | 0.62              |
| 3:AF:79:ARG:NH2   | 3:AF:186:SER:OG   | 2.33                     | 0.62              |
| 3:AF:258:THR:O    | 12:BF:117:GLU:HG3 | 1.99                     | 0.62              |
| 6:Ac:287:ASP:HB3  | 6:Ac:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Af:365:ASN:HB3  | 11:A8:72:HIS:CE1  | 2.33                     | 0.62              |
| 6:Ak:363:THR:HG23 | 11:A7:65:LEU:HD21 | 1.80                     | 0.62              |
| 9:Ax:160:GLN:HA   | 6:WE:166:VAL:HG22 | 1.81                     | 0.62              |
| 6:WO:196:HIS:HB3  | 6:WP:211:THR:HG21 | 1.80                     | 0.62              |
| 1:F:66:PHE:HE1    | 2:e:41:LEU:HD12   | 1.63                     | 0.62              |
| 2:i:220:THR:OG1   | 2:j:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:i:364:ILE:HD13  | 2:k:142:LEU:HB2   | 1.82                     | 0.62              |
| 2:k:364:ILE:HD13  | 2:m:142:LEU:HB2   | 1.82                     | 0.62              |
| 2:t:220:THR:OG1   | 2:u:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:y:319:LEU:HD21  | 2:z:264:MET:HE2   | 1.80                     | 0.62              |
| 3:1:193:ILE:CG2   | 5:AE:152:PRO:CD   | 2.66                     | 0.62              |
| 3:2:45:LEU:HD22   | 3:AF:98:LYS:HD2   | 1.82                     | 0.62              |
| 4:ZH:236:GLY:HA3  | 4:ZN:190:GLN:HE22 | 1.63                     | 0.62              |
| 4:ZN:34:SER:HB3   | 4:ZN:366:VAL:HG22 | 1.82                     | 0.62              |
| 4:ZW:322:ASN:HB3  | 4:ZW:340:SER:HA   | 1.82                     | 0.62              |
| 4:Zb:97:ASN:OD1   | 4:Zb:99:GLN:NE2   | 2.32                     | 0.62              |
| 5:AA:51:LEU:HD12  | 12:BB:19:LYS:HE2  | 1.82                     | 0.62              |
| 5:AA:70:GLN:HB2   | 3:AL:6:TRP:HB2    | 1.82                     | 0.62              |
| 5:AA:72:ASP:OD1   | 3:AL:6:TRP:CE3    | 2.52                     | 0.62              |
| 5:AC:217:MET:CE   | 3:AN:258:THR:CA   | 2.73                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AD:175:ASP:OD1  | 3:AI:48:THR:OG1   | 2.17                     | 0.62              |
| 6:Aj:235:LEU:HD22 | 6:Ak:244:ARG:HH12 | 1.63                     | 0.62              |
| 6:Al:394:LYS:HA   | 6:Al:394:LYS:HE3  | 1.80                     | 0.62              |
| 9:Ax:160:GLN:CA   | 6:WE:166:VAL:HG22 | 2.29                     | 0.62              |
| 11:A7:51:LYS:CB   | 11:A7:55:ARG:CZ   | 2.66                     | 0.62              |
| 6:WQ:128:GLU:HG2  | 6:WR:126:PHE:CD2  | 2.34                     | 0.62              |
| 6:BT:394:LYS:HA   | 6:BT:394:LYS:HE3  | 1.80                     | 0.62              |
| 1:C:62:TYR:HD1    | 2:a:129:VAL:HG11  | 1.62                     | 0.62              |
| 1:G:47:ALA:HB3    | 2:d:178:GLN:CG    | 2.26                     | 0.62              |
| 1:G:66:PHE:HE1    | 2:f:41:LEU:HD12   | 1.64                     | 0.62              |
| 1:H:66:PHE:HE1    | 2:g:41:LEU:HD12   | 1.64                     | 0.62              |
| 2:l:364:ILE:HD13  | 2:n:142:LEU:HB2   | 1.82                     | 0.62              |
| 2:t:35:SER:HB3    | 2:u:123:MET:HE1   | 1.80                     | 0.62              |
| 3:0:70:THR:CG2    | 5:AD:71:LEU:HB2   | 2.30                     | 0.62              |
| 3:2:49:ILE:HG21   | 3:2:66:LEU:HD23   | 1.82                     | 0.62              |
| 3:3:218:TYR:CZ    | 3:ZE:73:ARG:HD2   | 2.34                     | 0.62              |
| 3:8:36:ARG:HB3    | 3:8:224:VAL:HG22  | 1.81                     | 0.62              |
| 4:ZS:17:LEU:CD1   | 4:ZX:395:ILE:HD11 | 2.29                     | 0.62              |
| 4:ZS:65:THR:HG21  | 4:Zd:4:SER:CB     | 2.30                     | 0.62              |
| 5:AE:215:GLU:CD   | 3:AK:9:LYS:HZ1    | 2.07                     | 0.62              |
| 3:AL:49:ILE:HD12  | 3:AL:66:LEU:HD11  | 1.81                     | 0.62              |
| 6:Ad:287:ASP:HB3  | 6:Ad:290:LYS:HE2  | 1.80                     | 0.62              |
| 7:Aq:24:LEU:HD22  | 7:Aq:58:VAL:HG13  | 1.81                     | 0.62              |
| 9:Ax:159:LEU:HD23 | 6:WE:165:PHE:HD1  | 1.65                     | 0.62              |
| 6:UP:73:MET:HE3   | 6:UP:99:ARG:HD3   | 1.81                     | 0.62              |
| 6:WJ:186:LEU:HA   | 6:WJ:190:GLN:OE1  | 2.00                     | 0.62              |
| 6:BS:394:LYS:HA   | 6:BS:394:LYS:HE3  | 1.80                     | 0.62              |
| 1:J:181:SER:HB2   | 1:K:31:VAL:HG13   | 1.82                     | 0.62              |
| 2:r:220:THR:OG1   | 2:s:98:ARG:HD2    | 1.99                     | 0.62              |
| 2:s:35:SER:HB3    | 2:t:123:MET:HE1   | 1.80                     | 0.62              |
| 2:x:51:GLN:HE21   | 3:AH:125:ASN:HD22 | 1.47                     | 0.62              |
| 3:9:257:LEU:HD13  | 3:AM:230:LEU:HD12 | 1.81                     | 0.62              |
| 3:ZA:34:PHE:HB3   | 3:ZA:222:SER:HB3  | 1.82                     | 0.62              |
| 3:ZD:52:PRO:HA    | 3:ZD:65:GLY:H     | 1.63                     | 0.62              |
| 4:ZQ:382:TYR:CE1  | 4:ZV:395:ILE:HG23 | 2.34                     | 0.62              |
| 5:AB:206:LEU:CD2  | 3:AG:38:ARG:NH2   | 2.62                     | 0.62              |
| 5:AC:165:LYS:O    | 5:AC:189:ARG:NH2  | 2.32                     | 0.62              |
| 6:Ak:394:LYS:HE3  | 6:Ak:394:LYS:HA   | 1.80                     | 0.62              |
| 9:Av:67:ILE:HD12  | 9:Av:239:LEU:HD13 | 1.81                     | 0.62              |
| 9:Ay:67:ILE:HD11  | 9:Ay:96:LEU:HB3   | 1.81                     | 0.62              |
| 6:UM:161:LYS:O    | 6:UM:162:PRO:C    | 2.43                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WI:190:GLN:NE2  | 6:WJ:216:SER:O    | 2.33                     | 0.62              |
| 6:WI:200:SER:OG   | 6:WJ:175:SER:HB2  | 2.00                     | 0.62              |
| 6:WS:197:LEU:HD12 | 6:WT:175:SER:HB3  | 1.81                     | 0.62              |
| 1:C:66:PHE:HE1    | 2:b:41:LEU:HD12   | 1.64                     | 0.62              |
| 1:E:66:PHE:HE1    | 2:d:41:LEU:HD12   | 1.64                     | 0.62              |
| 1:F:62:TYR:HD1    | 2:d:129:VAL:HG11  | 1.62                     | 0.62              |
| 1:K:181:SER:HB2   | 1:L:31:VAL:HG13   | 1.82                     | 0.62              |
| 2:a:364:ILE:HD13  | 2:c:142:LEU:HB2   | 1.82                     | 0.62              |
| 2:h:364:ILE:HD13  | 2:j:142:LEU:HB2   | 1.82                     | 0.62              |
| 2:o:319:LEU:HD21  | 2:p:264:MET:HE2   | 1.80                     | 0.62              |
| 2:y:80:GLN:HE22   | 3:AM:200:ALA:CA   | 1.88                     | 0.62              |
| 3:2:238:ARG:O     | 3:2:241:GLU:N     | 2.32                     | 0.62              |
| 3:3:121:GLN:HE22  | 3:8:182:THR:HG21  | 1.64                     | 0.62              |
| 3:4:50:ARG:HD3    | 3:4:62:LEU:HD11   | 1.82                     | 0.62              |
| 3:7:167:PRO:HG2   | 4:ZI:338:GLN:OE1  | 1.99                     | 0.62              |
| 3:ZA:91:ASN:O     | 3:ZA:93:LYS:N     | 2.33                     | 0.62              |
| 4:ZI:102:LEU:O    | 4:ZN:322:ASN:HB2  | 2.00                     | 0.62              |
| 4:ZL:367:ASP:HB3  | 4:ZL:370:LYS:HG2  | 1.82                     | 0.62              |
| 4:ZU:270:ASN:ND2  | 4:Za:191:GLY:O    | 2.33                     | 0.62              |
| 4:Za:288:ASP:OD2  | 4:Zf:351:GLY:HA2  | 2.00                     | 0.62              |
| 5:AA:202:MET:SD   | 3:AL:44:LEU:HD23  | 2.39                     | 0.62              |
| 5:AE:91:GLN:HB2   | 5:AE:121:ILE:HD11 | 1.80                     | 0.62              |
| 6:AS:287:ASP:HB3  | 6:AS:290:LYS:HE2  | 1.80                     | 0.62              |
| 6:Ag:287:ASP:HB3  | 6:Ag:290:LYS:HE2  | 1.80                     | 0.62              |
| 7:As:46:GLU:HB2   | 7:As:49:LEU:HD23  | 1.82                     | 0.62              |
| 8:At:105:GLN:NE2  | 9:Au:216:THR:O    | 2.33                     | 0.62              |
| 8:At:158:PRO:CG   | 8:At:162:ASN:HD21 | 2.09                     | 0.62              |
| 9:Ax:153:LEU:HD21 | 6:WG:165:PHE:CZ   | 2.35                     | 0.62              |
| 6:UK:161:LYS:O    | 6:UK:162:PRO:C    | 2.43                     | 0.62              |
| 1:L:88:ALA:HB1    | 1:N:171:ILE:HD12  | 1.82                     | 0.61              |
| 1:N:62:TYR:HD1    | 2:l:129:VAL:HG11  | 1.62                     | 0.61              |
| 1:N:181:SER:HB2   | 1:O:31:VAL:HG13   | 1.82                     | 0.61              |
| 2:j:220:THR:OG1   | 2:k:98:ARG:HD2    | 1.99                     | 0.61              |
| 2:l:220:THR:OG1   | 2:m:98:ARG:HD2    | 1.99                     | 0.61              |
| 3:ZB:163:GLY:O    | 3:ZB:164:GLN:C    | 2.43                     | 0.61              |
| 4:ZL:375:MET:SD   | 4:ZQ:388:THR:HA   | 2.40                     | 0.61              |
| 4:ZN:165:PRO:HG2  | 4:ZN:201:VAL:HG23 | 1.82                     | 0.61              |
| 5:AC:49:LEU:HB2   | 11:A8:90:PRO:HG2  | 1.80                     | 0.61              |
| 5:AE:154:THR:O    | 5:AE:156:ALA:N    | 2.32                     | 0.61              |
| 5:AE:243:ARG:CZ   | 3:AF:259:GLN:OE1  | 2.48                     | 0.61              |
| 3:AG:256:LYS:HD2  | 3:AG:259:GLN:HE21 | 1.63                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AJ:142:ILE:HD13 | 3:AJ:149:ILE:HG12 | 1.82                     | 0.61              |
| 3:AL:3:SER:O      | 3:AL:5:LEU:N      | 2.32                     | 0.61              |
| 6:Ac:277:GLN:HB3  | 6:Ac:377:MET:HE1  | 1.82                     | 0.61              |
| 10:A5:11:ILE:CG2  | 6:BR:372:ILE:CG2  | 2.78                     | 0.61              |
| 6:UO:103:GLN:NE2  | 6:WU:182:PRO:CB   | 2.63                     | 0.61              |
| 6:WM:200:SER:HG   | 6:WN:175:SER:HB2  | 1.63                     | 0.61              |
| 6:WO:128:GLU:HG2  | 6:WP:126:PHE:HD2  | 1.64                     | 0.61              |
| 6:WP:128:GLU:HG3  | 6:WQ:126:PHE:CE2  | 2.35                     | 0.61              |
| 1:D:88:ALA:HB1    | 1:F:171:ILE:HD12  | 1.82                     | 0.61              |
| 1:M:88:ALA:HB1    | 1:O:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:Z:66:PHE:HE1    | 2:y:41:LEU:HD12   | 1.64                     | 0.61              |
| 2:a:264:MET:HE2   | 2:z:319:LEU:HD21  | 1.79                     | 0.61              |
| 2:b:364:ILE:HD13  | 2:d:142:LEU:HB2   | 1.82                     | 0.61              |
| 2:m:364:ILE:HD13  | 2:o:142:LEU:HB2   | 1.82                     | 0.61              |
| 2:z:21:ARG:HH21   | 2:z:246:VAL:HG21  | 1.65                     | 0.61              |
| 3:3:34:PHE:HB3    | 3:3:222:SER:HB3   | 1.83                     | 0.61              |
| 3:8:70:THR:HG22   | 3:8:71:GLY:H      | 1.66                     | 0.61              |
| 3:9:73:ARG:HD2    | 3:AM:218:TYR:HE2  | 1.64                     | 0.61              |
| 3:ZB:28:ASN:HD22  | 4:ZG:52:VAL:CG2   | 2.10                     | 0.61              |
| 4:ZG:297:ASP:OD2  | 4:ZG:314:GLN:NE2  | 2.31                     | 0.61              |
| 4:Za:269:GLN:CD   | 4:Zg:286:PRO:HG3  | 2.23                     | 0.61              |
| 5:AB:37:GLN:OE1   | 5:AB:173:ARG:NH1  | 2.30                     | 0.61              |
| 5:AD:214:VAL:HG13 | 3:AJ:12:LEU:HD13  | 1.81                     | 0.61              |
| 6:AS:235:LEU:HD22 | 6:AT:244:ARG:HH12 | 1.63                     | 0.61              |
| 6:AS:299:ASN:HD21 | 11:A0:78:VAL:HG12 | 1.62                     | 0.61              |
| 6:Ah:277:GLN:HB3  | 6:Ah:377:MET:HE1  | 1.82                     | 0.61              |
| 6:AO:297:GLN:HE22 | 11:A6:60:THR:HG23 | 1.66                     | 0.61              |
| 7:As:70:LEU:O     | 7:As:74:LEU:HG    | 2.01                     | 0.61              |
| 1:A:66:PHE:HE1    | 2:z:41:LEU:HD12   | 1.63                     | 0.61              |
| 1:B:66:PHE:HE1    | 2:a:41:LEU:HD12   | 1.64                     | 0.61              |
| 1:C:88:ALA:HB1    | 1:E:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:E:66:PHE:CE1    | 2:d:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:G:66:PHE:CE1    | 2:f:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:G:181:SER:HB2   | 1:H:31:VAL:HG13   | 1.82                     | 0.61              |
| 1:J:88:ALA:HB1    | 1:L:171:ILE:HD12  | 1.82                     | 0.61              |
| 1:N:88:ALA:HB1    | 1:P:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:O:88:ALA:HB1    | 1:Q:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:U:88:ALA:HB1    | 1:W:171:ILE:HD12  | 1.82                     | 0.61              |
| 3:6:85:ASN:HA     | 4:ZH:50:LEU:HD22  | 1.82                     | 0.61              |
| 3:ZA:240:TYR:OH   | 4:ZF:399:LEU:HD22 | 1.99                     | 0.61              |
| 3:ZE:85:ASN:HA    | 4:ZP:50:LEU:HD13  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZI:331:ASP:HA   | 4:ZN:40:ALA:HB1   | 1.82                     | 0.61              |
| 4:ZY:194:HIS:HB3  | 4:ZY:196:MET:HE3  | 1.82                     | 0.61              |
| 3:AF:9:LYS:HE3    | 12:BF:100:GLY:CA  | 2.29                     | 0.61              |
| 6:AQ:287:ASP:HB3  | 6:AQ:290:LYS:HE2  | 1.80                     | 0.61              |
| 10:A1:48:ARG:NH2  | 11:A7:6:ASP:OD1   | 2.32                     | 0.61              |
| 6:UL:161:LYS:O    | 6:UL:162:PRO:C    | 2.44                     | 0.61              |
| 6:WA:197:LEU:HA   | 6:WB:175:SER:OG   | 2.00                     | 0.61              |
| 6:WL:186:LEU:HA   | 6:WL:190:GLN:OE1  | 1.99                     | 0.61              |
| 6:BS:287:ASP:HB3  | 6:BS:290:LYS:HE2  | 1.81                     | 0.61              |
| 1:A:88:ALA:HB1    | 1:C:171:ILE:HD12  | 1.82                     | 0.61              |
| 1:B:88:ALA:HB1    | 1:D:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:E:88:ALA:HB1    | 1:G:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:H:88:ALA:HB1    | 1:J:171:ILE:HD12  | 1.82                     | 0.61              |
| 1:I:88:ALA:HB1    | 1:K:171:ILE:HD12  | 1.82                     | 0.61              |
| 1:J:66:PHE:CE1    | 2:i:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:K:88:ALA:HB1    | 1:M:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:L:66:PHE:CE1    | 2:k:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:W:181:SER:HB2   | 1:X:31:VAL:HG13   | 1.82                     | 0.61              |
| 2:a:21:ARG:HH21   | 2:a:246:VAL:HG21  | 1.65                     | 0.61              |
| 2:b:142:LEU:HB2   | 2:z:364:ILE:HD13  | 1.82                     | 0.61              |
| 2:c:364:ILE:HD13  | 2:e:142:LEU:HB2   | 1.82                     | 0.61              |
| 2:g:364:ILE:HD13  | 2:i:142:LEU:HB2   | 1.82                     | 0.61              |
| 2:s:78:ASN:ND2    | 3:AI:170:VAL:O    | 2.32                     | 0.61              |
| 3:2:28:ASN:ND2    | 3:7:43:ASP:OD1    | 2.33                     | 0.61              |
| 3:5:189:GLU:OE2   | 3:AN:215:TYR:OH   | 2.11                     | 0.61              |
| 3:8:164:GLN:C     | 3:8:166:ALA:H     | 2.07                     | 0.61              |
| 3:ZB:24:ASN:OD1   | 3:ZB:37:GLN:NE2   | 2.33                     | 0.61              |
| 3:ZB:28:ASN:ND2   | 4:ZG:52:VAL:CB    | 2.64                     | 0.61              |
| 3:ZB:240:TYR:CZ   | 4:ZG:399:LEU:HD11 | 2.35                     | 0.61              |
| 4:ZM:390:LYS:HB2  | 4:ZR:402:LEU:HD22 | 1.82                     | 0.61              |
| 4:ZR:373:VAL:HG11 | 4:ZX:7:VAL:HG22   | 1.83                     | 0.61              |
| 4:ZS:235:ASN:OD1  | 4:ZY:189:SER:OG   | 2.18                     | 0.61              |
| 4:ZY:104:GLU:OE2  | 4:ZY:104:GLU:N    | 2.26                     | 0.61              |
| 4:ZZ:184:VAL:HG13 | 4:ZZ:196:MET:HB2  | 1.83                     | 0.61              |
| 5:AD:200:ARG:HH22 | 3:AJ:189:GLU:HB3  | 1.64                     | 0.61              |
| 5:AE:16:LEU:HD23  | 3:AJ:253:MET:HE3  | 1.69                     | 0.61              |
| 6:Aa:277:GLN:HB3  | 6:Aa:377:MET:HE1  | 1.83                     | 0.61              |
| 9:Av:66:ARG:NE    | 9:Av:178:GLU:OE1  | 2.33                     | 0.61              |
| 6:UO:161:LYS:O    | 6:UO:162:PRO:C    | 2.43                     | 0.61              |
| 6:WK:193:ALA:CB   | 6:WL:213:VAL:CG2  | 2.76                     | 0.61              |
| 1:F:181:SER:HB2   | 1:G:31:VAL:HG13   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:88:ALA:HB1    | 1:I:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:P:88:ALA:HB1    | 1:R:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:S:66:PHE:CE1    | 2:r:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:V:88:ALA:HB1    | 1:X:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:W:88:ALA:HB1    | 1:Y:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:Z:62:TYR:HD1    | 2:x:129:VAL:HG11  | 1.62                     | 0.61              |
| 2:a:142:LEU:HB2   | 2:y:364:ILE:HD13  | 1.82                     | 0.61              |
| 2:n:364:ILE:HD13  | 2:p:142:LEU:HB2   | 1.82                     | 0.61              |
| 2:y:91:ALA:HB2    | 2:y:105:VAL:HG12  | 1.83                     | 0.61              |
| 2:z:91:ALA:HB2    | 2:z:105:VAL:HG12  | 1.83                     | 0.61              |
| 3:4:45:LEU:HD22   | 3:AH:98:LYS:HG3   | 1.83                     | 0.61              |
| 3:ZA:49:ILE:HG13  | 3:ZA:68:ILE:HD12  | 1.81                     | 0.61              |
| 3:ZB:175:LEU:HG   | 3:ZB:206:PRO:HG3  | 1.82                     | 0.61              |
| 3:ZE:19:MET:HE3   | 4:ZJ:395:ILE:HD12 | 1.83                     | 0.61              |
| 4:ZH:281:GLN:OE1  | 4:ZH:283:GLY:N    | 2.31                     | 0.61              |
| 5:AA:181:LEU:HD21 | 5:AA:193:LEU:HD11 | 1.81                     | 0.61              |
| 5:AD:49:LEU:HB2   | 11:A9:90:PRO:HG2  | 1.81                     | 0.61              |
| 5:AD:146:LEU:HD13 | 5:AD:155:VAL:HG22 | 1.82                     | 0.61              |
| 6:Ae:277:GLN:HB3  | 6:Ae:377:MET:HE1  | 1.83                     | 0.61              |
| 6:Af:277:GLN:HB3  | 6:Af:377:MET:HE1  | 1.83                     | 0.61              |
| 6:Ag:295:SER:CB   | 11:A8:72:HIS:CB   | 2.73                     | 0.61              |
| 6:AO:394:LYS:HE3  | 6:AO:394:LYS:HA   | 1.80                     | 0.61              |
| 7:Aq:89:GLY:C     | 6:WW:164:LEU:HD12 | 2.24                     | 0.61              |
| 8:At:106:MET:SD   | 8:At:225:GLY:HA3  | 2.40                     | 0.61              |
| 11:A9:103:ASP:OD1 | 12:BE:112:TYR:OH  | 2.11                     | 0.61              |
| 6:UM:103:GLN:CD   | 6:WQ:182:PRO:CB   | 2.71                     | 0.61              |
| 6:UN:73:MET:HE3   | 6:UN:99:ARG:HD3   | 1.81                     | 0.61              |
| 1:A:31:VAL:HG13   | 1:Z:181:SER:HB2   | 1.82                     | 0.61              |
| 1:B:171:ILE:HD12  | 1:Z:88:ALA:HB1    | 1.83                     | 0.61              |
| 1:F:88:ALA:HB1    | 1:H:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:R:66:PHE:CE1    | 2:q:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:S:88:ALA:HB1    | 1:U:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:T:88:ALA:HB1    | 1:V:171:ILE:HD12  | 1.83                     | 0.61              |
| 2:k:220:THR:OG1   | 2:l:98:ARG:HD2    | 1.99                     | 0.61              |
| 2:w:21:ARG:HH21   | 2:w:246:VAL:HG21  | 1.65                     | 0.61              |
| 2:x:91:ALA:HB2    | 2:x:105:VAL:HG12  | 1.83                     | 0.61              |
| 2:y:21:ARG:HH21   | 2:y:246:VAL:HG21  | 1.65                     | 0.61              |
| 3:4:79:ARG:NH2    | 3:4:184:LEU:O     | 2.30                     | 0.61              |
| 3:5:237:GLN:NE2   | 3:ZA:252:GLN:HB3  | 2.16                     | 0.61              |
| 4:ZH:270:ASN:HB2  | 4:ZN:191:GLY:C    | 2.25                     | 0.61              |
| 4:ZO:270:ASN:N    | 4:ZU:190:GLN:O    | 2.32                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZQ:307:GLU:OE1  | 4:Zb:92:VAL:HG22  | 2.01                     | 0.61              |
| 4:ZR:146:ALA:HB2  | 4:ZR:286:PRO:HD3  | 1.83                     | 0.61              |
| 3:AF:143:PRO:HG2  | 3:AF:161:GLN:HE22 | 1.65                     | 0.61              |
| 6:Ad:277:GLN:HB3  | 6:Ad:377:MET:HE1  | 1.83                     | 0.61              |
| 6:Ag:277:GLN:HB3  | 6:Ag:377:MET:HE1  | 1.83                     | 0.61              |
| 6:Aj:277:GLN:HB3  | 6:Aj:377:MET:HE1  | 1.83                     | 0.61              |
| 6:WB:212:LEU:HB3  | 6:WB:221:THR:HG23 | 1.81                     | 0.61              |
| 12:BC:3:LEU:HB3   | 12:BC:7:PHE:HB3   | 1.82                     | 0.61              |
| 1:I:66:PHE:CE1    | 2:h:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:M:181:SER:HB2   | 1:N:31:VAL:HG13   | 1.82                     | 0.61              |
| 1:T:66:PHE:CE1    | 2:s:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:U:181:SER:HB2   | 1:V:31:VAL:HG13   | 1.82                     | 0.61              |
| 1:X:88:ALA:HB1    | 1:Z:171:ILE:HD12  | 1.83                     | 0.61              |
| 2:x:21:ARG:HH21   | 2:x:246:VAL:HG21  | 1.65                     | 0.61              |
| 3:0:108:PRO:HG2   | 3:AI:153:ARG:NH2  | 2.15                     | 0.61              |
| 3:1:197:SER:HA    | 3:AK:124:GLN:HB3  | 1.82                     | 0.61              |
| 3:2:42:GLU:HB3    | 3:2:75:VAL:HG23   | 1.81                     | 0.61              |
| 3:4:254:LEU:O     | 3:4:258:THR:HG23  | 2.01                     | 0.61              |
| 3:8:45:LEU:HD13   | 3:AL:83:GLN:HG2   | 1.81                     | 0.61              |
| 3:9:259:GLN:O     | 3:9:260:LEU:C     | 2.44                     | 0.61              |
| 3:ZD:76:ALA:HA    | 4:ZI:47:LYS:CE    | 2.30                     | 0.61              |
| 4:ZO:160:SER:OG   | 4:ZU:192:ASN:OD1  | 2.18                     | 0.61              |
| 4:ZQ:379:GLN:HE21 | 4:ZV:394:GLN:HE22 | 1.48                     | 0.61              |
| 4:ZX:114:MET:HE1  | 4:ZX:333:VAL:HG21 | 1.82                     | 0.61              |
| 5:AB:211:VAL:O    | 3:AM:1:MET:HB3    | 1.99                     | 0.61              |
| 5:AC:59:ALA:C     | 3:AH:66:LEU:HD23  | 2.25                     | 0.61              |
| 5:AC:84:GLN:OE1   | 3:AN:48:THR:CG2   | 2.47                     | 0.61              |
| 5:AE:221:ILE:HG23 | 3:AK:251:ASP:OD2  | 2.01                     | 0.61              |
| 3:AJ:62:LEU:HG    | 12:BF:84:LEU:HD11 | 1.83                     | 0.61              |
| 6:AZ:277:GLN:HB3  | 6:AZ:377:MET:HE1  | 1.83                     | 0.61              |
| 6:Ai:277:GLN:HB3  | 6:Ai:377:MET:HE1  | 1.83                     | 0.61              |
| 7:Ar:21:ALA:HB2   | 9:Ax:199:VAL:HG22 | 1.81                     | 0.61              |
| 8:At:178:LEU:HD12 | 8:At:182:ASN:HD21 | 1.65                     | 0.61              |
| 9:Aw:106:ASP:OD2  | 10:A2:31:THR:N    | 2.33                     | 0.61              |
| 6:UP:161:LYS:O    | 6:UP:162:PRO:C    | 2.43                     | 0.61              |
| 6:WD:117:ASP:O    | 6:WD:118:GLN:C    | 2.44                     | 0.61              |
| 6:WG:212:LEU:HB3  | 6:WG:221:THR:HG23 | 1.82                     | 0.61              |
| 1:B:66:PHE:CE1    | 2:a:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:O:181:SER:HB2   | 1:P:31:VAL:HG13   | 1.82                     | 0.61              |
| 1:Q:88:ALA:HB1    | 1:S:171:ILE:HD12  | 1.83                     | 0.61              |
| 1:U:66:PHE:CE1    | 2:t:41:LEU:HD12   | 2.36                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:a:91:ALA:HB2   | 2:a:105:VAL:HG12  | 1.83                     | 0.61              |
| 2:b:21:ARG:HH21  | 2:b:246:VAL:HG21  | 1.65                     | 0.61              |
| 2:d:364:ILE:HD13 | 2:f:142:LEU:HB2   | 1.82                     | 0.61              |
| 2:w:91:ALA:HB2   | 2:w:105:VAL:HG12  | 1.83                     | 0.61              |
| 2:x:364:ILE:HD13 | 2:z:142:LEU:HB2   | 1.82                     | 0.61              |
| 3:0:226:VAL:HG21 | 3:ZB:1:MET:HB2    | 1.83                     | 0.61              |
| 3:3:22:ILE:HG21  | 3:3:233:MET:HG3   | 1.83                     | 0.61              |
| 3:3:58:GLU:N     | 5:AB:140:ASP:OD2  | 2.34                     | 0.61              |
| 3:4:51:GLN:NE2   | 5:AC:146:LEU:HD12 | 2.16                     | 0.61              |
| 3:6:56:SER:CB    | 5:AE:138:ALA:HB1  | 2.29                     | 0.61              |
| 3:8:56:SER:OG    | 3:AG:153:ARG:HG3  | 2.00                     | 0.61              |
| 4:ZO:65:THR:HG21 | 4:ZZ:4:SER:OG     | 2.00                     | 0.61              |
| 4:ZQ:188:ASP:HA  | 4:ZQ:257:ALA:HB2  | 1.82                     | 0.61              |
| 4:ZZ:269:GLN:HG2 | 4:Zf:286:PRO:CG   | 2.30                     | 0.61              |
| 5:AB:70:GLN:CG   | 3:AM:6:TRP:HE1    | 2.12                     | 0.61              |
| 3:AG:178:PHE:CE2 | 3:AG:184:LEU:HD21 | 2.36                     | 0.61              |
| 6:AR:277:GLN:HB3 | 6:AR:377:MET:HE1  | 1.83                     | 0.61              |
| 6:AY:277:GLN:HB3 | 6:AY:377:MET:HE1  | 1.83                     | 0.61              |
| 6:AZ:236:LYS:HE2 | 6:UP:167:ARG:NH1  | 2.15                     | 0.61              |
| 7:Ab:56:VAL:O    | 7:Ab:60:ILE:HG12  | 2.01                     | 0.61              |
| 6:Ak:277:GLN:HB3 | 6:Ak:377:MET:HE1  | 1.83                     | 0.61              |
| 7:As:14:MET:CE   | 8:At:229:MET:SD   | 2.89                     | 0.61              |
| 9:Ay:152:ARG:NH2 | 6:WJ:165:PHE:HA   | 2.16                     | 0.61              |
| 11:A7:51:LYS:NZ  | 11:A7:84:ASP:OD1  | 2.34                     | 0.61              |
| 6:WH:193:ALA:CB  | 6:WI:213:VAL:HG11 | 2.26                     | 0.61              |
| 6:WM:200:SER:O   | 6:WN:158:ALA:HB3  | 2.01                     | 0.61              |
| 6:WP:190:GLN:NE2 | 6:WQ:216:SER:O    | 2.33                     | 0.61              |
| 1:A:171:ILE:HD12 | 1:Y:88:ALA:HB1    | 1.83                     | 0.61              |
| 1:Q:66:PHE:CE1   | 2:p:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:Y:181:SER:HB2  | 1:Z:31:VAL:HG13   | 1.82                     | 0.61              |
| 2:v:21:ARG:HH21  | 2:v:246:VAL:HG21  | 1.65                     | 0.61              |
| 3:9:20:ASP:OD1   | 3:ZE:4:SER:OG     | 2.18                     | 0.61              |
| 3:ZB:248:SER:CB  | 4:ZG:402:LEU:HD22 | 2.29                     | 0.61              |
| 4:ZH:11:ASN:O    | 4:ZH:15:THR:HG23  | 2.00                     | 0.61              |
| 4:ZS:319:ASN:ND2 | 4:ZS:352:ASN:OD1  | 2.33                     | 0.61              |
| 4:ZU:294:ILE:O   | 4:ZU:358:ASN:ND2  | 2.30                     | 0.61              |
| 5:AA:76:ARG:CD   | 3:AF:80:LEU:CD1   | 2.78                     | 0.61              |
| 5:AE:151:PRO:HB2 | 5:AE:154:THR:HG23 | 1.83                     | 0.61              |
| 3:AF:73:ARG:HB2  | 12:BA:78:TYR:CE2  | 2.36                     | 0.61              |
| 3:AF:98:LYS:HE2  | 3:AL:187:ILE:O    | 2.01                     | 0.61              |
| 3:AM:52:PRO:HG2  | 12:BC:89:GLY:CA   | 2.30                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Av:152:ARG:HH12 | 6:WV:164:LEU:HB3  | 1.64                     | 0.61              |
| 6:WF:190:GLN:HA   | 6:WG:217:GLY:O    | 2.01                     | 0.61              |
| 6:BR:394:LYS:HA   | 6:BR:394:LYS:HE3  | 1.80                     | 0.61              |
| 1:B:181:SER:HB2   | 1:C:31:VAL:HG13   | 1.82                     | 0.61              |
| 1:D:66:PHE:CE1    | 2:c:41:LEU:HD12   | 2.36                     | 0.61              |
| 1:I:181:SER:HB2   | 1:J:31:VAL:HG13   | 1.82                     | 0.61              |
| 1:X:181:SER:HB2   | 1:Y:31:VAL:HG13   | 1.82                     | 0.61              |
| 2:b:91:ALA:HB2    | 2:b:105:VAL:HG12  | 1.83                     | 0.61              |
| 4:ZL:83:PHE:HB2   | 4:ZL:95:SER:O     | 2.01                     | 0.61              |
| 4:ZT:106:ARG:HH21 | 4:ZT:139:ILE:HG22 | 1.64                     | 0.61              |
| 4:ZX:80:ASN:OD1   | 4:ZX:81:GLY:N     | 2.34                     | 0.61              |
| 4:Zg:114:MET:HA   | 4:Zg:114:MET:HE3  | 1.82                     | 0.61              |
| 5:AE:57:VAL:HG11  | 12:BF:29:ALA:O    | 2.01                     | 0.61              |
| 9:Ax:160:GLN:HA   | 6:WE:166:VAL:HG23 | 1.81                     | 0.61              |
| 10:A4:14:LEU:HD23 | 6:BW:278:THR:HG21 | 1.83                     | 0.61              |
| 11:A6:22:ARG:HH22 | 12:BB:3:LEU:HD21  | 1.66                     | 0.61              |
| 11:A8:65:LEU:C    | 11:A8:65:LEU:HD12 | 2.25                     | 0.61              |
| 6:WV:190:GLN:NE2  | 6:WW:216:SER:O    | 2.34                     | 0.61              |
| 6:BR:287:ASP:HB3  | 6:BR:290:LYS:HE2  | 1.80                     | 0.61              |
| 6:BV:277:GLN:HB3  | 6:BV:377:MET:HE1  | 1.83                     | 0.61              |
| 1:A:66:PHE:CE1    | 2:z:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:R:88:ALA:HB1    | 1:T:171:ILE:HD12  | 1.83                     | 0.60              |
| 1:Z:66:PHE:CE1    | 2:y:41:LEU:HD12   | 2.36                     | 0.60              |
| 2:f:364:ILE:HD13  | 2:h:142:LEU:HB2   | 1.82                     | 0.60              |
| 2:u:21:ARG:HH21   | 2:u:246:VAL:HG21  | 1.65                     | 0.60              |
| 3:0:6:TRP:HZ2     | 3:AI:235:GLN:NE2  | 1.98                     | 0.60              |
| 3:5:70:THR:HG22   | 3:5:71:GLY:H      | 1.65                     | 0.60              |
| 3:6:257:LEU:HD21  | 3:AJ:227:ALA:HA   | 1.83                     | 0.60              |
| 4:ZK:112:GLN:N    | 4:ZK:112:GLN:OE1  | 2.33                     | 0.60              |
| 5:AA:229:MET:HG2  | 3:AG:258:THR:CG2  | 2.21                     | 0.60              |
| 5:AB:72:ASP:CB    | 3:AM:9:LYS:HZ3    | 2.09                     | 0.60              |
| 5:AB:214:VAL:HA   | 3:AM:257:LEU:HD21 | 1.83                     | 0.60              |
| 6:Ad:372:ILE:HG22 | 10:A2:11:ILE:CG2  | 2.31                     | 0.60              |
| 6:An:394:LYS:HA   | 6:An:394:LYS:HE3  | 1.80                     | 0.60              |
| 9:Ay:152:ARG:HH22 | 6:WJ:165:PHE:N    | 1.98                     | 0.60              |
| 10:A2:11:ILE:HD12 | 10:A2:12:SER:CA   | 2.31                     | 0.60              |
| 6:UI:73:MET:HE3   | 6:UI:99:ARG:HD3   | 1.81                     | 0.60              |
| 6:UO:73:MET:HE3   | 6:UO:99:ARG:HD3   | 1.81                     | 0.60              |
| 6:WR:212:LEU:HB3  | 6:WR:221:THR:HG23 | 1.82                     | 0.60              |
| 1:N:66:PHE:CE1    | 2:m:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:P:66:PHE:CE1    | 2:o:41:LEU:HD12   | 2.36                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:V:66:PHE:CE1    | 2:u:41:LEU:HD12   | 2.36                     | 0.60              |
| 2:n:208:ARG:O     | 2:n:212:SER:OG    | 2.16                     | 0.60              |
| 4:ZF:102:LEU:O    | 4:ZK:322:ASN:ND2  | 2.34                     | 0.60              |
| 4:ZF:107:ASN:ND2  | 4:ZF:138:THR:OG1  | 2.34                     | 0.60              |
| 4:ZJ:195:ASP:OD2  | 4:ZJ:216:SER:OG   | 2.17                     | 0.60              |
| 4:ZT:187:TYR:HE2  | 4:ZT:285:LYS:HB2  | 1.65                     | 0.60              |
| 5:AD:59:ALA:HB3   | 3:AI:66:LEU:HD11  | 1.83                     | 0.60              |
| 5:AD:74:THR:CG2   | 3:AI:38:ARG:HH12  | 1.98                     | 0.60              |
| 6:AX:277:GLN:HB3  | 6:AX:377:MET:HE1  | 1.83                     | 0.60              |
| 6:AI:277:GLN:HB3  | 6:AI:377:MET:HE1  | 1.83                     | 0.60              |
| 6:AQ:277:GLN:HB3  | 6:AQ:377:MET:HE1  | 1.83                     | 0.60              |
| 8:At:114:VAL:HG12 | 9:Av:213:PRO:HB3  | 1.81                     | 0.60              |
| 10:Az:86:ILE:HD13 | 10:A5:98:GLU:HG3  | 1.81                     | 0.60              |
| 10:A1:48:ARG:NH2  | 11:A7:6:ASP:CG    | 2.59                     | 0.60              |
| 10:A4:77:LYS:CE   | 11:A0:13:GLN:HE22 | 2.08                     | 0.60              |
| 6:UL:127:SER:O    | 6:UL:131:ASN:CB   | 2.50                     | 0.60              |
| 6:WH:197:LEU:HD12 | 6:WI:175:SER:HB3  | 1.83                     | 0.60              |
| 6:WI:190:GLN:HG2  | 6:WJ:217:GLY:HA3  | 1.82                     | 0.60              |
| 6:BU:277:GLN:HB3  | 6:BU:377:MET:HE1  | 1.83                     | 0.60              |
| 6:BW:277:GLN:HB3  | 6:BW:377:MET:HE1  | 1.83                     | 0.60              |
| 1:H:181:SER:HB2   | 1:I:31:VAL:HG13   | 1.82                     | 0.60              |
| 1:Q:62:TYR:HD1    | 2:o:129:VAL:HG11  | 1.62                     | 0.60              |
| 1:T:181:SER:HB2   | 1:U:31:VAL:HG13   | 1.82                     | 0.60              |
| 1:Y:66:PHE:CE1    | 2:x:41:LEU:HD12   | 2.36                     | 0.60              |
| 2:c:21:ARG:HH21   | 2:c:246:VAL:HG21  | 1.65                     | 0.60              |
| 2:h:91:ALA:HB2    | 2:h:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:o:364:ILE:HD13  | 2:q:142:LEU:HB2   | 1.82                     | 0.60              |
| 2:v:91:ALA:HB2    | 2:v:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:w:364:ILE:HD13  | 2:y:142:LEU:HB2   | 1.82                     | 0.60              |
| 3:ZD:208:LEU:O    | 3:ZD:210:GLY:N    | 2.35                     | 0.60              |
| 4:ZF:234:GLU:HB3  | 4:ZL:255:THR:HB   | 1.83                     | 0.60              |
| 4:ZZ:394:GLN:O    | 4:ZZ:398:THR:HG23 | 2.01                     | 0.60              |
| 6:AW:277:GLN:HB3  | 6:AW:377:MET:HE1  | 1.83                     | 0.60              |
| 6:Af:297:GLN:HE22 | 11:A8:76:GLN:H    | 1.46                     | 0.60              |
| 7:As:14:MET:HE2   | 8:At:229:MET:SD   | 2.42                     | 0.60              |
| 6:UI:161:LYS:O    | 6:UI:162:PRO:C    | 2.44                     | 0.60              |
| 6:WR:186:LEU:HA   | 6:WR:190:GLN:OE1  | 2.00                     | 0.60              |
| 6:WW:117:ASP:O    | 6:WW:118:GLN:C    | 2.44                     | 0.60              |
| 6:BR:277:GLN:HB3  | 6:BR:377:MET:HE1  | 1.83                     | 0.60              |
| 1:R:181:SER:HB2   | 1:S:31:VAL:HG13   | 1.82                     | 0.60              |
| 1:W:62:TYR:HD1    | 2:u:129:VAL:HG11  | 1.62                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:364:ILE:HD13  | 2:g:142:LEU:HB2   | 1.82                     | 0.60              |
| 2:g:91:ALA:HB2    | 2:g:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:i:91:ALA:HB2    | 2:i:105:VAL:HG12  | 1.83                     | 0.60              |
| 3:0:187:ILE:O     | 3:AI:98:LYS:NZ    | 2.31                     | 0.60              |
| 3:6:57:SER:CB     | 3:AK:108:PRO:HB3  | 2.06                     | 0.60              |
| 3:ZC:218:TYR:OH   | 4:ZN:53:LYS:CD    | 2.49                     | 0.60              |
| 4:ZK:104:GLU:HG2  | 4:ZP:338:GLN:O    | 2.02                     | 0.60              |
| 4:ZS:295:ASN:ND2  | 4:ZS:299:THR:OG1  | 2.34                     | 0.60              |
| 4:Zc:42:MET:HG2   | 4:Zc:53:LYS:HE3   | 1.83                     | 0.60              |
| 5:AC:249:SER:O    | 5:AC:250:MET:C    | 2.45                     | 0.60              |
| 5:AE:228:GLU:HB3  | 3:AK:258:THR:HG22 | 1.76                     | 0.60              |
| 3:AG:44:LEU:CD1   | 12:BB:78:TYR:HB2  | 2.29                     | 0.60              |
| 3:AN:22:ILE:HD11  | 3:AN:232:ASN:HB3  | 1.81                     | 0.60              |
| 6:AY:299:ASN:ND2  | 11:A9:78:VAL:C    | 2.48                     | 0.60              |
| 6:Ae:372:ILE:HD13 | 10:A2:3:ALA:C     | 2.26                     | 0.60              |
| 9:Au:162:PRO:HD2  | 9:Au:163:GLU:N    | 2.14                     | 0.60              |
| 12:BE:68:ILE:HD11 | 6:BP:312:VAL:HG21 | 1.84                     | 0.60              |
| 1:S:181:SER:HB2   | 1:T:31:VAL:HG13   | 1.82                     | 0.60              |
| 2:n:80:GLN:OE1    | 3:AJ:137:GLN:CG   | 2.49                     | 0.60              |
| 2:v:364:ILE:HD13  | 2:x:142:LEU:HB2   | 1.82                     | 0.60              |
| 3:2:56:SER:CA     | 5:AA:138:ALA:CB   | 2.79                     | 0.60              |
| 3:6:242:ILE:CD1   | 3:ZC:1:MET:HE1    | 2.32                     | 0.60              |
| 3:ZE:137:GLN:HA   | 3:ZE:139:ALA:H    | 1.67                     | 0.60              |
| 4:ZF:349:GLY:O    | 4:ZL:89:ASN:ND2   | 2.35                     | 0.60              |
| 4:ZJ:217:ASP:HB3  | 4:ZJ:220:ALA:HB2  | 1.84                     | 0.60              |
| 4:ZS:18:ASP:OD1   | 4:ZX:5:GLN:NE2    | 2.34                     | 0.60              |
| 4:ZV:269:GLN:HG3  | 4:Zb:286:PRO:HG2  | 1.82                     | 0.60              |
| 4:Zf:159:ASN:ND2  | 4:Zf:161:THR:OG1  | 2.34                     | 0.60              |
| 5:AD:217:MET:SD   | 3:AI:245:LYS:HG2  | 2.40                     | 0.60              |
| 6:Am:277:GLN:HB3  | 6:Am:377:MET:HE1  | 1.83                     | 0.60              |
| 6:UL:126:PHE:CE1  | 6:UL:130:VAL:CG2  | 2.84                     | 0.60              |
| 6:UM:127:SER:O    | 6:UM:131:ASN:CB   | 2.50                     | 0.60              |
| 6:WI:164:LEU:HD23 | 6:WI:165:PHE:HB3  | 1.83                     | 0.60              |
| 6:WK:197:LEU:HA   | 6:WL:175:SER:CB   | 2.32                     | 0.60              |
| 12:BE:12:SER:OG   | 12:BE:62:VAL:O    | 2.20                     | 0.60              |
| 1:I:62:TYR:HD1    | 2:g:129:VAL:HG11  | 1.62                     | 0.60              |
| 1:L:181:SER:HB2   | 1:M:31:VAL:HG13   | 1.82                     | 0.60              |
| 2:c:91:ALA:HB2    | 2:c:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:d:21:ARG:HH21   | 2:d:246:VAL:HG21  | 1.65                     | 0.60              |
| 2:n:21:ARG:HH21   | 2:n:246:VAL:HG21  | 1.65                     | 0.60              |
| 3:2:83:GLN:HG2    | 3:ZD:45:LEU:CD2   | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZO:71:ARG:HB2   | 4:ZO:74:ASP:OD1   | 2.02                     | 0.60              |
| 4:ZR:183:THR:OG1  | 4:Zc:132:ALA:HA   | 2.02                     | 0.60              |
| 4:ZU:150:THR:H    | 4:ZU:282:ASN:HD21 | 1.48                     | 0.60              |
| 4:ZV:196:MET:HA   | 4:ZV:196:MET:HE3  | 1.83                     | 0.60              |
| 5:AB:217:MET:HE3  | 3:AG:242:ILE:HD13 | 1.84                     | 0.60              |
| 3:AM:86:LEU:HD12  | 3:AM:218:TYR:HB3  | 1.84                     | 0.60              |
| 6:AS:402:LEU:HD12 | 6:AS:403:PRO:HD2  | 1.84                     | 0.60              |
| 6:Al:402:LEU:HD12 | 6:Al:403:PRO:HD2  | 1.84                     | 0.60              |
| 6:An:277:GLN:HB3  | 6:An:377:MET:HE1  | 1.83                     | 0.60              |
| 9:Ax:83:ALA:HB3   | 9:Ax:84:PRO:HD3   | 1.84                     | 0.60              |
| 9:Ax:152:ARG:HD3  | 6:WG:165:PHE:CD2  | 2.36                     | 0.60              |
| 6:UL:208:GLY:N    | 6:WG:187:ASP:OD2  | 2.33                     | 0.60              |
| 6:UP:127:SER:O    | 6:UP:131:ASN:CB   | 2.50                     | 0.60              |
| 1:K:66:PHE:CE1    | 2:j:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:T:62:TYR:HD1    | 2:r:129:VAL:HG11  | 1.62                     | 0.60              |
| 1:W:66:PHE:CE1    | 2:v:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:X:66:PHE:CE1    | 2:w:41:LEU:HD12   | 2.36                     | 0.60              |
| 2:f:91:ALA:HB2    | 2:f:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:j:91:ALA:HB2    | 2:j:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:k:208:ARG:O     | 2:k:212:SER:OG    | 2.16                     | 0.60              |
| 2:p:21:ARG:HH21   | 2:p:246:VAL:HG21  | 1.65                     | 0.60              |
| 2:t:21:ARG:HH21   | 2:t:246:VAL:HG21  | 1.65                     | 0.60              |
| 2:u:91:ALA:HB2    | 2:u:105:VAL:HG12  | 1.83                     | 0.60              |
| 3:ZE:85:ASN:HA    | 4:ZP:50:LEU:CD1   | 2.32                     | 0.60              |
| 4:ZN:65:THR:HG21  | 4:ZY:4:SER:HB2    | 1.83                     | 0.60              |
| 4:ZR:181:LYS:CD   | 4:Zc:129:GLN:NE2  | 2.64                     | 0.60              |
| 4:ZR:380:ARG:HD2  | 4:ZX:396:LEU:HB3  | 1.83                     | 0.60              |
| 4:Zc:382:TYR:CD1  | 4:Zh:395:ILE:HD11 | 2.36                     | 0.60              |
| 3:AG:45:LEU:HD23  | 12:BB:76:LEU:HD12 | 1.83                     | 0.60              |
| 3:AH:22:ILE:HG21  | 3:AH:233:MET:HG2  | 1.84                     | 0.60              |
| 3:AL:89:THR:C     | 3:AL:91:ASN:H     | 2.10                     | 0.60              |
| 6:AV:402:LEU:HD12 | 6:AV:403:PRO:HD2  | 1.84                     | 0.60              |
| 7:Ab:54:LYS:HD2   | 9:Av:207:LEU:HD23 | 1.82                     | 0.60              |
| 6:Ak:372:ILE:HG21 | 10:A1:4:ILE:HG13  | 1.82                     | 0.60              |
| 6:AP:278:THR:CG2  | 10:A5:21:ALA:CB   | 2.67                     | 0.60              |
| 6:UN:127:SER:O    | 6:UN:131:ASN:CB   | 2.50                     | 0.60              |
| 12:BB:27:ASN:OD1  | 12:BB:42:TYR:OH   | 2.19                     | 0.60              |
| 1:C:66:PHE:CE1    | 2:b:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:C:181:SER:HB2   | 1:D:31:VAL:HG13   | 1.82                     | 0.60              |
| 2:n:80:GLN:OE1    | 3:AJ:137:GLN:CD   | 2.45                     | 0.60              |
| 2:o:21:ARG:HH21   | 2:o:246:VAL:HG21  | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:q:21:ARG:HH21   | 2:q:246:VAL:HG21  | 1.65                     | 0.60              |
| 2:u:364:ILE:HD13  | 2:w:142:LEU:HB2   | 1.82                     | 0.60              |
| 3:0:257:LEU:HD21  | 5:AD:214:VAL:HA   | 1.83                     | 0.60              |
| 4:ZO:146:ALA:HB2  | 4:ZO:286:PRO:HD3  | 1.83                     | 0.60              |
| 4:ZV:181:LYS:CD   | 4:Zg:129:GLN:NE2  | 2.58                     | 0.60              |
| 4:ZW:382:TYR:CZ   | 4:Zb:395:ILE:HG23 | 2.37                     | 0.60              |
| 7:Aq:74:LEU:HD22  | 9:Aw:229:VAL:CG1  | 2.31                     | 0.60              |
| 6:UN:161:LYS:O    | 6:UN:162:PRO:C    | 2.44                     | 0.60              |
| 6:WC:193:ALA:HB1  | 6:WD:213:VAL:CG1  | 2.30                     | 0.60              |
| 6:WI:186:LEU:HA   | 6:WI:190:GLN:OE1  | 2.02                     | 0.60              |
| 6:WK:197:LEU:HD11 | 6:WL:156:HIS:CD2  | 2.36                     | 0.60              |
| 12:BD:109:SER:O   | 12:BD:113:GLN:HG3 | 2.02                     | 0.60              |
| 1:D:181:SER:HB2   | 1:E:31:VAL:HG13   | 1.82                     | 0.60              |
| 1:M:66:PHE:CE1    | 2:l:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:O:66:PHE:CE1    | 2:n:41:LEU:HD12   | 2.36                     | 0.60              |
| 2:j:21:ARG:HH21   | 2:j:246:VAL:HG21  | 1.65                     | 0.60              |
| 2:k:91:ALA:HB2    | 2:k:105:VAL:HG12  | 1.83                     | 0.60              |
| 2:p:364:ILE:HD13  | 2:r:142:LEU:HB2   | 1.82                     | 0.60              |
| 2:r:21:ARG:HH21   | 2:r:246:VAL:HG21  | 1.65                     | 0.60              |
| 3:1:100:GLN:OE1   | 3:1:100:GLN:N     | 2.30                     | 0.60              |
| 3:3:28:ASN:ND2    | 3:8:43:ASP:OD1    | 2.35                     | 0.60              |
| 4:ZX:242:GLY:O    | 4:ZX:263:PHE:N    | 2.30                     | 0.60              |
| 5:AC:229:MET:SD   | 12:BD:28:LEU:HD11 | 2.42                     | 0.60              |
| 3:AK:73:ARG:HD3   | 12:BF:78:TYR:CE1  | 2.37                     | 0.60              |
| 6:AV:277:GLN:HB3  | 6:AV:377:MET:HE1  | 1.83                     | 0.60              |
| 6:AY:295:SER:CB   | 11:A9:65:LEU:HB2  | 2.32                     | 0.60              |
| 6:Ak:402:LEU:HD12 | 6:Ak:403:PRO:HD2  | 1.84                     | 0.60              |
| 6:Al:294:ARG:CD   | 11:A7:68:THR:CG2  | 2.80                     | 0.60              |
| 9:Au:160:GLN:O    | 6:WP:165:PHE:CA   | 2.49                     | 0.60              |
| 9:Ax:232:TRP:O    | 9:Ax:236:MET:HG2  | 2.02                     | 0.60              |
| 9:Ay:184:GLN:O    | 9:Ay:188:THR:HG23 | 2.02                     | 0.60              |
| 10:Az:79:SER:HB2  | 10:A5:91:LYS:NZ   | 2.16                     | 0.60              |
| 6:UI:127:SER:O    | 6:UI:131:ASN:CB   | 2.50                     | 0.60              |
| 6:UJ:161:LYS:O    | 6:UJ:162:PRO:C    | 2.43                     | 0.60              |
| 6:WD:168:GLU:CG   | 6:WD:170:LYS:HE2  | 2.31                     | 0.60              |
| 6:WS:117:ASP:O    | 6:WS:118:GLN:C    | 2.44                     | 0.60              |
| 1:A:181:SER:HB2   | 1:B:31:VAL:HG13   | 1.82                     | 0.60              |
| 1:E:181:SER:HB2   | 1:F:31:VAL:HG13   | 1.82                     | 0.60              |
| 1:F:66:PHE:CE1    | 2:e:41:LEU:HD12   | 2.36                     | 0.60              |
| 1:V:181:SER:HB2   | 1:W:31:VAL:HG13   | 1.82                     | 0.60              |
| 2:e:21:ARG:HH21   | 2:e:246:VAL:HG21  | 1.65                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:e:91:ALA:HB2     | 2:e:105:VAL:HG12   | 1.83                     | 0.60              |
| 2:k:21:ARG:HH21    | 2:k:246:VAL:HG21   | 1.65                     | 0.60              |
| 2:m:21:ARG:HH21    | 2:m:246:VAL:HG21   | 1.65                     | 0.60              |
| 2:s:21:ARG:HH21    | 2:s:246:VAL:HG21   | 1.65                     | 0.60              |
| 3:ZA:91:ASN:HB2    | 3:ZA:94:ASP:OD2    | 2.02                     | 0.60              |
| 4:ZJ:18:ASP:HB3    | 4:ZO:5:GLN:HE22    | 1.67                     | 0.60              |
| 4:ZO:170:PHE:HE2   | 4:ZO:178:TYR:HB3   | 1.65                     | 0.60              |
| 4:ZO:248:THR:OG1   | 4:ZO:257:ALA:N     | 2.34                     | 0.60              |
| 4:ZY:330:GLY:HA2   | 4:Zd:41:ASP:OD1    | 2.02                     | 0.60              |
| 5:AB:9:MET:CG      | 12:BB:103:VAL:HG21 | 2.31                     | 0.60              |
| 5:AB:91:GLN:HB2    | 5:AB:121:ILE:HD11  | 1.83                     | 0.60              |
| 5:AB:224:ALA:N     | 3:AG:253:MET:HE3   | 2.15                     | 0.60              |
| 3:AH:189:GLU:HG2   | 3:AM:42:GLU:CD     | 2.27                     | 0.60              |
| 3:AL:3:SER:O       | 3:AL:6:TRP:N       | 2.35                     | 0.60              |
| 6:AT:402:LEU:HD12  | 6:AT:403:PRO:HD2   | 1.84                     | 0.60              |
| 6:AP:277:GLN:HB3   | 6:AP:377:MET:HE1   | 1.83                     | 0.60              |
| 7:Ar:36:SER:O      | 7:As:44:ILE:CD1    | 2.50                     | 0.60              |
| 9:Aw:140:ARG:O     | 6:WW:167:ARG:HD3   | 2.02                     | 0.60              |
| 9:Ay:105:ILE:HD13  | 10:A4:34:PHE:HZ    | 1.67                     | 0.60              |
| 6:UK:127:SER:O     | 6:UK:131:ASN:CB    | 2.50                     | 0.60              |
| 6:UO:127:SER:O     | 6:UO:131:ASN:CB    | 2.50                     | 0.60              |
| 6:BS:277:GLN:HB3   | 6:BS:377:MET:HE1   | 1.83                     | 0.60              |
| 6:BW:402:LEU:HD12  | 6:BW:403:PRO:HD2   | 1.84                     | 0.60              |
| 6:BX:402:LEU:HD12  | 6:BX:403:PRO:HD2   | 1.84                     | 0.60              |
| 1:H:66:PHE:CE1     | 2:g:41:LEU:HD12    | 2.36                     | 0.59              |
| 1:N:62:TYR:CD1     | 2:l:129:VAL:HG11   | 2.37                     | 0.59              |
| 2:t:364:ILE:HD13   | 2:v:142:LEU:HB2    | 1.82                     | 0.59              |
| 4:ZF:104:GLU:CD    | 4:ZK:341:GLY:HA2   | 2.27                     | 0.59              |
| 4:ZH:206:ASN:ND2   | 4:ZN:253:GLY:HA3   | 2.16                     | 0.59              |
| 4:ZS:289:LEU:HA    | 4:ZS:304:TYR:HA    | 1.83                     | 0.59              |
| 4:Za:24:ILE:O      | 4:Za:27:SER:OG     | 2.20                     | 0.59              |
| 4:Zc:382:TYR:CG    | 4:Zh:395:ILE:HD11  | 2.37                     | 0.59              |
| 5:AE:107:VAL:O     | 3:AJ:180:ASN:ND2   | 2.34                     | 0.59              |
| 3:AH:90:ASN:O      | 3:AH:91:ASN:C      | 2.45                     | 0.59              |
| 6:AW:402:LEU:HD12  | 6:AW:403:PRO:HD2   | 1.84                     | 0.59              |
| 7:As:89:GLY:C      | 9:Ay:143:ARG:HE    | 2.10                     | 0.59              |
| 11:A8:114:LEU:HD21 | 12:BD:126:MET:CE   | 2.32                     | 0.59              |
| 6:UL:73:MET:HE3    | 6:UL:99:ARG:HD3    | 1.81                     | 0.59              |
| 12:BA:112:TYR:CD1  | 12:BF:125:MET:HG3  | 2.37                     | 0.59              |
| 6:WI:212:LEU:HB3   | 6:WI:221:THR:HG23  | 1.84                     | 0.59              |
| 6:WP:128:GLU:HG2   | 6:WQ:126:PHE:CD2   | 2.37                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WS:193:ALA:HB1  | 6:WT:213:VAL:HG11  | 1.84                     | 0.59              |
| 1:N:144:PHE:CD2   | 1:O:171:ILE:HD11   | 2.38                     | 0.59              |
| 1:P:181:SER:HB2   | 1:Q:31:VAL:HG13    | 1.82                     | 0.59              |
| 1:Q:181:SER:HB2   | 1:R:31:VAL:HG13    | 1.82                     | 0.59              |
| 2:h:21:ARG:HH21   | 2:h:246:VAL:HG21   | 1.65                     | 0.59              |
| 2:l:91:ALA:HB2    | 2:l:105:VAL:HG12   | 1.83                     | 0.59              |
| 2:r:364:ILE:HD13  | 2:t:142:LEU:HB2    | 1.82                     | 0.59              |
| 3:1:6:TRP:CD1     | 5:AE:70:GLN:HB2    | 2.37                     | 0.59              |
| 3:2:40:VAL:O      | 3:2:75:VAL:N       | 2.33                     | 0.59              |
| 3:5:208:LEU:O     | 3:5:210:GLY:N      | 2.34                     | 0.59              |
| 3:9:73:ARG:CD     | 3:AM:218:TYR:CE2   | 2.85                     | 0.59              |
| 3:ZB:40:VAL:HG23  | 3:ZB:75:VAL:HB     | 1.84                     | 0.59              |
| 3:ZC:122:VAL:O    | 4:ZH:322:ASN:CG    | 2.44                     | 0.59              |
| 4:ZM:156:ILE:HB   | 4:ZM:276:ILE:HG23  | 1.84                     | 0.59              |
| 4:ZR:157:ASN:ND2  | 4:ZX:143:LEU:HD13  | 2.17                     | 0.59              |
| 4:ZV:178:TYR:HA   | 4:ZV:201:VAL:HG22  | 1.83                     | 0.59              |
| 4:Zg:385:ASN:O    | 4:Zg:388:THR:N     | 2.33                     | 0.59              |
| 5:AA:237:VAL:HG22 | 12:BB:21:LEU:HD21  | 1.84                     | 0.59              |
| 6:AY:295:SER:HB2  | 11:A9:65:LEU:HB2   | 1.84                     | 0.59              |
| 6:Af:402:LEU:HD12 | 6:Af:403:PRO:HD2   | 1.84                     | 0.59              |
| 6:Am:402:LEU:HD12 | 6:Am:403:PRO:HD2   | 1.84                     | 0.59              |
| 6:Ao:277:GLN:HB3  | 6:Ao:377:MET:HE1   | 1.83                     | 0.59              |
| 7:As:7:MET:HE2    | 8:At:233:MET:O     | 2.02                     | 0.59              |
| 9:Au:66:ARG:NH2   | 9:Au:243:PHE:O     | 2.36                     | 0.59              |
| 9:Av:48:ILE:HD12  | 11:A7:134:LEU:HD23 | 1.85                     | 0.59              |
| 10:A4:14:LEU:CD1  | 6:BX:370:ARG:HH21  | 2.10                     | 0.59              |
| 10:A4:75:MET:HE1  | 11:A9:122:VAL:HG22 | 1.84                     | 0.59              |
| 6:UJ:73:MET:HE3   | 6:UJ:99:ARG:HD3    | 1.81                     | 0.59              |
| 1:J:144:PHE:CD2   | 1:K:171:ILE:HD11   | 2.38                     | 0.59              |
| 1:Y:144:PHE:CD2   | 1:Z:171:ILE:HD11   | 2.38                     | 0.59              |
| 2:d:91:ALA:HB2    | 2:d:105:VAL:HG12   | 1.83                     | 0.59              |
| 2:i:21:ARG:HH21   | 2:i:246:VAL:HG21   | 1.65                     | 0.59              |
| 2:o:91:ALA:HB2    | 2:o:105:VAL:HG12   | 1.83                     | 0.59              |
| 2:p:91:ALA:HB2    | 2:p:105:VAL:HG12   | 1.83                     | 0.59              |
| 2:s:364:ILE:HD13  | 2:u:142:LEU:HB2    | 1.82                     | 0.59              |
| 3:4:238:ARG:NE    | 3:ZA:251:ASP:OD2   | 2.33                     | 0.59              |
| 3:ZC:10:THR:HG21  | 3:ZC:71:GLY:HA3    | 1.83                     | 0.59              |
| 3:ZD:24:ASN:ND2   | 4:ZI:49:GLY:CA     | 2.65                     | 0.59              |
| 4:ZT:42:MET:HE3   | 4:ZT:53:LYS:HB3    | 1.84                     | 0.59              |
| 4:Zc:71:ARG:NH1   | 4:Zc:74:ASP:OD1    | 2.35                     | 0.59              |
| 4:Ze:233:ASN:HD21 | 4:Ze:237:ILE:HB    | 1.67                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AD:174:SER:OG    | 5:AD:176:ASP:OD2   | 2.16                     | 0.59              |
| 5:AD:244:ALA:HB2   | 12:BE:116:ILE:HD11 | 1.84                     | 0.59              |
| 5:AE:51:LEU:HD11   | 12:BF:19:LYS:HD3   | 1.84                     | 0.59              |
| 3:AH:241:GLU:OE1   | 3:AN:258:THR:OG1   | 2.19                     | 0.59              |
| 6:AT:277:GLN:HB3   | 6:AT:377:MET:HE1   | 1.83                     | 0.59              |
| 6:AU:402:LEU:HD12  | 6:AU:403:PRO:HD2   | 1.84                     | 0.59              |
| 6:AW:299:ASN:HD21  | 11:A9:55:ARG:CZ    | 2.14                     | 0.59              |
| 6:Ae:402:LEU:HD12  | 6:Ae:403:PRO:HD2   | 1.84                     | 0.59              |
| 6:Aj:402:LEU:HD12  | 6:Aj:403:PRO:HD2   | 1.84                     | 0.59              |
| 6:Ak:372:ILE:HG22  | 10:A1:4:ILE:CG1    | 2.25                     | 0.59              |
| 9:Ay:116:PHE:CZ    | 11:A0:4:ARG:NH1    | 2.68                     | 0.59              |
| 11:A9:123:LEU:HD23 | 12:BD:132:LEU:HD11 | 1.84                     | 0.59              |
| 6:WA:175:SER:CB    | 6:WW:197:LEU:HA    | 2.31                     | 0.59              |
| 6:WB:197:LEU:CD1   | 6:WC:175:SER:OG    | 2.48                     | 0.59              |
| 6:BV:402:LEU:HD12  | 6:BV:403:PRO:HD2   | 1.84                     | 0.59              |
| 1:C:144:PHE:CD2    | 1:D:171:ILE:HD11   | 2.38                     | 0.59              |
| 1:O:144:PHE:CD2    | 1:P:171:ILE:HD11   | 2.38                     | 0.59              |
| 1:S:144:PHE:CD2    | 1:T:171:ILE:HD11   | 2.38                     | 0.59              |
| 1:X:144:PHE:CD2    | 1:Y:171:ILE:HD11   | 2.38                     | 0.59              |
| 1:X:201:ALA:HA     | 1:Y:149:THR:HG22   | 1.84                     | 0.59              |
| 2:g:21:ARG:HH21    | 2:g:246:VAL:HG21   | 1.65                     | 0.59              |
| 2:l:21:ARG:HH21    | 2:l:246:VAL:HG21   | 1.65                     | 0.59              |
| 2:n:91:ALA:HB2     | 2:n:105:VAL:HG12   | 1.83                     | 0.59              |
| 2:q:364:ILE:HD13   | 2:s:142:LEU:HB2    | 1.82                     | 0.59              |
| 3:O:257:LEU:HD22   | 5:AD:214:VAL:HG22  | 1.85                     | 0.59              |
| 3:1:52:PRO:CG      | 12:BF:80:PRO:HB3   | 2.32                     | 0.59              |
| 3:ZE:31:THR:HG22   | 4:ZJ:39:PHE:HB3    | 1.83                     | 0.59              |
| 4:ZO:268:GLN:HE22  | 4:ZU:190:GLN:HE22  | 1.49                     | 0.59              |
| 5:AB:234:ILE:CG2   | 12:BB:106:MET:HE1  | 2.31                     | 0.59              |
| 5:AE:76:ARG:NH2    | 5:AE:105:ILE:O     | 2.35                     | 0.59              |
| 3:AH:50:ARG:HD3    | 6:BL:322:PRO:HD3   | 1.84                     | 0.59              |
| 6:AY:402:LEU:HD12  | 6:AY:403:PRO:HD2   | 1.84                     | 0.59              |
| 7:Ab:8:MET:CE      | 6:WS:124:SER:CA    | 2.78                     | 0.59              |
| 7:Ab:8:MET:CE      | 6:WS:124:SER:N     | 2.65                     | 0.59              |
| 7:Ab:74:LEU:HD13   | 7:Ab:78:ARG:NH2    | 2.13                     | 0.59              |
| 6:Ag:402:LEU:HD12  | 6:Ag:403:PRO:HD2   | 1.84                     | 0.59              |
| 6:Al:294:ARG:HG2   | 11:A7:66:THR:OG1   | 2.03                     | 0.59              |
| 7:As:51:PHE:HB3    | 9:Ax:205:MET:HE3   | 1.84                     | 0.59              |
| 8:At:114:VAL:CG2   | 9:Ax:211:MET:HE1   | 2.29                     | 0.59              |
| 6:UJ:126:PHE:CE1   | 6:UJ:130:VAL:CG2   | 2.84                     | 0.59              |
| 6:UM:103:GLN:NE2   | 6:WQ:182:PRO:HB3   | 2.17                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UN:126:PHE:CE1  | 6:UN:130:VAL:CG2  | 2.84                     | 0.59              |
| 12:BA:20:ARG:HD3  | 12:BA:108:ALA:HB2 | 1.84                     | 0.59              |
| 6:WL:197:LEU:CD1  | 6:WM:175:SER:CB   | 2.72                     | 0.59              |
| 6:BT:277:GLN:HB3  | 6:BT:377:MET:HE1  | 1.83                     | 0.59              |
| 6:BX:277:GLN:HB3  | 6:BX:377:MET:HE1  | 1.83                     | 0.59              |
| 1:F:144:PHE:CD2   | 1:G:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:G:144:PHE:CD2   | 1:H:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:T:144:PHE:CD2   | 1:U:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:X:62:TYR:CD1    | 2:v:129:VAL:HG11  | 2.37                     | 0.59              |
| 1:Y:201:ALA:HA    | 1:Z:149:THR:HG22  | 1.85                     | 0.59              |
| 2:f:21:ARG:HH21   | 2:f:246:VAL:HG21  | 1.65                     | 0.59              |
| 2:f:54:GLN:HG2    | 3:AF:168:VAL:CG1  | 2.29                     | 0.59              |
| 2:m:91:ALA:HB2    | 2:m:105:VAL:HG12  | 1.83                     | 0.59              |
| 3:5:35:LYS:NZ     | 3:5:220:GLU:OE2   | 2.35                     | 0.59              |
| 4:ZF:346:GLY:HA3  | 4:ZF:353:PHE:CE2  | 2.37                     | 0.59              |
| 4:ZJ:382:TYR:CZ   | 4:ZO:395:ILE:HG23 | 2.38                     | 0.59              |
| 5:AC:104:ASN:HD21 | 3:AH:38:ARG:HH21  | 1.49                     | 0.59              |
| 5:AD:75:SER:O     | 5:AD:76:ARG:C     | 2.46                     | 0.59              |
| 3:AF:47:GLN:HE22  | 12:BA:73:PRO:HB2  | 1.65                     | 0.59              |
| 3:AJ:62:LEU:HD23  | 12:BF:83:PRO:CG   | 2.32                     | 0.59              |
| 6:AZ:402:LEU:HD12 | 6:AZ:403:PRO:HD2  | 1.84                     | 0.59              |
| 6:Ap:277:GLN:HB3  | 6:Ap:377:MET:HE1  | 1.83                     | 0.59              |
| 7:As:78:ARG:HG3   | 9:Ay:234:LEU:HD11 | 1.83                     | 0.59              |
| 9:Av:180:LYS:NZ   | 9:Aw:230:ASP:OD1  | 2.27                     | 0.59              |
| 6:UJ:127:SER:O    | 6:UJ:131:ASN:CB   | 2.50                     | 0.59              |
| 6:UP:126:PHE:CE1  | 6:UP:130:VAL:CG2  | 2.84                     | 0.59              |
| 6:WI:200:SER:O    | 6:WJ:158:ALA:HB2  | 2.02                     | 0.59              |
| 6:WJ:128:GLU:OE2  | 6:WK:127:SER:OG   | 2.20                     | 0.59              |
| 6:WL:197:LEU:HD12 | 6:WM:175:SER:HB3  | 1.80                     | 0.59              |
| 6:BU:402:LEU:HD12 | 6:BU:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:M:144:PHE:CD2   | 1:N:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:R:144:PHE:CD2   | 1:S:171:ILE:HD11  | 2.38                     | 0.59              |
| 2:t:91:ALA:HB2    | 2:t:105:VAL:HG12  | 1.83                     | 0.59              |
| 3:5:16:GLN:NE2    | 3:ZA:2:ILE:HG13   | 2.17                     | 0.59              |
| 3:5:115:THR:HB    | 3:5:191:LEU:HD23  | 1.85                     | 0.59              |
| 3:9:73:ARG:CD     | 3:AM:218:TYR:HE2  | 2.15                     | 0.59              |
| 3:ZC:185:GLU:OE1  | 4:ZH:46:SER:HB2   | 2.03                     | 0.59              |
| 4:ZT:314:GLN:NE2  | 4:ZT:347:THR:OG1  | 2.35                     | 0.59              |
| 5:AB:202:MET:HE2  | 3:AM:73:ARG:NE    | 2.15                     | 0.59              |
| 5:AE:106:GLN:HE22 | 3:AJ:182:THR:HG21 | 1.68                     | 0.59              |
| 6:AX:402:LEU:HD12 | 6:AX:403:PRO:HD2  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:Az:73:ALA:HB1  | 10:Az:77:LYS:NZ   | 2.18                     | 0.59              |
| 6:WK:203:ALA:HB1  | 6:WL:160:PRO:HA   | 1.84                     | 0.59              |
| 6:WP:193:ALA:HB1  | 6:WQ:213:VAL:CG1  | 2.32                     | 0.59              |
| 6:BT:402:LEU:HD12 | 6:BT:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:B:144:PHE:CD2   | 1:C:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:C:201:ALA:HA    | 1:D:149:THR:HG22  | 1.85                     | 0.59              |
| 1:D:201:ALA:HA    | 1:E:149:THR:HG22  | 1.85                     | 0.59              |
| 1:Y:62:TYR:CD1    | 2:w:129:VAL:HG11  | 2.37                     | 0.59              |
| 2:b:43:VAL:HG12   | 2:b:84:VAL:HG22   | 1.85                     | 0.59              |
| 2:c:43:VAL:HG12   | 2:c:84:VAL:HG22   | 1.85                     | 0.59              |
| 3:1:178:PHE:HE1   | 3:1:201:PRO:HB3   | 1.67                     | 0.59              |
| 3:3:88:GLN:HB2    | 3:3:218:TYR:CE2   | 2.37                     | 0.59              |
| 3:6:194:GLU:O     | 3:AJ:165:ALA:HB1  | 2.02                     | 0.59              |
| 3:9:231:VAL:HG11  | 4:ZF:7:VAL:HG22   | 1.84                     | 0.59              |
| 3:ZA:76:ALA:CB    | 4:ZF:47:LYS:HD3   | 2.33                     | 0.59              |
| 4:ZL:144:MET:SD   | 4:ZL:310:GLN:NE2  | 2.75                     | 0.59              |
| 4:ZN:382:TYR:CE1  | 4:ZS:395:ILE:HG23 | 2.37                     | 0.59              |
| 4:ZW:178:TYR:HA   | 4:ZW:201:VAL:HG22 | 1.83                     | 0.59              |
| 4:ZX:269:GLN:OE1  | 4:Zd:286:PRO:CG   | 2.51                     | 0.59              |
| 4:Zc:150:THR:OG1  | 4:Zc:282:ASN:ND2  | 2.35                     | 0.59              |
| 5:AA:109:PRO:HG3  | 3:AF:197:SER:CA   | 2.33                     | 0.59              |
| 5:AE:146:LEU:O    | 5:AE:147:ASN:C    | 2.46                     | 0.59              |
| 6:AU:277:GLN:HB3  | 6:AU:377:MET:HE1  | 1.83                     | 0.59              |
| 6:AO:402:LEU:HD12 | 6:AO:403:PRO:HD2  | 1.84                     | 0.59              |
| 8:At:188:LEU:HG   | 8:At:189:PRO:HD3  | 1.84                     | 0.59              |
| 11:A0:32:ASN:ND2  | 12:BE:60:GLY:O    | 2.35                     | 0.59              |
| 12:BA:50:GLN:HG3  | 12:BA:65:ALA:HB2  | 1.85                     | 0.59              |
| 6:WA:213:VAL:CG1  | 6:WW:193:ALA:HB1  | 2.32                     | 0.59              |
| 6:WK:212:LEU:HB3  | 6:WK:221:THR:HG23 | 1.84                     | 0.59              |
| 6:WS:196:HIS:HB3  | 6:WT:211:THR:HG21 | 1.84                     | 0.59              |
| 1:A:171:ILE:HD11  | 1:Z:144:PHE:CD2   | 2.38                     | 0.59              |
| 1:W:144:PHE:CD2   | 1:X:171:ILE:HD11  | 2.38                     | 0.59              |
| 2:q:91:ALA:HB2    | 2:q:105:VAL:HG12  | 1.83                     | 0.59              |
| 2:v:35:SER:HB3    | 2:w:123:MET:CE    | 2.33                     | 0.59              |
| 2:x:208:ARG:O     | 2:x:212:SER:OG    | 2.16                     | 0.59              |
| 3:0:83:GLN:HG2    | 3:ZB:45:LEU:HD13  | 1.84                     | 0.59              |
| 3:1:99:GLY:O      | 3:1:116:ARG:NH2   | 2.29                     | 0.59              |
| 3:9:45:LEU:HD22   | 3:AM:98:LYS:HG3   | 1.85                     | 0.59              |
| 3:ZD:77:THR:H     | 4:ZI:47:LYS:HD3   | 1.67                     | 0.59              |
| 3:ZE:231:VAL:HG11 | 4:ZK:7:VAL:HG22   | 1.84                     | 0.59              |
| 3:AG:35:LYS:HD2   | 3:AG:81:HIS:HA    | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Ab:35:ILE:HD11  | 7:Ab:53:PRO:HB2   | 1.85                     | 0.59              |
| 6:Ag:252:ILE:HD11 | 6:Ag:419:ALA:HB2  | 1.85                     | 0.59              |
| 6:An:402:LEU:HD12 | 6:An:403:PRO:HD2  | 1.84                     | 0.59              |
| 9:Aw:83:ALA:HB3   | 9:Aw:84:PRO:HD3   | 1.84                     | 0.59              |
| 9:Ax:48:ILE:HD11  | 10:A4:89:ARG:HH12 | 1.68                     | 0.59              |
| 10:A2:61:LEU:HD22 | 11:A7:50:LYS:HE2  | 1.83                     | 0.59              |
| 11:A6:46:ALA:O    | 11:A6:50:LYS:HG3  | 2.02                     | 0.59              |
| 6:BS:402:LEU:HD12 | 6:BS:403:PRO:HD2  | 1.84                     | 0.59              |
| 1:D:144:PHE:CD2   | 1:E:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:I:62:TYR:CD1    | 2:g:129:VAL:HG11  | 2.37                     | 0.59              |
| 1:I:144:PHE:CD2   | 1:J:171:ILE:HD11  | 2.38                     | 0.59              |
| 2:a:43:VAL:HG12   | 2:a:84:VAL:HG22   | 1.85                     | 0.59              |
| 2:d:43:VAL:HG12   | 2:d:84:VAL:HG22   | 1.85                     | 0.59              |
| 2:o:43:VAL:HG12   | 2:o:84:VAL:HG22   | 1.85                     | 0.59              |
| 2:p:43:VAL:HG12   | 2:p:84:VAL:HG22   | 1.85                     | 0.59              |
| 3:4:40:VAL:O      | 3:4:75:VAL:N      | 2.30                     | 0.59              |
| 4:ZQ:6:ALA:HB1    | 4:ZQ:389:ILE:HG12 | 1.85                     | 0.59              |
| 4:ZT:18:ASP:HB3   | 4:ZY:5:GLN:NE2    | 2.17                     | 0.59              |
| 4:Za:2:SER:OG     | 4:Za:3:PHE:N      | 2.34                     | 0.59              |
| 4:Zh:217:ASP:HB3  | 4:Zh:220:ALA:HB2  | 1.85                     | 0.59              |
| 5:AD:214:VAL:HG11 | 3:AJ:12:LEU:CB    | 2.32                     | 0.59              |
| 6:AS:277:GLN:HB3  | 6:AS:377:MET:HE1  | 1.83                     | 0.59              |
| 6:Ah:252:ILE:HD11 | 6:Ah:419:ALA:HB2  | 1.85                     | 0.59              |
| 6:Ah:402:LEU:HD12 | 6:Ah:403:PRO:HD2  | 1.84                     | 0.59              |
| 6:Aj:278:THR:HG21 | 10:A1:7:ILE:CG2   | 2.33                     | 0.59              |
| 6:AO:277:GLN:HB3  | 6:AO:377:MET:HE1  | 1.83                     | 0.59              |
| 6:AP:402:LEU:HD12 | 6:AP:403:PRO:HD2  | 1.84                     | 0.59              |
| 9:Av:116:PHE:CD2  | 11:A7:4:ARG:NH2   | 2.71                     | 0.59              |
| 6:UM:126:PHE:CE1  | 6:UM:130:VAL:CG2  | 2.84                     | 0.59              |
| 6:WM:197:LEU:CD1  | 6:WN:175:SER:OG   | 2.48                     | 0.59              |
| 1:A:149:THR:HG22  | 1:Z:201:ALA:HA    | 1.85                     | 0.59              |
| 1:K:144:PHE:CD2   | 1:L:171:ILE:HD11  | 2.38                     | 0.59              |
| 1:U:144:PHE:CD2   | 1:V:171:ILE:HD11  | 2.38                     | 0.59              |
| 2:a:123:MET:CE    | 2:z:35:SER:HB3    | 2.33                     | 0.59              |
| 2:e:43:VAL:HG12   | 2:e:84:VAL:HG22   | 1.85                     | 0.59              |
| 2:q:43:VAL:HG12   | 2:q:84:VAL:HG22   | 1.85                     | 0.59              |
| 2:s:35:SER:HB3    | 2:t:123:MET:CE    | 2.33                     | 0.59              |
| 2:z:43:VAL:HG12   | 2:z:84:VAL:HG22   | 1.85                     | 0.59              |
| 3:3:248:SER:O     | 3:3:252:GLN:HG2   | 2.02                     | 0.59              |
| 4:ZS:33:LYS:O     | 4:ZS:59:GLN:NE2   | 2.36                     | 0.59              |
| 4:ZS:105:ASN:HB2  | 4:ZS:107:ASN:HD21 | 1.68                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZW:208:TRP:NE1  | 4:ZW:268:GLN:OE1  | 2.35                     | 0.59              |
| 4:ZY:111:MET:HE1  | 4:Zd:58:THR:OG1   | 2.03                     | 0.59              |
| 4:ZZ:205:ASP:OD1  | 4:Zf:252:ASN:HA   | 2.03                     | 0.59              |
| 5:AC:107:VAL:O    | 3:AH:180:ASN:ND2  | 2.36                     | 0.59              |
| 5:AD:49:LEU:HB3   | 11:A9:90:PRO:HG2  | 1.83                     | 0.59              |
| 3:AL:52:PRO:HD3   | 12:BB:80:PRO:CB   | 2.32                     | 0.59              |
| 3:AN:115:THR:HB   | 3:AN:191:LEU:HD23 | 1.85                     | 0.59              |
| 6:AR:377:MET:N    | 6:AR:377:MET:SD   | 2.76                     | 0.59              |
| 6:AZ:377:MET:N    | 6:AZ:377:MET:SD   | 2.76                     | 0.59              |
| 7:Ab:89:GLY:CA    | 6:WS:165:PHE:HE1  | 2.07                     | 0.59              |
| 6:Ap:377:MET:N    | 6:Ap:377:MET:SD   | 2.76                     | 0.59              |
| 6:Ap:402:LEU:HD12 | 6:Ap:403:PRO:HD2  | 1.84                     | 0.59              |
| 6:WK:197:LEU:CD1  | 6:WL:175:SER:OG   | 2.51                     | 0.59              |
| 6:WT:116:LEU:HD13 | 6:WT:135:ALA:HB2  | 1.85                     | 0.59              |
| 1:P:144:PHE:CD2   | 1:Q:171:ILE:HD11  | 2.38                     | 0.58              |
| 2:n:43:VAL:HG12   | 2:n:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:s:91:ALA:HB2    | 2:s:105:VAL:HG12  | 1.83                     | 0.58              |
| 2:z:53:THR:HG21   | 3:AM:110:GLY:HA3  | 1.84                     | 0.58              |
| 3:2:85:ASN:O      | 3:2:221:THR:OG1   | 2.21                     | 0.58              |
| 3:4:85:ASN:OD1    | 4:ZF:50:LEU:HD23  | 2.02                     | 0.58              |
| 4:ZX:178:TYR:HA   | 4:ZX:201:VAL:HG22 | 1.85                     | 0.58              |
| 5:AB:26:LEU:CD2   | 3:AG:242:ILE:CG2  | 2.76                     | 0.58              |
| 5:AB:48:GLY:HA2   | 6:BK:324:ASN:HB3  | 1.84                     | 0.58              |
| 3:AJ:129:VAL:HG12 | 3:AJ:135:GLN:HA   | 1.84                     | 0.58              |
| 6:AU:377:MET:N    | 6:AU:377:MET:SD   | 2.76                     | 0.58              |
| 6:Ad:377:MET:N    | 6:Ad:377:MET:SD   | 2.76                     | 0.58              |
| 6:Ad:402:LEU:HD12 | 6:Ad:403:PRO:HD2  | 1.84                     | 0.58              |
| 6:Ak:370:ARG:NE   | 10:A1:7:ILE:HD11  | 2.17                     | 0.58              |
| 6:An:252:ILE:HD11 | 6:An:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:AP:377:MET:SD   | 6:AP:377:MET:N    | 2.76                     | 0.58              |
| 10:A2:61:LEU:CD1  | 11:A7:50:LYS:NZ   | 2.66                     | 0.58              |
| 11:A6:127:LEU:O   | 11:A6:131:MET:HG2 | 2.03                     | 0.58              |
| 6:WK:186:LEU:HD22 | 6:WK:190:GLN:CD   | 2.28                     | 0.58              |
| 6:WP:212:LEU:HB3  | 6:WP:221:THR:HG23 | 1.85                     | 0.58              |
| 6:WU:212:LEU:HB3  | 6:WU:221:THR:HG23 | 1.84                     | 0.58              |
| 6:BR:402:LEU:HD12 | 6:BR:403:PRO:HD2  | 1.84                     | 0.58              |
| 6:BV:252:ILE:HD11 | 6:BV:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:E:201:ALA:HA    | 1:F:149:THR:HG22  | 1.85                     | 0.58              |
| 1:W:62:TYR:CD1    | 2:u:129:VAL:HG11  | 2.37                     | 0.58              |
| 1:W:201:ALA:HA    | 1:X:149:THR:HG22  | 1.85                     | 0.58              |
| 2:r:43:VAL:HG12   | 2:r:84:VAL:HG22   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:91:ALA:HB2    | 2:r:105:VAL:HG12  | 1.83                     | 0.58              |
| 3:3:238:ARG:NE    | 3:9:251:ASP:OD2   | 2.35                     | 0.58              |
| 3:ZA:28:ASN:OD1   | 4:ZF:52:VAL:HB    | 2.03                     | 0.58              |
| 3:ZD:237:GLN:O    | 3:ZD:241:GLU:HG2  | 2.02                     | 0.58              |
| 4:ZI:99:GLN:HG3   | 4:ZI:361:LEU:HD21 | 1.84                     | 0.58              |
| 4:ZI:195:ASP:OD2  | 4:ZI:216:SER:OG   | 2.22                     | 0.58              |
| 4:ZN:373:VAL:HG11 | 4:ZT:7:VAL:HG22   | 1.84                     | 0.58              |
| 4:ZT:248:THR:OG1  | 4:ZT:257:ALA:N    | 2.37                     | 0.58              |
| 5:AA:96:ALA:HB3   | 5:AA:180:ARG:HH21 | 1.68                     | 0.58              |
| 5:AC:21:VAL:HG23  | 3:AH:68:ILE:CG2   | 2.27                     | 0.58              |
| 5:AD:76:ARG:HG2   | 5:AD:78:LEU:HB2   | 1.86                     | 0.58              |
| 5:AD:227:PHE:CE2  | 3:AI:253:MET:O    | 2.57                     | 0.58              |
| 6:AR:252:ILE:HD11 | 6:AR:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:AS:252:ILE:HD11 | 6:AS:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Aa:402:LEU:HD12 | 6:Aa:403:PRO:HD2  | 1.84                     | 0.58              |
| 6:Ac:252:ILE:HD11 | 6:Ac:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Ac:305:GLY:HA3  | 6:Ac:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:An:377:MET:N    | 6:An:377:MET:SD   | 2.76                     | 0.58              |
| 7:Ar:52:ILE:O     | 7:Ar:56:VAL:HG22  | 2.02                     | 0.58              |
| 8:At:145:TRP:HD1  | 6:WJ:164:LEU:CD1  | 2.02                     | 0.58              |
| 9:Ax:162:PRO:HD3  | 6:WE:167:ARG:NH2  | 2.13                     | 0.58              |
| 6:WD:197:LEU:HD12 | 6:WE:175:SER:HB3  | 1.85                     | 0.58              |
| 6:WM:193:ALA:CB   | 6:WN:213:VAL:HG11 | 2.27                     | 0.58              |
| 6:BU:252:ILE:HD11 | 6:BU:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:A:144:PHE:CD2   | 1:B:171:ILE:HD11  | 2.38                     | 0.58              |
| 1:B:201:ALA:HA    | 1:C:149:THR:HG22  | 1.85                     | 0.58              |
| 2:m:43:VAL:HG12   | 2:m:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:w:35:SER:HB3    | 2:x:123:MET:CE    | 2.33                     | 0.58              |
| 2:y:43:VAL:HG12   | 2:y:84:VAL:HG22   | 1.85                     | 0.58              |
| 3:6:86:LEU:HD12   | 4:ZH:42:MET:HE1   | 1.74                     | 0.58              |
| 3:7:238:ARG:HG2   | 3:ZD:254:LEU:HD13 | 1.84                     | 0.58              |
| 3:9:238:ARG:NH2   | 4:ZF:397:ASN:HB2  | 2.19                     | 0.58              |
| 3:ZA:233:MET:SD   | 4:ZF:388:THR:CB   | 2.92                     | 0.58              |
| 3:ZB:231:VAL:HG11 | 4:ZH:7:VAL:HG22   | 1.84                     | 0.58              |
| 3:ZD:115:THR:HB   | 3:ZD:191:LEU:HD23 | 1.84                     | 0.58              |
| 3:ZE:218:TYR:OH   | 4:ZP:53:LYS:HD2   | 2.02                     | 0.58              |
| 4:ZG:331:ASP:HA   | 4:ZL:40:ALA:HB1   | 1.83                     | 0.58              |
| 4:ZQ:22:ASN:OD1   | 4:ZQ:26:ASN:ND2   | 2.35                     | 0.58              |
| 4:ZR:183:THR:HG21 | 4:Zc:132:ALA:HA   | 1.83                     | 0.58              |
| 4:ZX:146:ALA:HB2  | 4:ZX:286:PRO:HD3  | 1.85                     | 0.58              |
| 4:Ze:60:ASP:O     | 4:Ze:365:ASN:ND2  | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AA:9:MET:HG3     | 12:BA:103:VAL:HG21 | 1.84                     | 0.58              |
| 5:AA:70:GLN:HB2    | 3:AL:6:TRP:CD1     | 2.39                     | 0.58              |
| 5:AC:62:PRO:CB     | 3:AH:63:PRO:HG2    | 2.33                     | 0.58              |
| 5:AD:76:ARG:HB3    | 5:AD:79:ASP:OD2    | 2.03                     | 0.58              |
| 5:AE:55:THR:CG2    | 12:BF:30:ASN:HD21  | 2.15                     | 0.58              |
| 5:AE:61:THR:HG23   | 3:AJ:66:LEU:HD12   | 1.84                     | 0.58              |
| 3:AL:22:ILE:HG21   | 3:AL:233:MET:HG3   | 1.84                     | 0.58              |
| 6:AS:377:MET:SD    | 6:AS:377:MET:N     | 2.76                     | 0.58              |
| 6:AW:377:MET:N     | 6:AW:377:MET:SD    | 2.76                     | 0.58              |
| 6:AX:305:GLY:HA3   | 6:AX:355:PRO:HG2   | 1.86                     | 0.58              |
| 6:AX:377:MET:N     | 6:AX:377:MET:SD    | 2.76                     | 0.58              |
| 6:Ad:305:GLY:HA3   | 6:Ad:355:PRO:HG2   | 1.86                     | 0.58              |
| 6:Ai:252:ILE:HD11  | 6:Ai:419:ALA:HB2   | 1.85                     | 0.58              |
| 6:Am:252:ILE:HD11  | 6:Am:419:ALA:HB2   | 1.85                     | 0.58              |
| 11:A8:120:LEU:HD11 | 12:BC:129:THR:OG1  | 2.03                     | 0.58              |
| 6:BS:377:MET:N     | 6:BS:377:MET:SD    | 2.76                     | 0.58              |
| 1:J:201:ALA:HA     | 1:K:149:THR:CG2    | 2.34                     | 0.58              |
| 1:M:62:TYR:CD1     | 2:k:129:VAL:HG11   | 2.37                     | 0.58              |
| 1:M:201:ALA:HA     | 1:N:149:THR:CG2    | 2.34                     | 0.58              |
| 1:N:201:ALA:HA     | 1:O:149:THR:HG22   | 1.85                     | 0.58              |
| 1:Q:144:PHE:CD2    | 1:R:171:ILE:HD11   | 2.38                     | 0.58              |
| 1:S:201:ALA:HA     | 1:T:149:THR:HG22   | 1.84                     | 0.58              |
| 2:f:43:VAL:HG12    | 2:f:84:VAL:HG22    | 1.85                     | 0.58              |
| 2:y:35:SER:HB3     | 2:z:123:MET:CE     | 2.33                     | 0.58              |
| 3:2:208:LEU:O      | 3:AL:162:GLN:NE2   | 2.36                     | 0.58              |
| 3:3:56:SER:CA      | 5:AB:138:ALA:HB1   | 2.34                     | 0.58              |
| 3:4:64:SER:O       | 3:4:64:SER:OG      | 2.19                     | 0.58              |
| 3:ZE:85:ASN:OD1    | 4:ZP:50:LEU:HD21   | 2.04                     | 0.58              |
| 4:ZT:180:LYS:HD3   | 4:ZT:274:ASN:HB3   | 1.85                     | 0.58              |
| 4:ZZ:309:GLU:N     | 4:ZZ:309:GLU:OE2   | 2.34                     | 0.58              |
| 4:Zc:281:GLN:NE2   | 4:Zc:283:GLY:O     | 2.36                     | 0.58              |
| 5:AC:170:GLU:OE1   | 5:AC:189:ARG:NH1   | 2.36                     | 0.58              |
| 5:AD:234:ILE:HG22  | 3:AI:260:LEU:HD11  | 1.84                     | 0.58              |
| 3:AF:260:LEU:HD21  | 12:BA:106:MET:HE1  | 1.84                     | 0.58              |
| 3:AJ:62:LEU:CD2    | 12:BF:83:PRO:CD    | 2.77                     | 0.58              |
| 6:Af:377:MET:N     | 6:Af:377:MET:SD    | 2.76                     | 0.58              |
| 6:Ai:402:LEU:HD12  | 6:Ai:403:PRO:HD2   | 1.84                     | 0.58              |
| 9:Ay:148:ALA:CA    | 6:WI:164:LEU:HD22  | 2.33                     | 0.58              |
| 9:Ay:159:LEU:HB2   | 6:WI:165:PHE:HD2   | 1.69                     | 0.58              |
| 11:A6:67:LEU:HD11  | 11:A6:74:PRO:HA    | 1.85                     | 0.58              |
| 6:WJ:212:LEU:HB3   | 6:WJ:221:THR:HG23  | 1.84                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WT:212:LEU:HB3  | 6:WT:221:THR:HG23 | 1.84                     | 0.58              |
| 1:E:144:PHE:CD2   | 1:F:171:ILE:HD11  | 2.38                     | 0.58              |
| 1:L:201:ALA:HA    | 1:M:149:THR:HG22  | 1.84                     | 0.58              |
| 1:M:201:ALA:HA    | 1:N:149:THR:HG22  | 1.84                     | 0.58              |
| 1:T:201:ALA:HA    | 1:U:149:THR:HG22  | 1.85                     | 0.58              |
| 2:e:88:MET:HG2    | 2:e:110:MET:HG3   | 1.86                     | 0.58              |
| 2:l:35:SER:HB3    | 2:m:123:MET:CE    | 2.33                     | 0.58              |
| 2:m:88:MET:HG2    | 2:m:110:MET:HG3   | 1.86                     | 0.58              |
| 2:s:43:VAL:HG12   | 2:s:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:x:35:SER:HB3    | 2:y:123:MET:CE    | 2.33                     | 0.58              |
| 4:ZH:162:ASP:O    | 4:ZH:202:LYS:NZ   | 2.33                     | 0.58              |
| 4:ZK:75:VAL:HG21  | 4:ZK:356:LEU:HD23 | 1.85                     | 0.58              |
| 4:ZK:165:PRO:HG2  | 4:ZK:201:VAL:HG13 | 1.84                     | 0.58              |
| 4:ZL:270:ASN:HB2  | 4:ZR:190:GLN:O    | 2.02                     | 0.58              |
| 5:AE:245:ASN:HD22 | 12:BE:113:GLN:CD  | 2.07                     | 0.58              |
| 3:AH:50:ARG:CD    | 6:BM:328:ILE:HD13 | 2.33                     | 0.58              |
| 3:AI:6:TRP:O      | 3:AI:10:THR:HG23  | 2.04                     | 0.58              |
| 6:AS:305:GLY:HA3  | 6:AS:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:AV:377:MET:N    | 6:AV:377:MET:SD   | 2.76                     | 0.58              |
| 6:Ag:377:MET:N    | 6:Ag:377:MET:SD   | 2.76                     | 0.58              |
| 6:AQ:377:MET:N    | 6:AQ:377:MET:SD   | 2.76                     | 0.58              |
| 10:Az:69:ASN:HD21 | 11:A6:20:ALA:HB2  | 1.68                     | 0.58              |
| 6:UN:208:GLY:N    | 6:WR:187:ASP:OD1  | 2.35                     | 0.58              |
| 6:BX:252:ILE:HD11 | 6:BX:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:A:201:ALA:HA    | 1:B:149:THR:HG22  | 1.84                     | 0.58              |
| 1:E:219:MET:SD    | 1:F:212:TYR:CG    | 2.97                     | 0.58              |
| 1:G:201:ALA:HA    | 1:H:149:THR:CG2   | 2.34                     | 0.58              |
| 1:H:219:MET:SD    | 1:I:212:TYR:CG    | 2.97                     | 0.58              |
| 1:J:219:MET:SD    | 1:K:212:TYR:CG    | 2.97                     | 0.58              |
| 1:K:201:ALA:HA    | 1:L:149:THR:HG22  | 1.85                     | 0.58              |
| 1:L:144:PHE:CD2   | 1:M:171:ILE:HD11  | 2.38                     | 0.58              |
| 1:M:219:MET:SD    | 1:N:212:TYR:CG    | 2.97                     | 0.58              |
| 1:U:201:ALA:HA    | 1:V:149:THR:CG2   | 2.34                     | 0.58              |
| 2:a:35:SER:HB3    | 2:b:123:MET:CE    | 2.33                     | 0.58              |
| 2:d:88:MET:HG2    | 2:d:110:MET:HG3   | 1.86                     | 0.58              |
| 2:g:43:VAL:HG12   | 2:g:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:l:88:MET:HG2    | 2:l:110:MET:HG3   | 1.86                     | 0.58              |
| 2:n:88:MET:HG2    | 2:n:110:MET:HG3   | 1.86                     | 0.58              |
| 2:q:88:MET:HG2    | 2:q:110:MET:HG3   | 1.86                     | 0.58              |
| 2:z:88:MET:HG2    | 2:z:110:MET:HG3   | 1.86                     | 0.58              |
| 3:1:49:ILE:HB     | 3:1:66:LEU:HD23   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:1:72:VAL:HB     | 3:AK:28:ASN:ND2   | 2.18                     | 0.58              |
| 3:ZD:165:ALA:O    | 3:ZD:166:ALA:C    | 2.47                     | 0.58              |
| 4:ZU:97:ASN:HB2   | 4:ZU:332:ASN:HD22 | 1.69                     | 0.58              |
| 4:ZW:103:ASP:HA   | 4:Zb:322:ASN:HD22 | 1.68                     | 0.58              |
| 4:ZZ:71:ARG:HG2   | 4:ZZ:73:LEU:H     | 1.68                     | 0.58              |
| 4:Zb:107:ASN:ND2  | 4:Zb:138:THR:OG1  | 2.37                     | 0.58              |
| 4:Zf:101:LYS:HD3  | 4:Zf:102:LEU:H    | 1.67                     | 0.58              |
| 3:AF:93:LYS:HE3   | 3:AF:149:ILE:HG21 | 1.84                     | 0.58              |
| 3:AI:260:LEU:HD23 | 12:BD:106:MET:SD  | 2.43                     | 0.58              |
| 6:AY:305:GLY:HA3  | 6:AY:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:AY:377:MET:N    | 6:AY:377:MET:SD   | 2.76                     | 0.58              |
| 6:Aa:252:ILE:HD11 | 6:Aa:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Ae:377:MET:N    | 6:Ae:377:MET:SD   | 2.76                     | 0.58              |
| 6:Af:252:ILE:HD11 | 6:Af:419:ALA:HB2  | 1.85                     | 0.58              |
| 7:Aq:51:PHE:CZ    | 7:Aq:55:ILE:HD11  | 2.38                     | 0.58              |
| 11:A8:42:ASP:OD1  | 11:A8:88:ARG:NH2  | 2.36                     | 0.58              |
| 6:UO:126:PHE:CE1  | 6:UO:130:VAL:CG2  | 2.84                     | 0.58              |
| 6:WA:175:SER:OG   | 6:WW:197:LEU:CD1  | 2.51                     | 0.58              |
| 6:WD:168:GLU:OE1  | 6:WD:170:LYS:CE   | 2.51                     | 0.58              |
| 6:WS:145:GLU:C    | 6:WS:147:LEU:H    | 2.12                     | 0.58              |
| 6:WT:145:GLU:C    | 6:WT:147:LEU:H    | 2.12                     | 0.58              |
| 6:BR:252:ILE:HD11 | 6:BR:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:BT:252:ILE:HD11 | 6:BT:419:ALA:HB2  | 1.85                     | 0.58              |
| 1:C:219:MET:SD    | 1:D:212:TYR:CG    | 2.97                     | 0.58              |
| 1:N:201:ALA:HA    | 1:O:149:THR:CG2   | 2.34                     | 0.58              |
| 1:S:201:ALA:HA    | 1:T:149:THR:CG2   | 2.34                     | 0.58              |
| 1:T:201:ALA:HA    | 1:U:149:THR:CG2   | 2.34                     | 0.58              |
| 1:V:144:PHE:CD2   | 1:W:171:ILE:HD11  | 2.38                     | 0.58              |
| 2:a:88:MET:HG2    | 2:a:110:MET:HG3   | 1.86                     | 0.58              |
| 2:b:208:ARG:O     | 2:b:212:SER:OG    | 2.16                     | 0.58              |
| 2:i:88:MET:HG2    | 2:i:110:MET:HG3   | 1.86                     | 0.58              |
| 2:k:35:SER:HB3    | 2:l:123:MET:CE    | 2.33                     | 0.58              |
| 2:m:35:SER:HB3    | 2:n:123:MET:CE    | 2.33                     | 0.58              |
| 2:m:80:GLN:HE22   | 3:AJ:204:SER:CB   | 2.17                     | 0.58              |
| 2:r:35:SER:HB3    | 2:s:123:MET:CE    | 2.33                     | 0.58              |
| 3:3:49:ILE:HG21   | 3:3:66:LEU:HD23   | 1.86                     | 0.58              |
| 3:4:124:GLN:HB2   | 3:9:199:GLY:HA2   | 1.85                     | 0.58              |
| 3:6:35:LYS:HB2    | 3:6:79:ARG:HD2    | 1.85                     | 0.58              |
| 3:ZD:37:GLN:CD    | 4:ZI:43:PHE:HE2   | 2.12                     | 0.58              |
| 4:ZQ:22:ASN:N     | 4:ZV:5:GLN:HE21   | 2.01                     | 0.58              |
| 5:AA:149:GLY:HA3  | 3:AF:210:GLY:HA2  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:239:GLU:OE1  | 12:BC:113:GLN:NE2 | 2.36                     | 0.58              |
| 5:AC:24:SER:N     | 3:AH:7:ILE:HG21   | 2.19                     | 0.58              |
| 3:AN:49:ILE:HD12  | 3:AN:66:LEU:HD11  | 1.86                     | 0.58              |
| 7:Ab:48:THR:HG21  | 9:Au:208:GLY:CA   | 2.34                     | 0.58              |
| 6:Aj:372:ILE:HB   | 10:A1:11:ILE:CG2  | 2.33                     | 0.58              |
| 6:Al:252:ILE:HD11 | 6:Al:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Al:377:MET:SD   | 6:Al:377:MET:N    | 2.76                     | 0.58              |
| 6:Am:377:MET:N    | 6:Am:377:MET:SD   | 2.76                     | 0.58              |
| 6:Ao:252:ILE:HD11 | 6:Ao:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Ao:402:LEU:HD12 | 6:Ao:403:PRO:HD2  | 1.84                     | 0.58              |
| 8:At:167:ASN:HD21 | 8:At:174:ARG:HH12 | 1.52                     | 0.58              |
| 9:Ay:83:ALA:O     | 9:Ay:84:PRO:C     | 2.46                     | 0.58              |
| 12:BB:94:PRO:HB2  | 12:BB:96:VAL:HG23 | 1.86                     | 0.58              |
| 6:WA:212:LEU:HB3  | 6:WA:221:THR:HG23 | 1.84                     | 0.58              |
| 6:WO:200:SER:O    | 6:WP:158:ALA:HB2  | 2.04                     | 0.58              |
| 6:BR:377:MET:SD   | 6:BR:377:MET:N    | 2.76                     | 0.58              |
| 6:BS:252:ILE:HD11 | 6:BS:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:BW:252:ILE:HD11 | 6:BW:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:BX:305:GLY:HA3  | 6:BX:355:PRO:HG2  | 1.85                     | 0.58              |
| 1:H:144:PHE:CD2   | 1:I:171:ILE:HD11  | 2.38                     | 0.58              |
| 1:K:201:ALA:HA    | 1:L:149:THR:CG2   | 2.34                     | 0.58              |
| 1:K:219:MET:SD    | 1:L:212:TYR:CG    | 2.97                     | 0.58              |
| 1:P:201:ALA:HA    | 1:Q:149:THR:HG22  | 1.85                     | 0.58              |
| 1:U:201:ALA:HA    | 1:V:149:THR:HG22  | 1.85                     | 0.58              |
| 1:V:201:ALA:HA    | 1:W:149:THR:CG2   | 2.34                     | 0.58              |
| 1:X:201:ALA:HA    | 1:Y:149:THR:CG2   | 2.34                     | 0.58              |
| 2:h:88:MET:HG2    | 2:h:110:MET:HG3   | 1.86                     | 0.58              |
| 2:j:35:SER:HB3    | 2:k:123:MET:CE    | 2.33                     | 0.58              |
| 2:l:43:VAL:HG12   | 2:l:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:n:35:SER:HB3    | 2:o:123:MET:CE    | 2.33                     | 0.58              |
| 2:p:88:MET:HG2    | 2:p:110:MET:HG3   | 1.86                     | 0.58              |
| 2:t:43:VAL:HG12   | 2:t:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:x:43:VAL:HG12   | 2:x:84:VAL:HG22   | 1.85                     | 0.58              |
| 3:2:86:LEU:HD12   | 3:ZD:44:LEU:HD22  | 1.85                     | 0.58              |
| 3:2:98:LYS:HB3    | 3:2:213:LEU:H     | 1.68                     | 0.58              |
| 3:3:180:ASN:O     | 3:3:181:ASP:C     | 2.43                     | 0.58              |
| 3:ZA:76:ALA:HA    | 4:ZF:47:LYS:HD3   | 1.85                     | 0.58              |
| 4:ZS:228:THR:HB   | 4:ZS:244:VAL:HG11 | 1.86                     | 0.58              |
| 5:AB:131:GLU:C    | 3:AG:179:MET:SD   | 2.86                     | 0.58              |
| 5:AB:224:ALA:CA   | 3:AG:253:MET:CE   | 2.81                     | 0.58              |
| 5:AC:82:LEU:HD13  | 5:AC:201:ILE:HG22 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AH:205:THR:HG22 | 3:AH:208:LEU:HD21 | 1.86                     | 0.58              |
| 6:AR:305:GLY:HA3  | 6:AR:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:AR:402:LEU:HD12 | 6:AR:403:PRO:HD2  | 1.84                     | 0.58              |
| 6:AT:252:ILE:HD11 | 6:AT:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:AT:305:GLY:HA3  | 6:AT:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:AU:252:ILE:HD11 | 6:AU:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:AW:305:GLY:HA3  | 6:AW:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:Ah:377:MET:N    | 6:Ah:377:MET:SD   | 2.76                     | 0.58              |
| 6:Ak:377:MET:N    | 6:Ak:377:MET:SD   | 2.76                     | 0.58              |
| 6:An:276:GLU:OE2  | 10:Az:11:ILE:CD1  | 2.52                     | 0.58              |
| 6:AQ:402:LEU:HD12 | 6:AQ:403:PRO:HD2  | 1.84                     | 0.58              |
| 6:WE:128:GLU:HB3  | 6:WF:126:PHE:CD2  | 2.38                     | 0.58              |
| 6:BU:377:MET:N    | 6:BU:377:MET:SD   | 2.76                     | 0.58              |
| 1:D:201:ALA:HA    | 1:E:149:THR:CG2   | 2.34                     | 0.58              |
| 1:O:219:MET:SD    | 1:P:212:TYR:CG    | 2.97                     | 0.58              |
| 1:P:201:ALA:HA    | 1:Q:149:THR:CG2   | 2.34                     | 0.58              |
| 1:R:201:ALA:HA    | 1:S:149:THR:HG22  | 1.84                     | 0.58              |
| 1:U:219:MET:SD    | 1:V:212:TYR:CG    | 2.97                     | 0.58              |
| 1:W:201:ALA:HA    | 1:X:149:THR:CG2   | 2.34                     | 0.58              |
| 2:c:88:MET:HG2    | 2:c:110:MET:HG3   | 1.86                     | 0.58              |
| 2:g:88:MET:HG2    | 2:g:110:MET:HG3   | 1.86                     | 0.58              |
| 2:k:88:MET:HG2    | 2:k:110:MET:HG3   | 1.86                     | 0.58              |
| 2:o:35:SER:HB3    | 2:p:123:MET:CE    | 2.33                     | 0.58              |
| 2:o:88:MET:HG2    | 2:o:110:MET:HG3   | 1.86                     | 0.58              |
| 2:t:35:SER:HB3    | 2:u:123:MET:CE    | 2.33                     | 0.58              |
| 2:y:88:MET:HG2    | 2:y:110:MET:HG3   | 1.86                     | 0.58              |
| 3:1:52:PRO:HG2    | 12:BF:89:GLY:HA3  | 1.85                     | 0.58              |
| 3:5:240:TYR:CE1   | 3:ZA:257:LEU:HB2  | 2.39                     | 0.58              |
| 3:6:180:ASN:OD1   | 3:6:183:GLY:N     | 2.35                     | 0.58              |
| 3:ZB:147:LEU:CD2  | 4:ZG:352:ASN:OD1  | 2.51                     | 0.58              |
| 4:ZG:263:PHE:O    | 4:ZG:266:SER:OG   | 2.18                     | 0.58              |
| 4:ZL:18:ASP:HB3   | 4:ZQ:5:GLN:HE22   | 1.69                     | 0.58              |
| 4:ZL:375:MET:HE1  | 4:ZQ:388:THR:OG1  | 2.03                     | 0.58              |
| 4:ZV:380:ARG:CZ   | 4:Zb:393:ASP:OD2  | 2.52                     | 0.58              |
| 4:ZW:285:LYS:O    | 4:ZW:306:ASN:ND2  | 2.29                     | 0.58              |
| 4:ZW:331:ASP:CA   | 4:Zb:40:ALA:HB1   | 2.24                     | 0.58              |
| 4:ZZ:69:THR:OG1   | 4:ZZ:74:ASP:OD2   | 2.21                     | 0.58              |
| 5:AA:220:MET:CE   | 3:AF:246:ALA:HA   | 2.28                     | 0.58              |
| 3:AG:73:ARG:HD3   | 12:BB:78:TYR:CD2  | 2.25                     | 0.58              |
| 3:AH:153:ARG:NH2  | 3:AN:108:PRO:HG2  | 2.18                     | 0.58              |
| 6:AT:377:MET:N    | 6:AT:377:MET:SD   | 2.76                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:Ah:305:GLY:HA3   | 6:Ah:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:Ai:305:GLY:HA3   | 6:Ai:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:Aj:252:ILE:HD11  | 6:Aj:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:AO:377:MET:N     | 6:AO:377:MET:SD   | 2.76                     | 0.58              |
| 9:Aw:162:PRO:HD3   | 6:WA:167:ARG:NH2  | 2.13                     | 0.58              |
| 9:Ay:116:PHE:CE1   | 11:A0:4:ARG:NH1   | 2.68                     | 0.58              |
| 11:A7:114:LEU:HD21 | 12:BC:126:MET:SD  | 2.43                     | 0.58              |
| 1:A:62:TYR:HD1     | 2:y:129:VAL:HG11  | 1.62                     | 0.58              |
| 1:F:201:ALA:HA     | 1:G:149:THR:HG22  | 1.85                     | 0.58              |
| 1:F:219:MET:SD     | 1:G:212:TYR:CG    | 2.97                     | 0.58              |
| 1:G:219:MET:SD     | 1:H:212:TYR:CG    | 2.97                     | 0.58              |
| 1:O:201:ALA:HA     | 1:P:149:THR:HG22  | 1.85                     | 0.58              |
| 1:R:201:ALA:HA     | 1:S:149:THR:CG2   | 2.34                     | 0.58              |
| 1:Y:201:ALA:HA     | 1:Z:149:THR:CG2   | 2.34                     | 0.58              |
| 2:b:88:MET:HG2     | 2:b:110:MET:HG3   | 1.86                     | 0.58              |
| 2:f:88:MET:HG2     | 2:f:110:MET:HG3   | 1.86                     | 0.58              |
| 2:h:43:VAL:HG12    | 2:h:84:VAL:HG22   | 1.85                     | 0.58              |
| 2:v:88:MET:HG2     | 2:v:110:MET:HG3   | 1.86                     | 0.58              |
| 3:8:98:LYS:NZ      | 3:ZE:187:ILE:O    | 2.36                     | 0.58              |
| 3:ZB:19:MET:HE1    | 3:ZB:233:MET:HG3  | 1.86                     | 0.58              |
| 4:ZI:212:THR:HG21  | 4:ZI:246:ILE:HD13 | 1.86                     | 0.58              |
| 4:ZK:150:THR:OG1   | 4:ZK:282:ASN:ND2  | 2.36                     | 0.58              |
| 4:ZO:211:TYR:CE2   | 4:ZO:226:ALA:HA   | 2.38                     | 0.58              |
| 5:AB:231:MET:SD    | 3:AG:260:LEU:CD1  | 2.92                     | 0.58              |
| 5:AD:26:LEU:HD21   | 5:AD:216:ALA:HB1  | 1.86                     | 0.58              |
| 3:AL:89:THR:C      | 3:AL:91:ASN:N     | 2.62                     | 0.58              |
| 6:AV:252:ILE:HD11  | 6:AV:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Ac:402:LEU:HD12  | 6:Ac:403:PRO:HD2  | 1.84                     | 0.58              |
| 6:Ad:252:ILE:HD11  | 6:Ad:419:ALA:HB2  | 1.85                     | 0.58              |
| 6:Ag:305:GLY:HA3   | 6:Ag:355:PRO:HG2  | 1.86                     | 0.58              |
| 6:WC:212:LEU:HB3   | 6:WC:221:THR:HG23 | 1.84                     | 0.58              |
| 6:WS:190:GLN:NE2   | 6:WT:216:SER:O    | 2.36                     | 0.58              |
| 6:WV:212:LEU:HB3   | 6:WV:221:THR:HG23 | 1.84                     | 0.58              |
| 12:BD:47:VAL:O     | 6:BN:313:PRO:CD   | 2.51                     | 0.58              |
| 6:BW:377:MET:N     | 6:BW:377:MET:SD   | 2.77                     | 0.58              |
| 1:L:219:MET:SD     | 1:M:212:TYR:CG    | 2.97                     | 0.57              |
| 1:Q:201:ALA:HA     | 1:R:149:THR:HG22  | 1.85                     | 0.57              |
| 1:Q:201:ALA:HA     | 1:R:149:THR:CG2   | 2.34                     | 0.57              |
| 1:V:62:TYR:CD1     | 2:t:129:VAL:HG11  | 2.37                     | 0.57              |
| 2:d:208:ARG:O      | 2:d:212:SER:OG    | 2.16                     | 0.57              |
| 2:j:88:MET:HG2     | 2:j:110:MET:HG3   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:88:MET:HG2    | 2:r:110:MET:HG3   | 1.86                     | 0.57              |
| 2:s:208:ARG:O     | 2:s:212:SER:OG    | 2.16                     | 0.57              |
| 3:8:24:ASN:ND2    | 3:ZD:70:THR:O     | 2.36                     | 0.57              |
| 3:ZB:7:ILE:HG23   | 3:ZB:71:GLY:HA2   | 1.86                     | 0.57              |
| 4:ZL:269:GLN:NE2  | 4:ZR:190:GLN:HA   | 2.18                     | 0.57              |
| 4:ZP:178:TYR:HA   | 4:ZP:201:VAL:HG12 | 1.85                     | 0.57              |
| 4:ZV:369:SER:HA   | 4:Zg:399:LEU:HD13 | 1.86                     | 0.57              |
| 4:Zb:80:ASN:OD1   | 4:Zb:81:GLY:N     | 2.37                     | 0.57              |
| 4:Ze:34:SER:HB3   | 4:Ze:366:VAL:HG12 | 1.85                     | 0.57              |
| 5:AD:131:GLU:HB2  | 3:AI:179:MET:HG2  | 1.86                     | 0.57              |
| 6:Ae:252:ILE:HD11 | 6:Ae:419:ALA:HB2  | 1.85                     | 0.57              |
| 9:Ax:40:LEU:HD22  | 11:A9:8:ALA:CB    | 2.34                     | 0.57              |
| 6:UJ:167:ARG:CZ   | 6:WB:188:GLU:OE2  | 2.52                     | 0.57              |
| 6:WB:186:LEU:HA   | 6:WB:190:GLN:OE1  | 2.04                     | 0.57              |
| 1:A:149:THR:CG2   | 1:Z:201:ALA:HA    | 2.34                     | 0.57              |
| 1:A:201:ALA:HA    | 1:B:149:THR:CG2   | 2.34                     | 0.57              |
| 1:A:219:MET:SD    | 1:B:212:TYR:CG    | 2.97                     | 0.57              |
| 1:C:62:TYR:CD1    | 2:a:129:VAL:HG11  | 2.37                     | 0.57              |
| 1:H:201:ALA:HA    | 1:I:149:THR:CG2   | 2.34                     | 0.57              |
| 1:I:201:ALA:HA    | 1:J:149:THR:HG22  | 1.84                     | 0.57              |
| 1:I:201:ALA:HA    | 1:J:149:THR:CG2   | 2.34                     | 0.57              |
| 1:J:201:ALA:HA    | 1:K:149:THR:HG22  | 1.85                     | 0.57              |
| 1:Q:62:TYR:CD1    | 2:o:129:VAL:HG11  | 2.37                     | 0.57              |
| 2:k:43:VAL:HG12   | 2:k:84:VAL:HG22   | 1.85                     | 0.57              |
| 2:p:35:SER:HB3    | 2:q:123:MET:CE    | 2.33                     | 0.57              |
| 2:p:208:ARG:O     | 2:p:212:SER:OG    | 2.16                     | 0.57              |
| 2:q:35:SER:HB3    | 2:r:123:MET:CE    | 2.33                     | 0.57              |
| 2:u:43:VAL:HG12   | 2:u:84:VAL:HG22   | 1.85                     | 0.57              |
| 2:u:88:MET:HG2    | 2:u:110:MET:HG3   | 1.86                     | 0.57              |
| 2:w:54:GLN:OE1    | 3:AH:141:THR:HG21 | 2.03                     | 0.57              |
| 2:w:88:MET:HG2    | 2:w:110:MET:HG3   | 1.86                     | 0.57              |
| 3:0:242:ILE:HG22  | 3:AJ:26:LEU:HD13  | 1.86                     | 0.57              |
| 3:1:38:ARG:HH22   | 3:AK:119:SER:HB2  | 1.69                     | 0.57              |
| 3:ZC:208:LEU:O    | 3:ZC:210:GLY:N    | 2.37                     | 0.57              |
| 3:ZD:37:GLN:CD    | 4:ZI:43:PHE:CE2   | 2.82                     | 0.57              |
| 4:ZL:27:SER:HB3   | 4:ZQ:381:ASN:OD1  | 2.05                     | 0.57              |
| 4:ZU:24:ILE:HD13  | 4:ZZ:384:SER:OG   | 2.04                     | 0.57              |
| 4:ZU:157:ASN:ND2  | 4:Za:143:LEU:HD22 | 2.19                     | 0.57              |
| 4:ZW:181:LYS:HZ2  | 4:Zh:129:GLN:HE21 | 1.52                     | 0.57              |
| 4:ZW:369:SER:HB3  | 4:Zc:382:TYR:OH   | 2.03                     | 0.57              |
| 4:ZX:50:LEU:H     | 4:ZX:50:LEU:HD22  | 1.68                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zd:144:MET:HE3  | 4:Zd:145:ALA:N    | 2.18                     | 0.57              |
| 4:Zd:208:TRP:NE1  | 4:Zd:268:GLN:OE1  | 2.37                     | 0.57              |
| 5:AC:91:GLN:HB2   | 5:AC:121:ILE:HD11 | 1.85                     | 0.57              |
| 5:AD:243:ARG:NH2  | 12:BE:113:GLN:HB2 | 2.18                     | 0.57              |
| 6:Aa:377:MET:SD   | 6:Aa:377:MET:N    | 2.76                     | 0.57              |
| 6:Ae:305:GLY:HA3  | 6:Ae:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:WI:170:LYS:O    | 6:WI:171:SER:OG   | 2.21                     | 0.57              |
| 6:WV:134:ARG:HB3  | 6:WV:134:ARG:HH21 | 1.69                     | 0.57              |
| 1:B:219:MET:SD    | 1:C:212:TYR:CG    | 2.97                     | 0.57              |
| 1:D:62:TYR:CD1    | 2:b:129:VAL:HG11  | 2.37                     | 0.57              |
| 1:F:201:ALA:HA    | 1:G:149:THR:CG2   | 2.34                     | 0.57              |
| 1:V:201:ALA:HA    | 1:W:149:THR:HG22  | 1.85                     | 0.57              |
| 1:X:219:MET:SD    | 1:Y:212:TYR:CG    | 2.97                     | 0.57              |
| 2:g:35:SER:HB3    | 2:h:123:MET:CE    | 2.33                     | 0.57              |
| 2:i:35:SER:HB3    | 2:j:123:MET:CE    | 2.33                     | 0.57              |
| 2:t:88:MET:HG2    | 2:t:110:MET:HG3   | 1.86                     | 0.57              |
| 2:w:54:GLN:OE1    | 3:AH:141:THR:HB   | 2.03                     | 0.57              |
| 3:9:83:GLN:NE2    | 3:9:97:ILE:O      | 2.37                     | 0.57              |
| 3:ZD:46:TYR:HA    | 3:ZD:69:GLY:HA2   | 1.85                     | 0.57              |
| 4:ZQ:196:MET:HA   | 4:ZQ:196:MET:HE3  | 1.86                     | 0.57              |
| 4:ZR:379:GLN:HG3  | 4:ZW:391:THR:HG23 | 1.86                     | 0.57              |
| 4:ZU:112:GLN:OE1  | 4:ZU:112:GLN:N    | 2.36                     | 0.57              |
| 4:Zc:217:ASP:HB3  | 4:Zc:220:ALA:HB2  | 1.86                     | 0.57              |
| 4:Zf:69:THR:OG1   | 4:Zf:74:ASP:OD2   | 2.20                     | 0.57              |
| 5:AE:215:GLU:CG   | 3:AK:9:LYS:HE3    | 2.30                     | 0.57              |
| 6:AU:305:GLY:HA3  | 6:AU:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:AZ:305:GLY:HA3  | 6:AZ:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:Ao:377:MET:SD   | 6:Ao:377:MET:N    | 2.76                     | 0.57              |
| 7:As:52:ILE:HD13  | 9:Ax:206:ALA:CB   | 2.32                     | 0.57              |
| 10:A4:11:ILE:HG22 | 6:BX:372:ILE:CB   | 2.34                     | 0.57              |
| 11:A8:67:LEU:HA   | 11:A8:72:HIS:NE2  | 2.18                     | 0.57              |
| 6:UM:73:MET:HE3   | 6:UM:99:ARG:HD3   | 1.81                     | 0.57              |
| 6:WA:213:VAL:HG21 | 6:WW:193:ALA:HB1  | 1.86                     | 0.57              |
| 6:WG:166:VAL:HG12 | 6:WG:168:GLU:HB3  | 1.87                     | 0.57              |
| 6:WK:196:HIS:HB3  | 6:WL:211:THR:CG2  | 2.22                     | 0.57              |
| 6:WN:203:ALA:HB2  | 6:WO:160:PRO:HA   | 1.86                     | 0.57              |
| 6:BX:377:MET:N    | 6:BX:377:MET:SD   | 2.76                     | 0.57              |
| 1:L:201:ALA:HA    | 1:M:149:THR:CG2   | 2.34                     | 0.57              |
| 1:Q:219:MET:SD    | 1:R:212:TYR:CG    | 2.97                     | 0.57              |
| 1:S:62:TYR:CD1    | 2:q:129:VAL:HG11  | 2.37                     | 0.57              |
| 2:e:35:SER:HB3    | 2:f:123:MET:CE    | 2.33                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:x:88:MET:HG2    | 2:x:110:MET:HG3   | 1.86                     | 0.57              |
| 3:2:154:ASP:OD2   | 3:2:154:ASP:N     | 2.36                     | 0.57              |
| 4:ZL:167:LYS:HA   | 4:ZL:167:LYS:HE3  | 1.86                     | 0.57              |
| 4:ZO:161:THR:HA   | 4:ZU:252:ASN:ND2  | 2.19                     | 0.57              |
| 4:ZO:367:ASP:O    | 4:ZO:371:GLU:HG2  | 2.04                     | 0.57              |
| 4:ZQ:380:ARG:HB3  | 4:ZW:396:LEU:HD13 | 1.86                     | 0.57              |
| 4:ZU:182:GLY:CA   | 4:Zf:131:GLY:HA3  | 2.20                     | 0.57              |
| 5:AB:71:LEU:CD2   | 3:AM:70:THR:CG2   | 2.81                     | 0.57              |
| 3:AJ:38:ARG:NH2   | 3:AJ:78:GLU:OE1   | 2.35                     | 0.57              |
| 3:AL:124:GLN:HG2  | 3:AL:125:ASN:H    | 1.69                     | 0.57              |
| 6:AZ:252:ILE:HD11 | 6:AZ:419:ALA:HB2  | 1.85                     | 0.57              |
| 6:Aj:377:MET:N    | 6:Aj:377:MET:SD   | 2.76                     | 0.57              |
| 6:AP:305:GLY:HA3  | 6:AP:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:AQ:305:GLY:HA3  | 6:AQ:355:PRO:HG2  | 1.85                     | 0.57              |
| 8:At:144:LEU:HB2  | 6:WJ:164:LEU:CD2  | 2.34                     | 0.57              |
| 11:A0:42:ASP:OD1  | 11:A0:43:ILE:N    | 2.38                     | 0.57              |
| 6:WC:196:HIS:HB3  | 6:WD:211:THR:HG21 | 1.87                     | 0.57              |
| 6:WU:200:SER:O    | 6:WV:158:ALA:CB   | 2.52                     | 0.57              |
| 1:B:62:TYR:CD1    | 2:z:129:VAL:HG11  | 2.37                     | 0.57              |
| 1:E:201:ALA:HA    | 1:F:149:THR:CG2   | 2.34                     | 0.57              |
| 1:R:219:MET:SD    | 1:S:212:TYR:CG    | 2.97                     | 0.57              |
| 1:T:219:MET:SD    | 1:U:212:TYR:CG    | 2.97                     | 0.57              |
| 1:V:219:MET:SD    | 1:W:212:TYR:CG    | 2.97                     | 0.57              |
| 2:d:35:SER:HB3    | 2:e:123:MET:CE    | 2.33                     | 0.57              |
| 2:i:43:VAL:HG12   | 2:i:84:VAL:HG22   | 1.85                     | 0.57              |
| 2:t:208:ARG:O     | 2:t:212:SER:OG    | 2.16                     | 0.57              |
| 2:w:43:VAL:HG12   | 2:w:84:VAL:HG22   | 1.85                     | 0.57              |
| 3:9:56:SER:OG     | 3:AH:153:ARG:HB2  | 2.04                     | 0.57              |
| 4:ZJ:165:PRO:HG2  | 4:ZJ:201:VAL:HG13 | 1.85                     | 0.57              |
| 4:ZQ:281:GLN:NE2  | 4:ZQ:283:GLY:O    | 2.38                     | 0.57              |
| 4:ZX:367:ASP:O    | 4:ZX:371:GLU:HG2  | 2.05                     | 0.57              |
| 3:AL:1:MET:HG3    | 3:AL:2:ILE:H      | 1.69                     | 0.57              |
| 6:AT:294:ARG:NE   | 11:A0:72:HIS:HE1  | 2.02                     | 0.57              |
| 6:Ai:377:MET:SD   | 6:Ai:377:MET:N    | 2.76                     | 0.57              |
| 6:AQ:252:ILE:HD11 | 6:AQ:419:ALA:HB2  | 1.85                     | 0.57              |
| 6:UL:69:GLN:HE22  | 6:WH:182:PRO:HG2  | 1.69                     | 0.57              |
| 6:WV:197:LEU:CD1  | 6:WW:175:SER:OG   | 2.53                     | 0.57              |
| 1:A:212:TYR:CG    | 1:Z:219:MET:SD    | 2.97                     | 0.57              |
| 1:H:62:TYR:CD1    | 2:f:129:VAL:HG11  | 2.37                     | 0.57              |
| 1:Y:219:MET:SD    | 1:Z:212:TYR:CG    | 2.97                     | 0.57              |
| 2:c:35:SER:HB3    | 2:d:123:MET:CE    | 2.33                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:h:35:SER:HB3     | 2:i:123:MET:CE    | 2.33                     | 0.57              |
| 2:j:43:VAL:HG12    | 2:j:84:VAL:HG22   | 1.85                     | 0.57              |
| 2:u:35:SER:HB3     | 2:v:123:MET:CE    | 2.33                     | 0.57              |
| 3:9:73:ARG:HD3     | 3:AM:218:TYR:CE2  | 2.40                     | 0.57              |
| 3:9:238:ARG:NE     | 4:ZF:393:ASP:OD1  | 2.35                     | 0.57              |
| 3:ZA:31:THR:HG22   | 4:ZF:39:PHE:HB2   | 1.85                     | 0.57              |
| 4:ZJ:373:VAL:O     | 4:ZJ:377:VAL:HG23 | 2.04                     | 0.57              |
| 4:ZP:107:ASN:HD22  | 4:ZP:138:THR:HG22 | 1.69                     | 0.57              |
| 4:ZU:154:MET:HE1   | 4:ZU:198:VAL:HG21 | 1.86                     | 0.57              |
| 4:ZU:373:VAL:O     | 4:ZU:376:ILE:N    | 2.36                     | 0.57              |
| 5:AB:51:LEU:HD12   | 12:BC:19:LYS:NZ   | 2.20                     | 0.57              |
| 5:AE:228:GLU:C     | 3:AK:258:THR:HG23 | 2.29                     | 0.57              |
| 3:AH:142:ILE:HD13  | 3:AH:149:ILE:HG12 | 1.86                     | 0.57              |
| 3:AJ:62:LEU:HD23   | 12:BF:83:PRO:CD   | 2.35                     | 0.57              |
| 3:AJ:257:LEU:HD21  | 12:BE:98:VAL:CG1  | 2.33                     | 0.57              |
| 3:AM:66:LEU:HD23   | 3:AM:66:LEU:H     | 1.69                     | 0.57              |
| 6:AR:276:GLU:OE2   | 10:A2:19:MET:HA   | 2.04                     | 0.57              |
| 6:AV:305:GLY:HA3   | 6:AV:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:Ae:372:ILE:CB    | 10:A2:4:ILE:HG12  | 2.34                     | 0.57              |
| 6:Af:365:ASN:ND2   | 11:A8:65:LEU:CD1  | 2.67                     | 0.57              |
| 6:Aj:305:GLY:HA3   | 6:Aj:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:Ap:305:GLY:HA3   | 6:Ap:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:AP:252:ILE:HD11  | 6:AP:419:ALA:HB2  | 1.85                     | 0.57              |
| 11:A9:117:GLN:HE22 | 12:BD:125:MET:CG  | 2.17                     | 0.57              |
| 6:WE:200:SER:O     | 6:WF:158:ALA:CB   | 2.52                     | 0.57              |
| 6:WV:160:PRO:HB2   | 6:WV:170:LYS:HB2  | 1.87                     | 0.57              |
| 1:B:201:ALA:HA     | 1:C:149:THR:CG2   | 2.34                     | 0.57              |
| 1:H:201:ALA:HA     | 1:I:149:THR:HG22  | 1.85                     | 0.57              |
| 1:I:219:MET:SD     | 1:J:212:TYR:CG    | 2.97                     | 0.57              |
| 2:f:35:SER:HB3     | 2:g:123:MET:CE    | 2.33                     | 0.57              |
| 2:s:88:MET:HG2     | 2:s:110:MET:HG3   | 1.86                     | 0.57              |
| 3:3:52:PRO:HB3     | 3:3:65:GLY:H      | 1.70                     | 0.57              |
| 3:8:22:ILE:HG21    | 3:8:233:MET:HG3   | 1.87                     | 0.57              |
| 3:ZE:233:MET:HE3   | 4:ZJ:391:THR:OG1  | 2.04                     | 0.57              |
| 4:ZO:140:PRO:HD2   | 4:ZO:312:LEU:CD2  | 2.34                     | 0.57              |
| 5:AC:26:LEU:HD22   | 3:AH:242:ILE:HG21 | 1.87                     | 0.57              |
| 6:AW:252:ILE:HD11  | 6:AW:419:ALA:HB2  | 1.85                     | 0.57              |
| 6:BQ:319:GLN:NE2   | 6:BV:355:PRO:HB3  | 2.19                     | 0.57              |
| 6:BR:305:GLY:HA3   | 6:BR:355:PRO:HG2  | 1.86                     | 0.57              |
| 1:D:219:MET:SD     | 1:E:212:TYR:CG    | 2.97                     | 0.57              |
| 1:E:62:TYR:CD1     | 2:c:129:VAL:HG11  | 2.37                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:219:MET:SD    | 1:O:212:TYR:CG    | 2.97                     | 0.57              |
| 2:h:78:ASN:HB3    | 3:AK:209:ASN:OD1  | 2.04                     | 0.57              |
| 2:y:80:GLN:NE2    | 3:AM:200:ALA:CA   | 2.58                     | 0.57              |
| 3:O:179:MET:SD    | 3:AJ:126:GLY:N    | 2.78                     | 0.57              |
| 3:8:45:LEU:HD21   | 3:AL:98:LYS:HG3   | 1.87                     | 0.57              |
| 3:8:47:GLN:N      | 3:8:68:ILE:O      | 2.37                     | 0.57              |
| 3:ZD:122:VAL:O    | 4:ZI:322:ASN:CG   | 2.48                     | 0.57              |
| 4:ZG:112:GLN:HG2  | 4:ZG:331:ASP:HB3  | 1.87                     | 0.57              |
| 4:ZK:102:LEU:HD21 | 4:ZK:106:ARG:HD3  | 1.86                     | 0.57              |
| 4:ZS:159:ASN:ND2  | 4:ZS:162:ASP:OD1  | 2.38                     | 0.57              |
| 5:AE:225:ARG:NE   | 3:AK:251:ASP:OD2  | 2.34                     | 0.57              |
| 3:AF:62:LEU:HD11  | 12:BB:84:LEU:CD1  | 2.35                     | 0.57              |
| 3:AI:257:LEU:CD1  | 12:BD:99:VAL:HG22 | 2.29                     | 0.57              |
| 6:AX:252:ILE:HD11 | 6:AX:419:ALA:HB2  | 1.85                     | 0.57              |
| 6:Ac:377:MET:N    | 6:Ac:377:MET:SD   | 2.76                     | 0.57              |
| 6:An:305:GLY:HA3  | 6:An:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:UN:208:GLY:HA3  | 6:WR:187:ASP:OD1  | 2.05                     | 0.57              |
| 6:WB:187:ASP:CG   | 6:WB:190:GLN:HG3  | 2.30                     | 0.57              |
| 6:BW:305:GLY:HA3  | 6:BW:355:PRO:HG2  | 1.86                     | 0.57              |
| 1:O:201:ALA:HA    | 1:P:149:THR:CG2   | 2.34                     | 0.57              |
| 1:P:219:MET:SD    | 1:Q:212:TYR:CG    | 2.97                     | 0.57              |
| 1:R:62:TYR:CD1    | 2:p:129:VAL:HG11  | 2.37                     | 0.57              |
| 1:X:62:TYR:HD1    | 2:v:129:VAL:HG11  | 1.62                     | 0.57              |
| 2:b:35:SER:HB3    | 2:c:123:MET:CE    | 2.33                     | 0.57              |
| 2:r:51:GLN:HG2    | 3:AI:138:PRO:HB3  | 1.86                     | 0.57              |
| 2:u:193:ASP:HB3   | 2:u:196:MET:HB2   | 1.87                     | 0.57              |
| 2:v:43:VAL:HG12   | 2:v:84:VAL:HG22   | 1.85                     | 0.57              |
| 2:v:193:ASP:HB3   | 2:v:196:MET:HB2   | 1.87                     | 0.57              |
| 3:O:22:ILE:HG21   | 3:O:233:MET:HG3   | 1.87                     | 0.57              |
| 3:8:227:ALA:HB1   | 4:ZJ:399:LEU:CD2  | 2.35                     | 0.57              |
| 3:ZA:26:LEU:HD22  | 4:ZF:384:SER:OG   | 2.05                     | 0.57              |
| 3:ZC:240:TYR:CE2  | 4:ZH:399:LEU:HD11 | 2.40                     | 0.57              |
| 3:ZE:85:ASN:CG    | 4:ZP:50:LEU:HD21  | 2.30                     | 0.57              |
| 4:ZG:180:LYS:HD2  | 4:ZG:181:LYS:H    | 1.70                     | 0.57              |
| 4:ZO:186:VAL:HG23 | 4:ZO:194:HIS:HB2  | 1.87                     | 0.57              |
| 4:ZQ:155:GLN:HG3  | 4:ZQ:278:ALA:HB3  | 1.86                     | 0.57              |
| 4:ZQ:155:GLN:NE2  | 4:ZQ:277:VAL:HB   | 2.19                     | 0.57              |
| 4:ZR:107:ASN:ND2  | 4:ZR:138:THR:OG1  | 2.38                     | 0.57              |
| 4:ZR:181:LYS:HD2  | 4:Zc:129:GLN:HE22 | 1.69                     | 0.57              |
| 4:ZU:71:ARG:NH1   | 4:ZZ:324:GLU:OE2  | 2.38                     | 0.57              |
| 4:ZZ:196:MET:HE3  | 4:ZZ:196:MET:HA   | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zd:102:LEU:HD11 | 4:Zd:139:ILE:HD12 | 1.87                     | 0.57              |
| 4:Ze:106:ARG:HH22 | 4:Ze:141:ASN:HB3  | 1.68                     | 0.57              |
| 5:AA:217:MET:HE2  | 3:AL:257:LEU:C    | 2.30                     | 0.57              |
| 3:AF:255:GLN:O    | 3:AF:259:GLN:HG2  | 2.05                     | 0.57              |
| 6:AV:355:PRO:CB   | 6:BO:319:GLN:NE2  | 2.67                     | 0.57              |
| 6:Ad:278:THR:HG21 | 10:A2:7:ILE:CB    | 2.11                     | 0.57              |
| 6:AO:252:ILE:HD11 | 6:AO:419:ALA:HB2  | 1.85                     | 0.57              |
| 6:AO:305:GLY:HA3  | 6:AO:355:PRO:HG2  | 1.86                     | 0.57              |
| 7:As:55:ILE:CD1   | 9:Ax:205:MET:CE   | 2.55                     | 0.57              |
| 10:A5:11:ILE:HG22 | 6:BR:372:ILE:HG21 | 1.85                     | 0.57              |
| 11:A8:32:ASN:ND2  | 12:BC:62:VAL:HG22 | 2.20                     | 0.57              |
| 6:UJ:103:GLN:CD   | 6:WD:182:PRO:HB3  | 2.28                     | 0.57              |
| 6:UP:126:PHE:O    | 6:UP:130:VAL:HB   | 2.05                     | 0.57              |
| 6:WA:201:ALA:C    | 6:WB:158:ALA:HB2  | 2.28                     | 0.57              |
| 6:WG:149:PRO:HG2  | 6:WG:190:GLN:NE2  | 2.19                     | 0.57              |
| 6:WJ:162:PRO:HA   | 6:WJ:169:GLN:CD   | 2.30                     | 0.57              |
| 6:BV:377:MET:N    | 6:BV:377:MET:SD   | 2.76                     | 0.57              |
| 1:C:201:ALA:HA    | 1:D:149:THR:CG2   | 2.34                     | 0.57              |
| 2:s:193:ASP:HB3   | 2:s:196:MET:HB2   | 1.87                     | 0.57              |
| 2:t:193:ASP:HB3   | 2:t:196:MET:HB2   | 1.87                     | 0.57              |
| 3:0:2:ILE:HG21    | 5:AD:212:LYS:HG2  | 1.86                     | 0.57              |
| 3:9:115:THR:HB    | 3:9:191:LEU:HD23  | 1.87                     | 0.57              |
| 3:9:128:LEU:HD12  | 3:9:140:ILE:HB    | 1.87                     | 0.57              |
| 3:ZB:56:SER:HA    | 3:AJ:152:GLY:CA   | 2.35                     | 0.57              |
| 4:ZG:165:PRO:HG2  | 4:ZG:201:VAL:HG13 | 1.86                     | 0.57              |
| 4:ZJ:159:ASN:ND2  | 4:ZJ:161:THR:OG1  | 2.38                     | 0.57              |
| 4:ZQ:111:MET:HB3  | 4:ZV:55:ALA:HB1   | 1.86                     | 0.57              |
| 4:ZW:6:ALA:HB1    | 4:ZW:389:ILE:HG12 | 1.87                     | 0.57              |
| 4:ZX:102:LEU:O    | 4:Zc:322:ASN:HB2  | 2.05                     | 0.57              |
| 4:Zc:382:TYR:CD2  | 4:Zh:395:ILE:HD11 | 2.40                     | 0.57              |
| 4:Zd:71:ARG:NH1   | 4:Zd:74:ASP:OD1   | 2.38                     | 0.57              |
| 5:AC:11:ALA:HB2   | 12:BD:29:ALA:HB1  | 1.85                     | 0.57              |
| 5:AC:152:PRO:HB2  | 3:AN:195:THR:HG22 | 1.86                     | 0.57              |
| 5:AE:175:ASP:HA   | 3:AJ:46:TYR:HB2   | 1.86                     | 0.57              |
| 6:AS:365:ASN:CB   | 11:A0:72:HIS:CD2  | 2.60                     | 0.57              |
| 6:Aa:305:GLY:HA3  | 6:Aa:355:PRO:HG2  | 1.86                     | 0.57              |
| 6:An:278:THR:HG21 | 10:Az:14:LEU:CB   | 2.35                     | 0.57              |
| 9:Aw:66:ARG:HG3   | 9:Aw:182:ALA:HB2  | 1.87                     | 0.57              |
| 6:UK:73:MET:HE3   | 6:UK:99:ARG:HD3   | 1.81                     | 0.57              |
| 6:UN:126:PHE:O    | 6:UN:130:VAL:HB   | 2.05                     | 0.57              |
| 1:G:201:ALA:HA    | 1:H:149:THR:HG22  | 1.85                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:219:MET:SD    | 1:T:212:TYR:CG    | 2.97                     | 0.56              |
| 2:w:193:ASP:HB3   | 2:w:196:MET:HB2   | 1.87                     | 0.56              |
| 2:y:193:ASP:HB3   | 2:y:196:MET:HB2   | 1.87                     | 0.56              |
| 2:z:193:ASP:HB3   | 2:z:196:MET:HB2   | 1.87                     | 0.56              |
| 2:z:208:ARG:O     | 2:z:212:SER:OG    | 2.16                     | 0.56              |
| 3:ZD:70:THR:HG22  | 3:ZD:71:GLY:H     | 1.70                     | 0.56              |
| 4:ZH:319:ASN:HB2  | 4:ZH:353:PHE:HE1  | 1.69                     | 0.56              |
| 4:ZM:27:SER:HB2   | 4:ZR:381:ASN:ND2  | 2.20                     | 0.56              |
| 4:ZN:319:ASN:ND2  | 4:ZN:352:ASN:O    | 2.38                     | 0.56              |
| 4:ZV:373:VAL:HG21 | 4:Zb:10:LEU:HD22  | 1.87                     | 0.56              |
| 5:AD:2:ASP:OD2    | 5:AD:4:ALA:N      | 2.31                     | 0.56              |
| 5:AE:116:GLN:HG3  | 5:AE:118:HIS:HD2  | 1.70                     | 0.56              |
| 5:AE:173:ARG:NH1  | 3:AJ:46:TYR:HE1   | 2.01                     | 0.56              |
| 6:AV:278:THR:CG2  | 10:A3:21:ALA:HB1  | 2.35                     | 0.56              |
| 6:Af:305:GLY:HA3  | 6:Af:355:PRO:HG2  | 1.86                     | 0.56              |
| 6:Ak:252:ILE:HD11 | 6:Ak:419:ALA:HB2  | 1.86                     | 0.56              |
| 6:Ao:305:GLY:HA3  | 6:Ao:355:PRO:HG2  | 1.86                     | 0.56              |
| 6:Ap:252:ILE:HD11 | 6:Ap:419:ALA:HB2  | 1.85                     | 0.56              |
| 7:As:54:LYS:HZ1   | 8:At:215:VAL:C    | 2.12                     | 0.56              |
| 10:A5:8:GLU:O     | 10:A5:11:ILE:HG13 | 2.05                     | 0.56              |
| 11:A7:34:ASP:OD1  | 12:BB:20:ARG:NH2  | 2.37                     | 0.56              |
| 6:UK:207:PRO:HG2  | 6:WE:187:ASP:CG   | 2.29                     | 0.56              |
| 6:WG:197:LEU:HD12 | 6:WH:175:SER:CB   | 2.35                     | 0.56              |
| 6:WU:197:LEU:HD12 | 6:WV:175:SER:HB3  | 1.87                     | 0.56              |
| 1:W:219:MET:SD    | 1:X:212:TYR:CG    | 2.97                     | 0.56              |
| 2:q:193:ASP:HB3   | 2:q:196:MET:HB2   | 1.87                     | 0.56              |
| 2:r:193:ASP:HB3   | 2:r:196:MET:HB2   | 1.87                     | 0.56              |
| 2:x:193:ASP:HB3   | 2:x:196:MET:HB2   | 1.87                     | 0.56              |
| 3:1:197:SER:C     | 3:AK:124:GLN:HB3  | 2.31                     | 0.56              |
| 3:2:9:LYS:HE3     | 3:AK:228:GLU:HG3  | 1.85                     | 0.56              |
| 3:3:7:ILE:HG23    | 3:3:71:GLY:HA2    | 1.87                     | 0.56              |
| 3:5:20:ASP:OD2    | 3:ZA:3:SER:HB3    | 2.04                     | 0.56              |
| 3:ZB:208:LEU:O    | 3:ZB:210:GLY:N    | 2.38                     | 0.56              |
| 3:ZB:227:ALA:HA   | 4:ZM:399:LEU:HD23 | 1.87                     | 0.56              |
| 3:ZD:52:PRO:HG3   | 3:ZD:67:GLN:HE21  | 1.70                     | 0.56              |
| 3:ZE:153:ARG:HD2  | 3:ZE:213:LEU:HD13 | 1.86                     | 0.56              |
| 4:ZF:18:ASP:OD1   | 4:ZK:2:SER:HB2    | 2.05                     | 0.56              |
| 4:Za:17:LEU:CD2   | 4:Zf:391:THR:HG21 | 2.35                     | 0.56              |
| 5:AA:227:PHE:HE2  | 3:AF:253:MET:O    | 1.87                     | 0.56              |
| 5:AD:200:ARG:HH22 | 3:AJ:189:GLU:CB   | 2.18                     | 0.56              |
| 3:AK:6:TRP:CE2    | 12:BF:77:VAL:CG1  | 2.80                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AM:52:PRO:HD3   | 12:BC:80:PRO:HB3  | 1.87                     | 0.56              |
| 6:AY:252:ILE:HD11 | 6:AY:419:ALA:HB2  | 1.85                     | 0.56              |
| 7:As:24:LEU:HD13  | 9:Ay:203:VAL:HG21 | 1.87                     | 0.56              |
| 9:Ay:152:ARG:NH2  | 6:WJ:165:PHE:CA   | 2.69                     | 0.56              |
| 6:UK:126:PHE:CE1  | 6:UK:130:VAL:CG2  | 2.84                     | 0.56              |
| 6:UO:51:TYR:OH    | 6:UO:76:PRO:HB2   | 2.06                     | 0.56              |
| 6:UP:51:TYR:OH    | 6:UP:76:PRO:HB2   | 2.06                     | 0.56              |
| 6:WE:212:LEU:HB3  | 6:WE:221:THR:HG23 | 1.85                     | 0.56              |
| 6:BT:305:GLY:HA3  | 6:BT:355:PRO:HG2  | 1.86                     | 0.56              |
| 6:BT:377:MET:N    | 6:BT:377:MET:SD   | 2.76                     | 0.56              |
| 6:BU:305:GLY:HA3  | 6:BU:355:PRO:HG2  | 1.86                     | 0.56              |
| 1:A:62:TYR:CD1    | 2:y:129:VAL:HG11  | 2.37                     | 0.56              |
| 1:F:62:TYR:CD1    | 2:d:129:VAL:HG11  | 2.37                     | 0.56              |
| 1:L:62:TYR:CD1    | 2:j:129:VAL:HG11  | 2.37                     | 0.56              |
| 1:U:62:TYR:CD1    | 2:s:129:VAL:HG11  | 2.37                     | 0.56              |
| 2:a:193:ASP:HB3   | 2:a:196:MET:HB2   | 1.87                     | 0.56              |
| 2:b:193:ASP:HB3   | 2:b:196:MET:HB2   | 1.87                     | 0.56              |
| 2:m:208:ARG:O     | 2:m:212:SER:OG    | 2.16                     | 0.56              |
| 2:p:193:ASP:HB3   | 2:p:196:MET:HB2   | 1.87                     | 0.56              |
| 3:0:151:ILE:HG12  | 3:0:157:VAL:HG22  | 1.86                     | 0.56              |
| 3:4:139:ALA:O     | 3:4:140:ILE:C     | 2.49                     | 0.56              |
| 3:7:1:MET:HB2     | 3:AK:226:VAL:CG2  | 2.35                     | 0.56              |
| 3:8:45:LEU:CD1    | 3:AL:83:GLN:NE2   | 2.68                     | 0.56              |
| 3:8:122:VAL:O     | 3:ZD:180:ASN:ND2  | 2.39                     | 0.56              |
| 3:ZD:28:ASN:OD1   | 4:ZI:52:VAL:HG22  | 2.05                     | 0.56              |
| 3:ZD:54:ALA:HB1   | 3:AL:150:THR:CG2  | 2.29                     | 0.56              |
| 4:ZJ:367:ASP:O    | 4:ZJ:371:GLU:HG2  | 2.05                     | 0.56              |
| 4:ZK:122:THR:OG1  | 4:ZK:129:GLN:HG3  | 2.04                     | 0.56              |
| 4:ZM:171:SER:O    | 4:ZM:177:SER:OG   | 2.23                     | 0.56              |
| 4:ZV:281:GLN:NE2  | 4:ZV:283:GLY:O    | 2.34                     | 0.56              |
| 4:ZW:101:LYS:NZ   | 4:Zb:322:ASN:HD21 | 2.03                     | 0.56              |
| 4:ZX:128:ILE:H    | 4:ZX:128:ILE:HD12 | 1.71                     | 0.56              |
| 4:ZX:159:ASN:ND2  | 4:ZX:161:THR:OG1  | 2.34                     | 0.56              |
| 4:ZZ:83:PHE:HB2   | 4:ZZ:95:SER:O     | 2.05                     | 0.56              |
| 4:Za:373:VAL:HG21 | 4:Zg:10:LEU:HD22  | 1.85                     | 0.56              |
| 4:Zc:395:ILE:O    | 4:Zc:398:THR:HG22 | 2.06                     | 0.56              |
| 4:Zd:159:ASN:ND2  | 4:Zd:162:ASP:OD2  | 2.39                     | 0.56              |
| 5:AA:16:LEU:CD2   | 3:AF:253:MET:HE3  | 2.36                     | 0.56              |
| 5:AB:70:GLN:HE21  | 3:AM:1:MET:H3     | 1.41                     | 0.56              |
| 5:AB:84:GLN:OE1   | 3:AM:48:THR:HG22  | 2.05                     | 0.56              |
| 5:AB:165:LYS:HG3  | 5:AB:199:ILE:HD11 | 1.85                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AC:34:PHE:HE1    | 3:AH:46:TYR:HH    | 1.49                     | 0.56              |
| 5:AC:59:ALA:HB3    | 3:AH:66:LEU:CD2   | 2.33                     | 0.56              |
| 5:AD:82:LEU:CD2    | 5:AD:88:LEU:HG    | 2.32                     | 0.56              |
| 5:AD:232:LYS:HZ1   | 12:BE:106:MET:CG  | 2.19                     | 0.56              |
| 3:AI:50:ARG:HD3    | 6:BN:322:PRO:CG   | 2.32                     | 0.56              |
| 6:Aj:372:ILE:HB    | 10:A1:11:ILE:HG21 | 1.87                     | 0.56              |
| 6:Am:305:GLY:HA3   | 6:Am:355:PRO:HG2  | 1.85                     | 0.56              |
| 8:At:166:SER:C     | 8:At:168:ALA:N    | 2.64                     | 0.56              |
| 9:Ax:142:THR:O     | 6:WD:165:PHE:CB   | 2.33                     | 0.56              |
| 10:A2:11:ILE:CD1   | 10:A2:12:SER:N    | 2.55                     | 0.56              |
| 11:A0:114:LEU:HD22 | 12:BF:126:MET:SD  | 2.45                     | 0.56              |
| 6:UJ:126:PHE:O     | 6:UJ:130:VAL:HB   | 2.05                     | 0.56              |
| 6:UK:207:PRO:HG2   | 6:WE:187:ASP:OD2  | 2.05                     | 0.56              |
| 6:UN:51:TYR:OH     | 6:UN:76:PRO:HB2   | 2.05                     | 0.56              |
| 12:BA:22:ASN:CB    | 6:BG:315:ALA:HB2  | 2.32                     | 0.56              |
| 6:WP:145:GLU:C     | 6:WP:147:LEU:H    | 2.14                     | 0.56              |
| 12:BD:57:GLN:O     | 12:BD:59:THR:N    | 2.36                     | 0.56              |
| 6:BS:305:GLY:HA3   | 6:BS:355:PRO:HG2  | 1.86                     | 0.56              |
| 2:c:193:ASP:HB3    | 2:c:196:MET:HB2   | 1.87                     | 0.56              |
| 2:d:193:ASP:HB3    | 2:d:196:MET:HB2   | 1.87                     | 0.56              |
| 3:1:258:THR:CA     | 5:AE:217:MET:HE3  | 2.25                     | 0.56              |
| 3:3:56:SER:HA      | 5:AB:138:ALA:HB1  | 1.88                     | 0.56              |
| 3:ZC:22:ILE:HG21   | 3:ZC:233:MET:HG3  | 1.87                     | 0.56              |
| 4:ZK:233:ASN:ND2   | 4:ZK:237:ILE:O    | 2.38                     | 0.56              |
| 4:ZK:310:GLN:O     | 4:ZK:312:LEU:HD12 | 2.05                     | 0.56              |
| 4:ZR:18:ASP:CG     | 4:ZW:5:GLN:HE22   | 2.14                     | 0.56              |
| 4:Zb:331:ASP:HA    | 4:Zg:40:ALA:HB1   | 1.87                     | 0.56              |
| 5:AA:70:GLN:CD     | 3:AL:3:SER:CB     | 2.79                     | 0.56              |
| 5:AC:70:GLN:HB2    | 3:AN:6:TRP:CZ3    | 2.34                     | 0.56              |
| 6:Al:305:GLY:HA3   | 6:Al:355:PRO:HG2  | 1.86                     | 0.56              |
| 8:At:149:LEU:O     | 8:At:153:THR:HG23 | 2.05                     | 0.56              |
| 9:Ax:161:GLY:N     | 6:WE:167:ARG:HD2  | 2.21                     | 0.56              |
| 10:A1:8:GLU:O      | 10:A1:11:ILE:HG13 | 2.06                     | 0.56              |
| 10:A4:11:ILE:CG2   | 6:BX:372:ILE:CG2  | 2.83                     | 0.56              |
| 11:A6:114:LEU:HD11 | 12:BB:7:PHE:CZ    | 2.39                     | 0.56              |
| 6:UI:51:TYR:OH     | 6:UI:76:PRO:HB2   | 2.05                     | 0.56              |
| 6:UI:126:PHE:CE1   | 6:UI:130:VAL:CG2  | 2.84                     | 0.56              |
| 6:WA:216:SER:O     | 6:WW:190:GLN:NE2  | 2.39                     | 0.56              |
| 6:WK:170:LYS:O     | 6:WK:171:SER:C    | 2.47                     | 0.56              |
| 6:WU:200:SER:O     | 6:WV:158:ALA:HB2  | 2.05                     | 0.56              |
| 12:BF:86:ASP:OD1   | 12:BF:86:ASP:N    | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:110:MET:O     | 2:j:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:u:110:MET:O     | 2:v:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:v:110:MET:O     | 2:w:84:VAL:CG2    | 2.54                     | 0.56              |
| 3:0:226:VAL:CG2   | 3:ZB:1:MET:HB2    | 2.36                     | 0.56              |
| 3:6:226:VAL:HG11  | 3:ZB:242:ILE:HD13 | 1.88                     | 0.56              |
| 4:ZH:75:VAL:CG1   | 4:ZH:356:LEU:HB3  | 2.35                     | 0.56              |
| 4:ZO:236:GLY:O    | 4:ZO:237:ILE:C    | 2.49                     | 0.56              |
| 5:AA:173:ARG:CD   | 3:AF:46:TYR:CE2   | 2.88                     | 0.56              |
| 3:AH:140:ILE:HG23 | 3:AH:171:GLY:HA3  | 1.87                     | 0.56              |
| 7:Ar:4:GLU:C      | 7:Ar:6:VAL:H      | 2.13                     | 0.56              |
| 9:Av:152:ARG:HH12 | 6:WV:164:LEU:CB   | 2.17                     | 0.56              |
| 6:UJ:55:PHE:HB2   | 6:UJ:58:LEU:HD11  | 1.88                     | 0.56              |
| 6:UO:126:PHE:O    | 6:UO:130:VAL:HB   | 2.05                     | 0.56              |
| 2:e:110:MET:O     | 2:f:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:e:193:ASP:HB3   | 2:e:196:MET:HB2   | 1.87                     | 0.56              |
| 2:f:193:ASP:HB3   | 2:f:196:MET:HB2   | 1.87                     | 0.56              |
| 2:g:208:ARG:O     | 2:g:212:SER:OG    | 2.16                     | 0.56              |
| 2:h:110:MET:O     | 2:i:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:l:110:MET:O     | 2:m:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:o:110:MET:O     | 2:p:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:o:193:ASP:HB3   | 2:o:196:MET:HB2   | 1.87                     | 0.56              |
| 2:r:110:MET:O     | 2:s:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:s:110:MET:O     | 2:t:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:v:208:ARG:O     | 2:v:212:SER:OG    | 2.16                     | 0.56              |
| 3:8:56:SER:O      | 3:AG:152:GLY:CA   | 2.53                     | 0.56              |
| 4:ZM:196:MET:HA   | 4:ZM:196:MET:HE3  | 1.86                     | 0.56              |
| 4:ZN:269:GLN:HB3  | 4:ZT:286:PRO:HG2  | 1.87                     | 0.56              |
| 4:ZS:180:LYS:HD2  | 4:ZS:181:LYS:H    | 1.71                     | 0.56              |
| 4:ZS:183:THR:HB   | 4:Zd:131:GLY:C    | 2.31                     | 0.56              |
| 4:ZT:294:ILE:O    | 4:ZT:358:ASN:ND2  | 2.39                     | 0.56              |
| 5:AA:47:ASP:O     | 6:BI:324:ASN:HB2  | 2.05                     | 0.56              |
| 3:AK:6:TRP:CZ2    | 12:BF:77:VAL:HG11 | 2.40                     | 0.56              |
| 6:WG:197:LEU:HA   | 6:WH:175:SER:OG   | 2.05                     | 0.56              |
| 6:WM:201:ALA:C    | 6:WN:158:ALA:HB2  | 2.30                     | 0.56              |
| 2:f:110:MET:O     | 2:g:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:q:51:GLN:CG     | 3:AI:209:ASN:HD21 | 2.19                     | 0.56              |
| 2:y:110:MET:O     | 2:z:84:VAL:CG2    | 2.54                     | 0.56              |
| 3:1:91:ASN:ND2    | 3:1:94:ASP:OD1    | 2.39                     | 0.56              |
| 3:ZA:257:LEU:HD21 | 3:AN:230:LEU:HD12 | 1.88                     | 0.56              |
| 4:ZL:165:PRO:HG3  | 4:ZL:179:ASN:ND2  | 2.20                     | 0.56              |
| 4:ZM:129:GLN:HE21 | 4:ZM:132:ALA:HB2  | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Za:387:GLN:OE1  | 4:Zg:400:VAL:O    | 2.24                     | 0.56              |
| 5:AA:148:PRO:HB2  | 3:AF:210:GLY:HA3  | 1.88                     | 0.56              |
| 5:AB:26:LEU:HB3   | 3:AG:243:ASN:OD1  | 2.06                     | 0.56              |
| 5:AC:72:ASP:CG    | 3:AN:9:LYS:HZ1    | 2.14                     | 0.56              |
| 3:AK:22:ILE:HG21  | 3:AK:233:MET:HG3  | 1.88                     | 0.56              |
| 6:Ak:305:GLY:HA3  | 6:Ak:355:PRO:HG2  | 1.86                     | 0.56              |
| 7:Aq:89:GLY:O     | 6:WW:164:LEU:HB2  | 2.05                     | 0.56              |
| 8:At:101:PHE:CE2  | 9:Au:223:LEU:HD11 | 2.40                     | 0.56              |
| 9:Au:147:LEU:HD12 | 6:WO:166:VAL:HG11 | 1.87                     | 0.56              |
| 10:A4:8:GLU:O     | 10:A4:11:ILE:HG13 | 2.06                     | 0.56              |
| 2:j:208:ARG:O     | 2:j:212:SER:OG    | 2.16                     | 0.56              |
| 2:n:193:ASP:HB3   | 2:n:196:MET:HB2   | 1.87                     | 0.56              |
| 3:3:107:LEU:HD12  | 3:3:111:THR:HG23  | 1.88                     | 0.56              |
| 3:ZE:26:LEU:CD2   | 4:ZJ:384:SER:OG   | 2.52                     | 0.56              |
| 4:ZI:71:ARG:NH1   | 4:ZI:74:ASP:OD1   | 2.39                     | 0.56              |
| 4:ZM:150:THR:OG1  | 4:ZM:282:ASN:ND2  | 2.38                     | 0.56              |
| 4:ZR:375:MET:CE   | 4:ZW:388:THR:HG23 | 2.32                     | 0.56              |
| 4:ZS:322:ASN:HB3  | 4:ZS:340:SER:HA   | 1.87                     | 0.56              |
| 4:ZU:16:ASN:O     | 4:ZU:20:ILE:HG13  | 2.06                     | 0.56              |
| 4:ZV:101:LYS:HZ1  | 4:ZV:111:MET:HG3  | 1.70                     | 0.56              |
| 4:ZY:369:SER:HB3  | 4:Ze:382:TYR:OH   | 2.06                     | 0.56              |
| 5:AC:229:MET:HG2  | 12:BD:102:MET:CE  | 2.34                     | 0.56              |
| 7:Ab:51:PHE:CZ    | 9:Au:202:SER:HA   | 2.41                     | 0.56              |
| 8:At:145:TRP:CG   | 6:WJ:164:LEU:HD13 | 2.37                     | 0.56              |
| 10:A3:8:GLU:O     | 10:A3:11:ILE:HG13 | 2.05                     | 0.56              |
| 10:A4:14:LEU:CB   | 6:BW:278:THR:HG21 | 2.31                     | 0.56              |
| 6:UI:126:PHE:O    | 6:UI:130:VAL:HB   | 2.05                     | 0.56              |
| 6:UM:51:TYR:OH    | 6:UM:76:PRO:HB2   | 2.05                     | 0.56              |
| 6:WC:170:LYS:H    | 6:WC:170:LYS:HD2  | 1.69                     | 0.56              |
| 6:WQ:145:GLU:C    | 6:WQ:147:LEU:H    | 2.13                     | 0.56              |
| 2:g:193:ASP:HB3   | 2:g:196:MET:HB2   | 1.87                     | 0.56              |
| 2:x:110:MET:O     | 2:y:84:VAL:CG2    | 2.54                     | 0.56              |
| 3:3:180:ASN:O     | 3:3:182:THR:N     | 2.39                     | 0.56              |
| 3:9:64:SER:O      | 3:9:64:SER:OG     | 2.20                     | 0.56              |
| 3:ZA:240:TYR:HE2  | 4:ZF:395:ILE:HG23 | 1.60                     | 0.56              |
| 4:ZK:25:ALA:HB1   | 4:ZP:52:VAL:HG12  | 1.87                     | 0.56              |
| 4:ZM:24:ILE:O     | 4:ZM:27:SER:OG    | 2.22                     | 0.56              |
| 4:ZU:65:THR:CG2   | 4:Zf:4:SER:HB3    | 2.30                     | 0.56              |
| 4:Ze:156:ILE:HG13 | 4:Ze:276:ILE:HA   | 1.87                     | 0.56              |
| 3:AF:26:LEU:HD13  | 3:AK:242:ILE:HG22 | 1.87                     | 0.56              |
| 6:AS:294:ARG:HD3  | 11:A0:68:THR:CG2  | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A7:51:LYS:HG2  | 11:A7:55:ARG:NH1  | 2.20                     | 0.56              |
| 12:BB:72:ALA:O    | 12:BB:95:ASN:ND2  | 2.38                     | 0.56              |
| 12:BE:17:GLN:NE2  | 12:BE:111:SER:OG  | 2.39                     | 0.56              |
| 6:BV:305:GLY:HA3  | 6:BV:355:PRO:HG2  | 1.86                     | 0.56              |
| 2:b:110:MET:O     | 2:c:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:h:193:ASP:HB3   | 2:h:196:MET:HB2   | 1.87                     | 0.56              |
| 2:k:110:MET:O     | 2:l:84:VAL:CG2    | 2.54                     | 0.56              |
| 2:p:110:MET:O     | 2:q:84:VAL:CG2    | 2.54                     | 0.56              |
| 3:3:1:MET:HB2     | 3:AG:226:VAL:HG21 | 1.88                     | 0.56              |
| 3:3:19:MET:HB2    | 3:3:236:VAL:HG11  | 1.87                     | 0.56              |
| 3:4:22:ILE:HG21   | 3:4:233:MET:HG2   | 1.88                     | 0.56              |
| 3:5:45:LEU:HD22   | 3:AI:98:LYS:HG3   | 1.87                     | 0.56              |
| 3:5:240:TYR:OH    | 3:ZA:257:LEU:HD22 | 2.06                     | 0.56              |
| 3:ZA:99:GLY:O     | 3:ZA:116:ARG:NH2  | 2.39                     | 0.56              |
| 4:ZL:8:SER:OG     | 4:ZL:52:VAL:O     | 2.23                     | 0.56              |
| 4:ZO:304:TYR:HE1  | 4:ZO:310:GLN:HB3  | 1.71                     | 0.56              |
| 4:ZV:111:MET:N    | 4:ZV:111:MET:SD   | 2.79                     | 0.56              |
| 4:ZW:228:THR:HB   | 4:ZW:244:VAL:HG21 | 1.87                     | 0.56              |
| 5:AB:68:PRO:HG3   | 3:AM:47:GLN:HB2   | 1.88                     | 0.56              |
| 5:AD:137:ILE:HD13 | 5:AD:143:ILE:HG12 | 1.87                     | 0.56              |
| 7:Ab:84:LEU:HD21  | 9:Av:185:ILE:HG23 | 1.87                     | 0.56              |
| 8:At:176:GLY:HA2  | 8:At:179:ILE:HD12 | 1.87                     | 0.56              |
| 9:Ay:86:ASN:O     | 9:Ay:87:GLN:C     | 2.49                     | 0.56              |
| 6:UJ:102:GLN:HG2  | 6:UJ:193:ALA:HB2  | 1.88                     | 0.56              |
| 6:WD:118:GLN:O    | 6:WD:119:GLU:C    | 2.49                     | 0.56              |
| 6:WO:128:GLU:HG2  | 6:WP:126:PHE:CD2  | 2.40                     | 0.56              |
| 1:P:62:TYR:CD1    | 2:n:129:VAL:HG11  | 2.37                     | 0.55              |
| 2:c:110:MET:O     | 2:d:84:VAL:CG2    | 2.54                     | 0.55              |
| 3:7:238:ARG:HB3   | 3:ZD:1:MET:HE1    | 1.88                     | 0.55              |
| 3:8:56:SER:C      | 3:AG:153:ARG:H    | 2.13                     | 0.55              |
| 3:ZD:140:ILE:HD13 | 3:ZD:157:VAL:HG21 | 1.88                     | 0.55              |
| 3:ZE:31:THR:HG22  | 4:ZJ:39:PHE:C     | 2.30                     | 0.55              |
| 4:ZP:164:VAL:HG22 | 4:ZP:202:LYS:HG2  | 1.87                     | 0.55              |
| 4:ZT:102:LEU:O    | 4:ZY:322:ASN:CB   | 2.53                     | 0.55              |
| 4:ZT:187:TYR:CE2  | 4:ZT:285:LYS:HB2  | 2.41                     | 0.55              |
| 4:ZU:379:GLN:NE2  | 4:ZZ:394:GLN:HB2  | 2.21                     | 0.55              |
| 4:ZV:330:GLY:O    | 4:ZV:333:VAL:HG12 | 2.06                     | 0.55              |
| 5:AA:213:PRO:HG3  | 3:AL:1:MET:HE2    | 1.88                     | 0.55              |
| 5:AC:70:GLN:HB3   | 3:AN:6:TRP:HE3    | 1.67                     | 0.55              |
| 5:AC:181:LEU:HD11 | 5:AC:193:LEU:HG   | 1.86                     | 0.55              |
| 5:AE:196:ASP:HB3  | 5:AE:199:ILE:HD12 | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AF:124:GLN:O    | 3:AK:179:MET:HG2  | 2.06                     | 0.55              |
| 3:AI:3:SER:O      | 3:AI:7:ILE:HD12   | 2.06                     | 0.55              |
| 10:A2:61:LEU:CD1  | 11:A7:50:LYS:HZ3  | 2.18                     | 0.55              |
| 11:A7:51:LYS:CE   | 11:A7:55:ARG:NH2  | 2.67                     | 0.55              |
| 6:UK:126:PHE:CD1  | 6:UK:130:VAL:CG2  | 2.90                     | 0.55              |
| 6:UO:102:GLN:HG2  | 6:UO:193:ALA:HB2  | 1.89                     | 0.55              |
| 6:WM:197:LEU:HD11 | 6:WN:156:HIS:HD2  | 1.71                     | 0.55              |
| 2:m:193:ASP:HB3   | 2:m:196:MET:HB2   | 1.87                     | 0.55              |
| 2:r:208:ARG:O     | 2:r:212:SER:OG    | 2.16                     | 0.55              |
| 3:2:34:PHE:HB3    | 3:2:222:SER:HB3   | 1.87                     | 0.55              |
| 3:5:74:PRO:HB2    | 3:ZA:66:LEU:HD11  | 1.88                     | 0.55              |
| 3:7:19:MET:O      | 3:7:20:ASP:C      | 2.48                     | 0.55              |
| 3:ZD:35:LYS:HB2   | 3:ZD:79:ARG:HD3   | 1.87                     | 0.55              |
| 4:ZL:102:LEU:O    | 4:ZQ:322:ASN:HB2  | 2.06                     | 0.55              |
| 4:ZQ:330:GLY:N    | 4:ZV:43:PHE:HB2   | 2.21                     | 0.55              |
| 4:ZV:144:MET:HG2  | 4:ZV:287:GLY:H    | 1.70                     | 0.55              |
| 4:ZY:217:ASP:HB3  | 4:ZY:220:ALA:HB2  | 1.88                     | 0.55              |
| 5:AA:226:ARG:O    | 5:AA:230:GLN:HG2  | 2.05                     | 0.55              |
| 5:AE:240:ASN:HD21 | 12:BF:109:SER:CB  | 2.19                     | 0.55              |
| 6:AX:372:ILE:HB   | 10:A3:11:ILE:HG22 | 1.88                     | 0.55              |
| 6:Aj:372:ILE:CG1  | 10:A1:11:ILE:HG22 | 2.31                     | 0.55              |
| 7:As:24:LEU:CD1   | 9:Ay:203:VAL:HG21 | 2.36                     | 0.55              |
| 7:As:68:TRP:HE1   | 6:WF:122:GLY:HA2  | 1.71                     | 0.55              |
| 8:At:158:PRO:HG2  | 8:At:162:ASN:ND2  | 2.15                     | 0.55              |
| 9:Aw:109:TYR:CB   | 10:A2:32:VAL:HG21 | 2.37                     | 0.55              |
| 9:Ay:67:ILE:CD1   | 9:Ay:96:LEU:HB3   | 2.36                     | 0.55              |
| 10:Az:8:GLU:O     | 10:Az:11:ILE:HG13 | 2.05                     | 0.55              |
| 10:A1:87:GLN:O    | 10:A1:91:LYS:HG2  | 2.06                     | 0.55              |
| 6:UL:55:PHE:HB2   | 6:UL:58:LEU:HD11  | 1.88                     | 0.55              |
| 6:UL:216:SER:C    | 6:UL:218:HIS:H    | 2.14                     | 0.55              |
| 6:UM:102:GLN:HG2  | 6:UM:193:ALA:HB2  | 1.88                     | 0.55              |
| 6:WA:156:HIS:HD2  | 6:WW:197:LEU:HD11 | 1.71                     | 0.55              |
| 6:WG:190:GLN:NE2  | 6:WH:216:SER:O    | 2.39                     | 0.55              |
| 6:WK:187:ASP:OD1  | 6:WK:187:ASP:N    | 2.38                     | 0.55              |
| 6:WW:118:GLN:O    | 6:WW:119:GLU:C    | 2.49                     | 0.55              |
| 1:B:165:GLY:CA    | 1:C:35:THR:HG22   | 2.37                     | 0.55              |
| 1:G:62:TYR:CD1    | 2:e:129:VAL:HG11  | 2.37                     | 0.55              |
| 2:i:193:ASP:HB3   | 2:i:196:MET:HB2   | 1.87                     | 0.55              |
| 2:j:110:MET:O     | 2:k:84:VAL:CG2    | 2.54                     | 0.55              |
| 2:m:110:MET:O     | 2:n:84:VAL:CG2    | 2.54                     | 0.55              |
| 2:n:110:MET:O     | 2:o:84:VAL:CG2    | 2.54                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:v:273:CYS:CB    | 2:w:264:MET:O     | 2.42                     | 0.55              |
| 3:0:70:THR:HG22   | 5:AD:71:LEU:HB2   | 1.87                     | 0.55              |
| 3:4:55:GLN:NE2    | 3:4:57:SER:O      | 2.40                     | 0.55              |
| 3:4:74:PRO:HB2    | 3:9:66:LEU:HD11   | 1.88                     | 0.55              |
| 3:ZA:233:MET:SD   | 4:ZF:388:THR:HA   | 2.47                     | 0.55              |
| 4:ZL:18:ASP:CB    | 4:ZQ:5:GLN:HE22   | 2.18                     | 0.55              |
| 4:ZL:22:ASN:ND2   | 4:ZQ:49:GLY:HA3   | 2.21                     | 0.55              |
| 4:ZP:17:LEU:HD13  | 4:ZU:395:ILE:CD1  | 2.37                     | 0.55              |
| 4:ZT:382:TYR:CE1  | 4:ZY:395:ILE:HG23 | 2.40                     | 0.55              |
| 4:ZX:71:ARG:NH1   | 4:ZX:100:PHE:O    | 2.36                     | 0.55              |
| 4:ZZ:160:SER:O    | 4:ZZ:202:LYS:NZ   | 2.39                     | 0.55              |
| 4:Zf:109:VAL:HG12 | 4:Zf:115:GLN:HA   | 1.88                     | 0.55              |
| 5:AA:58:THR:CG2   | 3:AF:50:ARG:HH22  | 2.19                     | 0.55              |
| 5:AA:220:MET:HE1  | 3:AF:246:ALA:HB2  | 1.84                     | 0.55              |
| 3:AJ:126:GLY:O    | 3:AJ:127:GLN:HB2  | 2.05                     | 0.55              |
| 3:AM:44:LEU:HD23  | 3:AM:73:ARG:HD2   | 1.88                     | 0.55              |
| 8:At:166:SER:O    | 8:At:167:ASN:C    | 2.49                     | 0.55              |
| 10:A2:12:SER:O    | 10:A2:15:GLN:HG3  | 2.06                     | 0.55              |
| 11:A8:3:ASP:O     | 11:A8:7:ALA:N     | 2.35                     | 0.55              |
| 11:A9:32:ASN:ND2  | 12:BD:62:VAL:HG12 | 2.21                     | 0.55              |
| 11:A0:36:PRO:O    | 6:BP:310:GLY:HA2  | 2.06                     | 0.55              |
| 6:UP:55:PHE:HB2   | 6:UP:58:LEU:HD11  | 1.88                     | 0.55              |
| 6:WB:197:LEU:HD12 | 6:WC:175:SER:HB3  | 1.87                     | 0.55              |
| 6:WI:145:GLU:C    | 6:WI:147:LEU:H    | 2.13                     | 0.55              |
| 6:WQ:196:HIS:CD2  | 6:WR:219:LEU:HD22 | 2.40                     | 0.55              |
| 6:WT:190:GLN:NE2  | 6:WU:216:SER:O    | 2.39                     | 0.55              |
| 2:a:84:VAL:CG2    | 2:z:110:MET:O     | 2.54                     | 0.55              |
| 2:w:273:CYS:CB    | 2:x:264:MET:O     | 2.42                     | 0.55              |
| 3:4:32:ASN:HD21   | 3:9:38:ARG:HH22   | 1.53                     | 0.55              |
| 3:5:239:ALA:HB2   | 3:ZB:1:MET:HE1    | 1.88                     | 0.55              |
| 3:ZE:154:ASP:OD2  | 3:ZE:154:ASP:N    | 2.37                     | 0.55              |
| 4:ZF:352:ASN:OD1  | 4:ZF:352:ASN:N    | 2.39                     | 0.55              |
| 4:ZN:107:ASN:ND2  | 4:ZN:138:THR:OG1  | 2.39                     | 0.55              |
| 4:ZO:156:ILE:HG21 | 4:ZO:200:PHE:HE2  | 1.71                     | 0.55              |
| 4:Zh:97:ASN:OD1   | 4:Zh:99:GLN:NE2   | 2.40                     | 0.55              |
| 5:AB:229:MET:HE3  | 3:AH:258:THR:HG22 | 1.89                     | 0.55              |
| 3:AF:140:ILE:HG23 | 3:AF:170:VAL:CG1  | 2.37                     | 0.55              |
| 3:AJ:62:LEU:CD1   | 12:BF:84:LEU:HD11 | 2.37                     | 0.55              |
| 6:AV:264:ALA:HB2  | 6:AV:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:AX:278:THR:CG2  | 10:A3:7:ILE:CG2   | 2.80                     | 0.55              |
| 6:Al:295:SER:HB2  | 11:A7:65:LEU:HD22 | 1.86                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AO:264:ALA:HB2  | 6:AO:389:VAL:HG13 | 1.89                     | 0.55              |
| 7:As:59:PHE:HZ    | 9:Ax:198:LEU:HD12 | 1.71                     | 0.55              |
| 8:At:144:LEU:CB   | 6:WJ:164:LEU:CD2  | 2.84                     | 0.55              |
| 8:At:170:MET:O    | 8:At:174:ARG:N    | 2.26                     | 0.55              |
| 9:Av:58:LEU:O     | 9:Av:62:THR:OG1   | 2.22                     | 0.55              |
| 11:A7:90:PRO:HB3  | 11:A7:99:THR:HB   | 1.88                     | 0.55              |
| 6:UI:55:PHE:HB2   | 6:UI:58:LEU:HD11  | 1.88                     | 0.55              |
| 6:UK:126:PHE:O    | 6:UK:130:VAL:HB   | 2.05                     | 0.55              |
| 6:UN:102:GLN:HG2  | 6:UN:193:ALA:HB2  | 1.88                     | 0.55              |
| 6:WB:193:ALA:HB1  | 6:WC:213:VAL:CG1  | 2.36                     | 0.55              |
| 6:WM:190:GLN:HG3  | 6:WN:217:GLY:HA3  | 1.88                     | 0.55              |
| 6:WV:128:GLU:HG3  | 6:WW:126:PHE:CE2  | 2.41                     | 0.55              |
| 6:BR:264:ALA:HB2  | 6:BR:389:VAL:HG13 | 1.89                     | 0.55              |
| 2:j:193:ASP:HB3   | 2:j:196:MET:HB2   | 1.87                     | 0.55              |
| 2:w:110:MET:O     | 2:x:84:VAL:CG2    | 2.54                     | 0.55              |
| 3:0:180:ASN:HD22  | 3:AJ:122:VAL:HG23 | 1.71                     | 0.55              |
| 3:4:54:ALA:HB1    | 5:AC:136:THR:CG2  | 2.36                     | 0.55              |
| 3:8:164:GLN:O     | 3:8:166:ALA:N     | 2.40                     | 0.55              |
| 3:9:85:ASN:ND2    | 4:ZK:4:SER:CB     | 2.26                     | 0.55              |
| 3:ZA:260:LEU:HD11 | 3:AN:234:ILE:HD11 | 1.89                     | 0.55              |
| 4:ZG:212:THR:HG21 | 4:ZG:246:ILE:HD13 | 1.87                     | 0.55              |
| 4:ZP:87:ASP:OD1   | 4:ZP:87:ASP:N     | 2.36                     | 0.55              |
| 5:AB:27:ALA:O     | 3:AG:72:VAL:HG11  | 2.07                     | 0.55              |
| 5:AC:250:MET:HB2  | 12:BD:123:LYS:HE3 | 1.86                     | 0.55              |
| 5:AE:76:ARG:NH1   | 5:AE:79:ASP:OD1   | 2.40                     | 0.55              |
| 3:AH:75:VAL:HA    | 3:AM:51:GLN:HE22  | 1.71                     | 0.55              |
| 3:AI:62:LEU:HD23  | 12:BE:84:LEU:HD23 | 1.87                     | 0.55              |
| 3:AJ:194:GLU:OE1  | 3:AJ:201:PRO:HD3  | 2.06                     | 0.55              |
| 3:AK:73:ARG:HG3   | 12:BF:78:TYR:CE2  | 2.41                     | 0.55              |
| 7:Ab:6:VAL:HG21   | 9:Aw:228:LEU:HD21 | 1.88                     | 0.55              |
| 6:Aj:372:ILE:CB   | 10:A1:11:ILE:HG22 | 2.32                     | 0.55              |
| 6:Ao:409:MET:HE2  | 6:Ao:409:MET:HA   | 1.89                     | 0.55              |
| 7:Aq:74:LEU:HD22  | 9:Aw:229:VAL:HG13 | 1.88                     | 0.55              |
| 7:Ar:84:LEU:HD21  | 9:Ax:185:ILE:HG23 | 1.89                     | 0.55              |
| 11:A6:73:ILE:HG13 | 6:BR:295:SER:HB2  | 1.88                     | 0.55              |
| 6:UL:51:TYR:OH    | 6:UL:76:PRO:HB2   | 2.05                     | 0.55              |
| 6:UM:211:THR:HG23 | 6:UM:219:LEU:HD11 | 1.89                     | 0.55              |
| 6:UP:102:GLN:HG2  | 6:UP:193:ALA:HB2  | 1.89                     | 0.55              |
| 1:C:165:GLY:CA    | 1:D:35:THR:HG22   | 2.37                     | 0.55              |
| 1:E:219:MET:SD    | 1:F:212:TYR:CB    | 2.95                     | 0.55              |
| 1:F:219:MET:SD    | 1:G:212:TYR:CB    | 2.95                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:219:MET:SD    | 1:I:212:TYR:CB    | 2.95                     | 0.55              |
| 1:Q:165:GLY:CA    | 1:R:35:THR:HG22   | 2.37                     | 0.55              |
| 1:R:165:GLY:CA    | 1:S:35:THR:HG22   | 2.37                     | 0.55              |
| 1:V:165:GLY:CA    | 1:W:35:THR:HG22   | 2.37                     | 0.55              |
| 1:W:165:GLY:CA    | 1:X:35:THR:HG22   | 2.37                     | 0.55              |
| 2:g:110:MET:O     | 2:h:84:VAL:CG2    | 2.54                     | 0.55              |
| 2:q:110:MET:O     | 2:r:84:VAL:CG2    | 2.54                     | 0.55              |
| 2:u:273:CYS:CB    | 2:v:264:MET:O     | 2.42                     | 0.55              |
| 2:x:273:CYS:CB    | 2:y:264:MET:O     | 2.42                     | 0.55              |
| 3:0:89:THR:O      | 3:0:91:ASN:N      | 2.40                     | 0.55              |
| 4:ZI:144:MET:HE2  | 4:ZI:310:GLN:NE2  | 2.20                     | 0.55              |
| 4:ZM:105:ASN:HB2  | 4:ZM:107:ASN:HD21 | 1.70                     | 0.55              |
| 4:ZR:183:THR:CG2  | 4:Zc:132:ALA:HA   | 2.36                     | 0.55              |
| 4:ZT:319:ASN:OD1  | 4:ZT:320:PHE:N    | 2.39                     | 0.55              |
| 4:ZW:196:MET:HE1  | 4:ZW:214:ASP:HB2  | 1.88                     | 0.55              |
| 4:Zc:93:PHE:HD1   | 4:Zc:114:MET:HE1  | 1.71                     | 0.55              |
| 5:AB:104:ASN:HD22 | 3:AG:40:VAL:HG11  | 1.71                     | 0.55              |
| 5:AE:213:PRO:HB3  | 3:AJ:242:ILE:CD1  | 2.33                     | 0.55              |
| 3:AF:62:LEU:CD2   | 12:BB:83:PRO:CG   | 2.83                     | 0.55              |
| 9:Au:135:ARG:O    | 9:Au:136:ALA:C    | 2.48                     | 0.55              |
| 9:Ax:163:GLU:N    | 9:Ax:163:GLU:OE2  | 2.39                     | 0.55              |
| 9:Ay:66:ARG:HG2   | 9:Ay:243:PHE:HZ   | 1.72                     | 0.55              |
| 10:Az:72:MET:O    | 10:Az:76:GLN:HG2  | 2.06                     | 0.55              |
| 6:UI:211:THR:HG23 | 6:UI:219:LEU:HD11 | 1.89                     | 0.55              |
| 6:UJ:51:TYR:OH    | 6:UJ:76:PRO:HB2   | 2.06                     | 0.55              |
| 6:UJ:260:THR:HG23 | 6:UJ:268:LEU:HD11 | 1.89                     | 0.55              |
| 6:UN:211:THR:HG23 | 6:UN:219:LEU:HD11 | 1.89                     | 0.55              |
| 6:UO:211:THR:HG23 | 6:UO:219:LEU:HD11 | 1.89                     | 0.55              |
| 6:WJ:200:SER:O    | 6:WK:158:ALA:CB   | 2.54                     | 0.55              |
| 6:WL:190:GLN:NE2  | 6:WM:216:SER:O    | 2.39                     | 0.55              |
| 6:WQ:124:SER:O    | 6:WQ:127:SER:N    | 2.37                     | 0.55              |
| 6:BU:264:ALA:HB2  | 6:BU:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:BX:264:ALA:HB2  | 6:BX:389:VAL:HG13 | 1.89                     | 0.55              |
| 1:A:165:GLY:CA    | 1:B:35:THR:HG22   | 2.37                     | 0.55              |
| 1:D:219:MET:SD    | 1:E:212:TYR:CB    | 2.95                     | 0.55              |
| 1:G:219:MET:SD    | 1:H:212:TYR:CB    | 2.95                     | 0.55              |
| 1:I:219:MET:SD    | 1:J:212:TYR:CB    | 2.95                     | 0.55              |
| 1:Z:62:TYR:CD1    | 2:x:129:VAL:HG11  | 2.37                     | 0.55              |
| 2:l:193:ASP:HB3   | 2:l:196:MET:HB2   | 1.87                     | 0.55              |
| 2:t:110:MET:O     | 2:u:84:VAL:CG2    | 2.54                     | 0.55              |
| 3:4:73:ARG:HB2    | 3:AH:218:TYR:OH   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:5:257:LEU:HD21  | 3:AI:227:ALA:HA   | 1.87                     | 0.55              |
| 4:ZJ:370:LYS:HE2  | 4:ZP:11:ASN:CG    | 2.31                     | 0.55              |
| 4:ZS:247:THR:HG23 | 4:ZS:258:THR:HG22 | 1.88                     | 0.55              |
| 4:ZU:66:THR:O     | 4:Zf:42:MET:HE1   | 2.07                     | 0.55              |
| 4:ZZ:337:THR:HG22 | 4:ZZ:339:ALA:H    | 1.72                     | 0.55              |
| 4:Za:382:TYR:CE1  | 4:Zf:395:ILE:HG23 | 2.41                     | 0.55              |
| 4:Zb:217:ASP:HB3  | 4:Zb:220:ALA:HB2  | 1.88                     | 0.55              |
| 4:Zd:33:LYS:NZ    | 4:Zd:362:GLU:OE1  | 2.39                     | 0.55              |
| 4:Zd:381:ASN:OD1  | 4:Zd:385:ASN:ND2  | 2.39                     | 0.55              |
| 3:AF:147:LEU:HD11 | 3:AF:162:GLN:HA   | 1.88                     | 0.55              |
| 3:AN:229:GLU:O    | 3:AN:233:MET:HG3  | 2.06                     | 0.55              |
| 6:AS:264:ALA:HB2  | 6:AS:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:AX:264:ALA:HB2  | 6:AX:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:AX:370:ARG:HH21 | 10:A3:14:LEU:HD11 | 1.71                     | 0.55              |
| 6:AY:264:ALA:HB2  | 6:AY:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:An:409:MET:HA   | 6:An:409:MET:HE2  | 1.89                     | 0.55              |
| 6:AO:409:MET:HE2  | 6:AO:409:MET:HA   | 1.89                     | 0.55              |
| 9:Au:83:ALA:HB3   | 9:Au:84:PRO:HD3   | 1.89                     | 0.55              |
| 9:Ay:159:LEU:HB2  | 6:WI:165:PHE:CD2  | 2.42                     | 0.55              |
| 11:A0:31:ALA:HB1  | 12:BE:13:ALA:HB2  | 1.88                     | 0.55              |
| 6:UI:102:GLN:HG2  | 6:UI:193:ALA:HB2  | 1.89                     | 0.55              |
| 6:UK:102:GLN:HG2  | 6:UK:193:ALA:HB2  | 1.88                     | 0.55              |
| 6:UM:55:PHE:HB2   | 6:UM:58:LEU:HD11  | 1.88                     | 0.55              |
| 6:UN:55:PHE:HB2   | 6:UN:58:LEU:HD11  | 1.88                     | 0.55              |
| 6:WA:193:ALA:HB1  | 6:WB:213:VAL:HG11 | 1.89                     | 0.55              |
| 6:WB:143:THR:OG1  | 6:WC:154:ARG:HG2  | 2.06                     | 0.55              |
| 6:WD:143:THR:OG1  | 6:WE:154:ARG:HG2  | 2.06                     | 0.55              |
| 6:WP:197:LEU:HD12 | 6:WQ:175:SER:HB3  | 1.89                     | 0.55              |
| 6:WR:197:LEU:HA   | 6:WS:175:SER:OG   | 2.07                     | 0.55              |
| 1:C:219:MET:SD    | 1:D:212:TYR:CB    | 2.95                     | 0.55              |
| 1:J:219:MET:SD    | 1:K:212:TYR:CB    | 2.95                     | 0.55              |
| 1:P:165:GLY:CA    | 1:Q:35:THR:HG22   | 2.37                     | 0.55              |
| 1:T:62:TYR:CD1    | 2:r:129:VAL:HG11  | 2.37                     | 0.55              |
| 1:X:165:GLY:CA    | 1:Y:35:THR:HG22   | 2.37                     | 0.55              |
| 2:k:193:ASP:HB3   | 2:k:196:MET:HB2   | 1.87                     | 0.55              |
| 3:l:38:ARG:NH1    | 3:AK:94:ASP:OD2   | 2.38                     | 0.55              |
| 3:6:73:ARG:NH2    | 3:AJ:215:TYR:HE1  | 2.05                     | 0.55              |
| 4:ZW:181:LYS:NZ   | 4:Zh:129:GLN:NE2  | 2.54                     | 0.55              |
| 4:ZZ:33:LYS:O     | 4:ZZ:59:GLN:NE2   | 2.38                     | 0.55              |
| 4:Za:150:THR:OG1  | 4:Za:282:ASN:ND2  | 2.34                     | 0.55              |
| 5:AC:51:LEU:HD13  | 12:BD:19:LYS:HE2  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AF:47:GLN:NE2   | 12:BA:73:PRO:CB   | 2.69                     | 0.55              |
| 6:Aa:264:ALA:HB2  | 6:Aa:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:Al:409:MET:HE2  | 6:Al:409:MET:HA   | 1.89                     | 0.55              |
| 6:Ao:264:ALA:HB2  | 6:Ao:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:AO:297:GLN:NE2  | 11:A6:60:THR:HG23 | 2.21                     | 0.55              |
| 6:AP:264:ALA:HB2  | 6:AP:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:AP:409:MET:HE2  | 6:AP:409:MET:HA   | 1.89                     | 0.55              |
| 10:A3:57:GLU:HG2  | 11:A8:11:PHE:CD2  | 2.42                     | 0.55              |
| 10:A5:89:ARG:NH2  | 10:A5:90:ASN:OD1  | 2.39                     | 0.55              |
| 6:UO:55:PHE:HB2   | 6:UO:58:LEU:HD11  | 1.88                     | 0.55              |
| 12:BB:47:VAL:O    | 6:BJ:313:PRO:HD2  | 2.06                     | 0.55              |
| 6:BS:409:MET:HE2  | 6:BS:409:MET:HA   | 1.89                     | 0.55              |
| 1:I:165:GLY:CA    | 1:J:35:THR:HG22   | 2.37                     | 0.55              |
| 2:q:208:ARG:O     | 2:q:212:SER:OG    | 2.16                     | 0.55              |
| 3:0:16:GLN:HE22   | 3:5:2:ILE:HD11    | 1.72                     | 0.55              |
| 3:2:108:PRO:HG3   | 3:ZC:60:THR:HG21  | 1.88                     | 0.55              |
| 3:2:233:MET:O     | 3:2:236:VAL:HG22  | 2.06                     | 0.55              |
| 3:8:79:ARG:NH2    | 3:8:184:LEU:O     | 2.40                     | 0.55              |
| 4:ZN:71:ARG:NH1   | 4:ZN:74:ASP:OD1   | 2.40                     | 0.55              |
| 4:ZN:112:GLN:HG2  | 4:ZN:331:ASP:HB3  | 1.88                     | 0.55              |
| 4:ZR:210:VAL:HB   | 4:ZR:228:THR:HG22 | 1.88                     | 0.55              |
| 4:ZU:373:VAL:HG11 | 4:Za:7:VAL:HG22   | 1.87                     | 0.55              |
| 4:ZW:183:THR:HG21 | 4:Zh:133:ASN:N    | 2.22                     | 0.55              |
| 4:ZX:80:ASN:ND2   | 4:ZX:352:ASN:OD1  | 2.39                     | 0.55              |
| 4:ZY:251:ILE:HG22 | 4:ZY:252:ASN:OD1  | 2.07                     | 0.55              |
| 6:AU:264:ALA:HB2  | 6:AU:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:Am:409:MET:HE2  | 6:Am:409:MET:HA   | 1.89                     | 0.55              |
| 6:Ap:409:MET:HE2  | 6:Ap:409:MET:HA   | 1.89                     | 0.55              |
| 9:Ay:160:GLN:O    | 6:WI:167:ARG:CG   | 2.50                     | 0.55              |
| 6:UI:126:PHE:CD1  | 6:UI:130:VAL:CG2  | 2.90                     | 0.55              |
| 6:UK:55:PHE:HB2   | 6:UK:58:LEU:HD11  | 1.88                     | 0.55              |
| 6:UL:102:GLN:HG2  | 6:UL:193:ALA:HB2  | 1.88                     | 0.55              |
| 6:UL:126:PHE:CD1  | 6:UL:130:VAL:CG2  | 2.90                     | 0.55              |
| 6:UL:167:ARG:O    | 6:UL:168:GLU:C    | 2.49                     | 0.55              |
| 6:UP:211:THR:HG23 | 6:UP:219:LEU:HD11 | 1.89                     | 0.55              |
| 6:WT:145:GLU:O    | 6:WT:147:LEU:N    | 2.40                     | 0.55              |
| 6:WU:130:VAL:O    | 6:WU:134:ARG:HG3  | 2.07                     | 0.55              |
| 6:BV:264:ALA:HB2  | 6:BV:389:VAL:HG13 | 1.89                     | 0.55              |
| 1:B:219:MET:SD    | 1:C:212:TYR:CB    | 2.95                     | 0.55              |
| 1:D:165:GLY:CA    | 1:E:35:THR:HG22   | 2.37                     | 0.55              |
| 1:S:219:MET:SD    | 1:T:212:TYR:CB    | 2.95                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:73:ARG:HB2    | 3:AG:218:TYR:OH   | 2.06                     | 0.55              |
| 3:9:56:SER:C      | 3:AH:153:ARG:H    | 2.15                     | 0.55              |
| 4:ZH:285:LYS:O    | 4:ZH:306:ASN:ND2  | 2.40                     | 0.55              |
| 4:ZM:367:ASP:O    | 4:ZM:371:GLU:HG2  | 2.07                     | 0.55              |
| 4:ZS:117:THR:HG22 | 4:ZS:136:PRO:HA   | 1.88                     | 0.55              |
| 4:ZU:183:THR:CB   | 4:Zf:131:GLY:O    | 2.54                     | 0.55              |
| 4:ZY:234:GLU:HB3  | 4:Ze:255:THR:OG1  | 2.06                     | 0.55              |
| 4:Zh:294:ILE:O    | 4:Zh:358:ASN:ND2  | 2.40                     | 0.55              |
| 5:AB:70:GLN:HB3   | 3:AM:6:TRP:CG     | 2.37                     | 0.55              |
| 5:AC:75:SER:O     | 5:AC:75:SER:OG    | 2.23                     | 0.55              |
| 3:AG:178:PHE:CE1  | 3:AG:201:PRO:HB3  | 2.42                     | 0.55              |
| 3:AI:77:THR:HG23  | 3:AN:66:LEU:HB2   | 1.87                     | 0.55              |
| 6:AY:409:MET:HE2  | 6:AY:409:MET:HA   | 1.89                     | 0.55              |
| 9:Ay:143:ARG:HB2  | 9:Ay:146:ASP:OD2  | 2.07                     | 0.55              |
| 6:UK:51:TYR:OH    | 6:UK:76:PRO:HB2   | 2.06                     | 0.55              |
| 6:UL:126:PHE:O    | 6:UL:130:VAL:HB   | 2.05                     | 0.55              |
| 6:UP:103:GLN:CB   | 6:WW:182:PRO:HB3  | 2.33                     | 0.55              |
| 6:WJ:139:GLU:HB3  | 6:WK:154:ARG:HH21 | 1.70                     | 0.55              |
| 6:WQ:172:PRO:HD2  | 6:WQ:204:GLY:O    | 2.07                     | 0.55              |
| 6:WS:145:GLU:O    | 6:WS:147:LEU:N    | 2.39                     | 0.55              |
| 6:WS:172:PRO:HD2  | 6:WS:204:GLY:O    | 2.07                     | 0.55              |
| 6:WV:113:PHE:O    | 6:WV:116:LEU:HB3  | 2.07                     | 0.55              |
| 12:BF:3:LEU:H     | 6:BG:319:GLN:HE21 | 1.55                     | 0.55              |
| 6:BS:264:ALA:HB2  | 6:BS:389:VAL:HG13 | 1.89                     | 0.55              |
| 6:BV:409:MET:HE2  | 6:BV:409:MET:HA   | 1.89                     | 0.55              |
| 1:A:219:MET:SD    | 1:B:212:TYR:CB    | 2.95                     | 0.54              |
| 1:H:165:GLY:CA    | 1:I:35:THR:HG22   | 2.37                     | 0.54              |
| 1:J:165:GLY:CA    | 1:K:35:THR:HG22   | 2.37                     | 0.54              |
| 1:O:165:GLY:CA    | 1:P:35:THR:HG22   | 2.37                     | 0.54              |
| 1:S:165:GLY:CA    | 1:T:35:THR:HG22   | 2.37                     | 0.54              |
| 1:U:165:GLY:CA    | 1:V:35:THR:HG22   | 2.37                     | 0.54              |
| 1:Y:165:GLY:CA    | 1:Z:35:THR:HG22   | 2.37                     | 0.54              |
| 2:t:273:CYS:CB    | 2:u:264:MET:O     | 2.42                     | 0.54              |
| 2:y:273:CYS:CB    | 2:z:264:MET:O     | 2.42                     | 0.54              |
| 3:4:52:PRO:HB3    | 3:4:65:GLY:H      | 1.72                     | 0.54              |
| 4:ZI:160:SER:OG   | 4:ZO:192:ASN:OD1  | 2.25                     | 0.54              |
| 4:ZQ:184:VAL:HG13 | 4:ZQ:196:MET:HB2  | 1.89                     | 0.54              |
| 4:ZS:349:GLY:O    | 4:ZY:89:ASN:ND2   | 2.40                     | 0.54              |
| 4:ZU:178:TYR:HA   | 4:ZU:201:VAL:HG22 | 1.89                     | 0.54              |
| 4:ZW:70:GLY:N     | 4:ZW:359:GLY:O    | 2.38                     | 0.54              |
| 4:ZZ:331:ASP:HA   | 4:Ze:40:ALA:HB1   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AD:247:LEU:HD21 | 12:BE:119:LEU:HD12 | 1.89                     | 0.54              |
| 5:AE:87:TRP:HB3   | 5:AE:99:TYR:HB3    | 1.90                     | 0.54              |
| 3:AG:62:LEU:HD11  | 12:BC:84:LEU:HD11  | 1.88                     | 0.54              |
| 6:AK:409:MET:HE2  | 6:AK:409:MET:HA    | 1.89                     | 0.54              |
| 8:AT:233:MET:O    | 8:AT:236:ILE:HG12  | 2.07                     | 0.54              |
| 9:AX:160:GLN:CA   | 6:WE:166:VAL:CG2   | 2.84                     | 0.54              |
| 10:A4:7:ILE:HG22  | 6:BX:278:THR:HG21  | 1.78                     | 0.54              |
| 6:UJ:126:PHE:CD1  | 6:UJ:130:VAL:CG2   | 2.90                     | 0.54              |
| 6:WF:200:SER:O    | 6:WG:158:ALA:CB    | 2.55                     | 0.54              |
| 6:WH:186:LEU:HD22 | 6:WH:190:GLN:CD    | 2.32                     | 0.54              |
| 6:WP:197:LEU:HA   | 6:WQ:175:SER:OG    | 2.08                     | 0.54              |
| 6:WR:123:ILE:HB   | 6:WR:127:SER:OG    | 2.06                     | 0.54              |
| 6:BT:409:MET:HA   | 6:BT:409:MET:HE2   | 1.89                     | 0.54              |
| 1:A:35:THR:HG22   | 1:Z:165:GLY:CA     | 2.37                     | 0.54              |
| 1:K:165:GLY:CA    | 1:L:35:THR:HG22    | 2.37                     | 0.54              |
| 1:K:219:MET:SD    | 1:L:212:TYR:CB     | 2.95                     | 0.54              |
| 1:T:165:GLY:CA    | 1:U:35:THR:HG22    | 2.37                     | 0.54              |
| 1:W:219:MET:SD    | 1:X:212:TYR:CB     | 2.95                     | 0.54              |
| 2:I:78:ASN:HD21   | 5:AE:154:THR:HG21  | 1.73                     | 0.54              |
| 3:2:35:LYS:NZ     | 3:2:220:GLU:OE2    | 2.40                     | 0.54              |
| 3:3:33:GLY:N      | 3:3:220:GLU:O      | 2.40                     | 0.54              |
| 3:4:42:GLU:OE2    | 3:4:73:ARG:NE      | 2.28                     | 0.54              |
| 3:ZE:16:GLN:HE22  | 4:ZJ:392:GLN:NE2   | 2.05                     | 0.54              |
| 3:ZE:22:ILE:HG21  | 3:ZE:233:MET:HG3   | 1.89                     | 0.54              |
| 4:ZH:269:GLN:OE1  | 4:ZN:146:ALA:N     | 2.40                     | 0.54              |
| 4:ZK:118:GLY:HA2  | 4:ZK:316:VAL:HG12  | 1.87                     | 0.54              |
| 4:Za:106:ARG:NH1  | 4:Zf:321:ALA:HB2   | 2.22                     | 0.54              |
| 5:AA:44:VAL:HG21  | 6:BH:320:PRO:HG3   | 1.90                     | 0.54              |
| 5:AA:76:ARG:CD    | 3:AF:80:LEU:HD13   | 2.38                     | 0.54              |
| 5:AB:51:LEU:O     | 5:AB:52:ALA:C      | 2.51                     | 0.54              |
| 3:AF:95:VAL:HG12  | 3:AF:216:GLN:HA    | 1.89                     | 0.54              |
| 6:An:264:ALA:HB2  | 6:An:389:VAL:HG13  | 1.89                     | 0.54              |
| 8:AT:249:ASN:HB2  | 6:WK:162:PRO:HB2   | 1.89                     | 0.54              |
| 9:Ay:68:ILE:O     | 9:Ay:69:ILE:C      | 2.50                     | 0.54              |
| 6:UM:126:PHE:O    | 6:UM:130:VAL:HB    | 2.05                     | 0.54              |
| 6:WD:145:GLU:C    | 6:WD:147:LEU:H     | 2.15                     | 0.54              |
| 6:WQ:124:SER:O    | 6:WQ:125:GLN:C     | 2.50                     | 0.54              |
| 6:WV:128:GLU:HG3  | 6:WW:126:PHE:CD2   | 2.43                     | 0.54              |
| 12:BC:6:ILE:CG2   | 12:BC:122:VAL:HG21 | 2.33                     | 0.54              |
| 6:BR:409:MET:HE2  | 6:BR:409:MET:HA    | 1.89                     | 0.54              |
| 1:G:165:GLY:CA    | 1:H:35:THR:HG22    | 2.37                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:O:62:TYR:CD1    | 2:m:129:VAL:HG11   | 2.37                     | 0.54              |
| 1:T:219:MET:SD    | 1:U:212:TYR:CB     | 2.95                     | 0.54              |
| 1:V:219:MET:SD    | 1:W:212:TYR:CB     | 2.95                     | 0.54              |
| 3:ZA:45:LEU:HD13  | 3:AN:83:GLN:CG     | 2.35                     | 0.54              |
| 4:ZM:184:VAL:HG13 | 4:ZM:196:MET:HB2   | 1.88                     | 0.54              |
| 4:ZU:165:PRO:HG2  | 4:ZU:201:VAL:HG13  | 1.89                     | 0.54              |
| 5:AE:247:LEU:CD1  | 12:BF:116:ILE:HG23 | 2.38                     | 0.54              |
| 3:AI:45:LEU:CD2   | 12:BD:76:LEU:CD1   | 2.86                     | 0.54              |
| 3:AK:73:ARG:CG    | 12:BF:78:TYR:CE2   | 2.89                     | 0.54              |
| 3:AN:22:ILE:HG21  | 3:AN:233:MET:HG2   | 1.89                     | 0.54              |
| 6:Aa:409:MET:HE2  | 6:Aa:409:MET:HA    | 1.89                     | 0.54              |
| 6:Aj:409:MET:HE2  | 6:Aj:409:MET:HA    | 1.89                     | 0.54              |
| 6:AQ:409:MET:HE2  | 6:AQ:409:MET:HA    | 1.89                     | 0.54              |
| 7:Ar:84:LEU:HD23  | 9:Ax:238:SER:OG    | 2.07                     | 0.54              |
| 11:A8:36:PRO:HB3  | 11:A8:96:ASP:HB2   | 1.89                     | 0.54              |
| 6:UK:211:THR:HG23 | 6:UK:219:LEU:HD11  | 1.89                     | 0.54              |
| 6:WJ:190:GLN:HG2  | 6:WK:216:SER:O     | 2.07                     | 0.54              |
| 6:BU:409:MET:HE2  | 6:BU:409:MET:HA    | 1.89                     | 0.54              |
| 1:L:165:GLY:CA    | 1:M:35:THR:HG22    | 2.37                     | 0.54              |
| 1:X:219:MET:SD    | 1:Y:212:TYR:CB     | 2.95                     | 0.54              |
| 2:w:54:GLN:OE1    | 3:AH:141:THR:CB    | 2.55                     | 0.54              |
| 3:0:89:THR:C      | 3:0:91:ASN:N       | 2.61                     | 0.54              |
| 3:5:237:GLN:HE21  | 3:ZA:252:GLN:CB    | 2.20                     | 0.54              |
| 3:8:164:GLN:C     | 3:8:166:ALA:N      | 2.65                     | 0.54              |
| 3:8:205:THR:OG1   | 3:8:208:LEU:HD23   | 2.08                     | 0.54              |
| 3:ZC:257:LEU:O    | 3:ZC:260:LEU:HB2   | 2.07                     | 0.54              |
| 3:ZD:164:GLN:O    | 3:ZD:165:ALA:C     | 2.50                     | 0.54              |
| 3:ZE:28:ASN:OD1   | 4:ZJ:52:VAL:CG2    | 2.55                     | 0.54              |
| 4:ZK:99:GLN:HG3   | 4:ZK:361:LEU:HD11  | 1.88                     | 0.54              |
| 4:ZN:93:PHE:HB3   | 4:ZN:333:VAL:HG13  | 1.89                     | 0.54              |
| 4:ZN:331:ASP:HA   | 4:ZS:40:ALA:HB1    | 1.90                     | 0.54              |
| 4:ZP:201:VAL:HG23 | 4:ZP:209:ALA:HB3   | 1.90                     | 0.54              |
| 4:ZU:146:ALA:HB2  | 4:ZU:286:PRO:HD3   | 1.88                     | 0.54              |
| 5:AC:70:GLN:HG2   | 3:AN:3:SER:HA      | 1.90                     | 0.54              |
| 5:AC:248:LEU:HD21 | 11:A8:106:ARG:HG2  | 1.88                     | 0.54              |
| 5:AD:17:ASN:HD22  | 3:AI:66:LEU:HD21   | 1.72                     | 0.54              |
| 5:AE:214:VAL:HG11 | 3:AK:12:LEU:CB     | 2.37                     | 0.54              |
| 3:AJ:50:ARG:HD3   | 6:BP:322:PRO:HD3   | 1.89                     | 0.54              |
| 3:AJ:187:ILE:HG13 | 3:AJ:191:LEU:HB2   | 1.90                     | 0.54              |
| 6:Al:264:ALA:HB2  | 6:Al:389:VAL:HG13  | 1.89                     | 0.54              |
| 7:Ar:36:SER:C     | 7:As:44:ILE:HD12   | 2.33                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Au:152:ARG:NH1  | 6:WR:164:LEU:HG   | 2.23                     | 0.54              |
| 9:Ay:148:ALA:HA   | 6:WI:164:LEU:HD22 | 1.88                     | 0.54              |
| 6:UL:211:THR:HG23 | 6:UL:219:LEU:HD11 | 1.89                     | 0.54              |
| 6:UO:126:PHE:CD1  | 6:UO:130:VAL:CG2  | 2.90                     | 0.54              |
| 12:BA:113:GLN:O   | 12:BA:117:GLU:HG2 | 2.07                     | 0.54              |
| 6:BW:409:MET:HA   | 6:BW:409:MET:HE2  | 1.89                     | 0.54              |
| 1:A:212:TYR:CB    | 1:Z:219:MET:SD    | 2.95                     | 0.54              |
| 1:L:219:MET:SD    | 1:M:212:TYR:CB    | 2.95                     | 0.54              |
| 1:N:219:MET:SD    | 1:O:212:TYR:CB    | 2.95                     | 0.54              |
| 1:O:219:MET:SD    | 1:P:212:TYR:CB    | 2.95                     | 0.54              |
| 1:R:219:MET:SD    | 1:S:212:TYR:CB    | 2.95                     | 0.54              |
| 1:U:219:MET:SD    | 1:V:212:TYR:CB    | 2.95                     | 0.54              |
| 2:d:110:MET:O     | 2:e:84:VAL:CG2    | 2.54                     | 0.54              |
| 3:3:124:GLN:HB2   | 3:8:199:GLY:HA2   | 1.90                     | 0.54              |
| 3:6:42:GLU:OE1    | 3:6:73:ARG:NH2    | 2.32                     | 0.54              |
| 3:ZD:37:GLN:OE1   | 4:ZI:43:PHE:CE2   | 2.61                     | 0.54              |
| 4:ZG:97:ASN:OD1   | 4:ZG:98:GLY:N     | 2.40                     | 0.54              |
| 4:ZU:368:LEU:HD13 | 4:Zf:396:LEU:HD11 | 1.90                     | 0.54              |
| 4:Za:24:ILE:CG2   | 4:Zf:384:SER:OG   | 2.55                     | 0.54              |
| 4:Za:157:ASN:HD21 | 4:Zg:143:LEU:HD13 | 1.68                     | 0.54              |
| 4:Zb:57:ILE:HD12  | 4:Zg:47:LYS:HB2   | 1.88                     | 0.54              |
| 4:Zb:83:PHE:HB2   | 4:Zb:95:SER:O     | 2.08                     | 0.54              |
| 4:Ze:322:ASN:HB3  | 4:Ze:340:SER:HA   | 1.89                     | 0.54              |
| 4:Zf:79:GLN:O     | 4:Zf:96:ARG:NH2   | 2.40                     | 0.54              |
| 5:AD:55:THR:HG1   | 12:BE:45:LYS:HZ1  | 1.46                     | 0.54              |
| 5:AE:51:LEU:HB2   | 5:AE:53:THR:HG23  | 1.90                     | 0.54              |
| 6:AR:264:ALA:HB2  | 6:AR:389:VAL:HG13 | 1.89                     | 0.54              |
| 6:Ai:409:MET:HE2  | 6:Ai:409:MET:HA   | 1.89                     | 0.54              |
| 6:Ap:264:ALA:HB2  | 6:Ap:389:VAL:HG13 | 1.89                     | 0.54              |
| 6:AQ:264:ALA:HB2  | 6:AQ:389:VAL:HG13 | 1.89                     | 0.54              |
| 9:Ay:152:ARG:NH2  | 6:WJ:165:PHE:N    | 2.55                     | 0.54              |
| 6:WD:186:LEU:HD22 | 6:WD:190:GLN:CD   | 2.32                     | 0.54              |
| 6:WF:212:LEU:HB3  | 6:WF:221:THR:HG23 | 1.90                     | 0.54              |
| 12:BD:57:GLN:C    | 12:BD:59:THR:N    | 2.63                     | 0.54              |
| 12:BF:85:ALA:HB1  | 12:BF:89:GLY:HA2  | 1.89                     | 0.54              |
| 1:K:62:TYR:CD1    | 2:i:129:VAL:HG11  | 2.37                     | 0.54              |
| 1:P:219:MET:SD    | 1:Q:212:TYR:CB    | 2.95                     | 0.54              |
| 3:1:251:ASP:OD1   | 3:AJ:238:ARG:NH2  | 2.40                     | 0.54              |
| 3:2:163:GLY:HA2   | 3:ZD:111:THR:HG21 | 1.89                     | 0.54              |
| 3:7:56:SER:HB3    | 3:7:62:LEU:HB2    | 1.88                     | 0.54              |
| 3:7:238:ARG:HD2   | 3:ZD:254:LEU:HB3  | 1.88                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZN:248:THR:OG1  | 4:ZN:257:ALA:N     | 2.40                     | 0.54              |
| 4:ZV:2:SER:OG     | 4:ZV:392:GLN:OE1   | 2.21                     | 0.54              |
| 4:ZV:373:VAL:HG21 | 4:Zb:10:LEU:CD2    | 2.37                     | 0.54              |
| 4:Za:14:ALA:HB2   | 4:Za:382:TYR:HE2   | 1.72                     | 0.54              |
| 6:Ae:372:ILE:CG2  | 10:A2:4:ILE:HG12   | 2.37                     | 0.54              |
| 7:Aq:62:ILE:O     | 7:Aq:66:GLY:N      | 2.39                     | 0.54              |
| 10:Az:69:ASN:HD21 | 11:A6:20:ALA:CB    | 2.20                     | 0.54              |
| 10:A4:7:ILE:HG22  | 6:BX:278:THR:CG2   | 2.32                     | 0.54              |
| 6:UM:103:GLN:NE2  | 6:WQ:182:PRO:CB    | 2.71                     | 0.54              |
| 12:BA:80:PRO:HB3  | 12:BA:89:GLY:HA3   | 1.90                     | 0.54              |
| 6:WO:197:LEU:HA   | 6:WP:175:SER:OG    | 2.07                     | 0.54              |
| 6:BK:330:THR:HB   | 6:BK:331:PRO:HD3   | 1.89                     | 0.54              |
| 6:BT:264:ALA:HB2  | 6:BT:389:VAL:HG13  | 1.89                     | 0.54              |
| 1:E:165:GLY:CA    | 1:F:35:THR:HG22    | 2.37                     | 0.54              |
| 1:F:165:GLY:CA    | 1:G:35:THR:HG22    | 2.37                     | 0.54              |
| 1:M:165:GLY:CA    | 1:N:35:THR:HG22    | 2.37                     | 0.54              |
| 1:M:219:MET:SD    | 1:N:212:TYR:CB     | 2.95                     | 0.54              |
| 1:Q:219:MET:SD    | 1:R:212:TYR:CB     | 2.95                     | 0.54              |
| 1:Y:219:MET:SD    | 1:Z:212:TYR:CB     | 2.95                     | 0.54              |
| 2:a:264:MET:O     | 2:z:273:CYS:CB     | 2.42                     | 0.54              |
| 3:1:42:GLU:CD     | 3:AK:189:GLU:HG3   | 2.33                     | 0.54              |
| 3:3:165:ALA:HB1   | 3:ZE:194:GLU:HG2   | 1.89                     | 0.54              |
| 3:4:19:MET:HB2    | 3:4:236:VAL:HG11   | 1.90                     | 0.54              |
| 3:8:19:MET:HE1    | 3:8:233:MET:HG2    | 1.88                     | 0.54              |
| 3:9:241:GLU:HG2   | 3:ZE:256:LYS:HG3   | 1.90                     | 0.54              |
| 3:ZC:240:TYR:HE2  | 4:ZH:399:LEU:HD11  | 1.72                     | 0.54              |
| 4:ZM:81:GLY:HA3   | 4:ZM:317:LEU:HD23  | 1.89                     | 0.54              |
| 4:ZU:183:THR:N    | 4:Zf:131:GLY:O     | 2.40                     | 0.54              |
| 4:ZV:159:ASN:ND2  | 4:ZV:162:ASP:OD2   | 2.38                     | 0.54              |
| 4:Ze:130:GLN:H    | 4:Ze:130:GLN:CD    | 2.15                     | 0.54              |
| 5:AB:213:PRO:HD2  | 3:AM:2:ILE:CD1     | 2.29                     | 0.54              |
| 5:AE:57:VAL:HG13  | 12:BF:29:ALA:HB1   | 1.90                     | 0.54              |
| 3:AH:98:LYS:NZ    | 3:AN:187:ILE:O     | 2.33                     | 0.54              |
| 3:AH:241:GLU:HG3  | 3:AM:256:LYS:HE3   | 1.88                     | 0.54              |
| 3:AN:180:ASN:ND2  | 3:AN:197:SER:O     | 2.38                     | 0.54              |
| 8:At:38:ILE:HB    | 8:At:43:LYS:HE2    | 1.90                     | 0.54              |
| 8:At:236:ILE:O    | 8:At:240:CYS:N     | 2.36                     | 0.54              |
| 9:Ay:63:SER:O     | 9:Ay:67:ILE:HB     | 2.07                     | 0.54              |
| 9:Ay:64:PHE:O     | 9:Ay:67:ILE:HG22   | 2.08                     | 0.54              |
| 10:A4:75:MET:CE   | 11:A9:122:VAL:HG22 | 2.37                     | 0.54              |
| 6:UM:126:PHE:CD1  | 6:UM:130:VAL:CG2   | 2.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WN:145:GLU:C    | 6:WN:147:LEU:H    | 2.15                     | 0.54              |
| 6:WO:200:SER:O    | 6:WP:158:ALA:CB   | 2.55                     | 0.54              |
| 6:WU:196:HIS:HB3  | 6:WV:211:THR:HG21 | 1.89                     | 0.54              |
| 6:BX:409:MET:HE2  | 6:BX:409:MET:HA   | 1.89                     | 0.54              |
| 1:N:165:GLY:CA    | 1:O:35:THR:HG22   | 2.37                     | 0.54              |
| 3:2:108:PRO:HG3   | 3:ZC:60:THR:CG2   | 2.38                     | 0.54              |
| 3:3:184:LEU:HB3   | 3:3:192:TYR:HB3   | 1.90                     | 0.54              |
| 4:ZH:234:GLU:OE2  | 4:ZN:255:THR:CB   | 2.46                     | 0.54              |
| 4:ZJ:102:LEU:O    | 4:ZO:322:ASN:HB2  | 2.08                     | 0.54              |
| 4:ZV:112:GLN:HG2  | 4:ZV:331:ASP:HB3  | 1.89                     | 0.54              |
| 4:ZV:383:GLN:O    | 4:ZV:387:GLN:HG2  | 2.07                     | 0.54              |
| 5:AA:173:ARG:HD3  | 3:AF:46:TYR:CZ    | 2.42                     | 0.54              |
| 5:AB:16:LEU:CD2   | 3:AG:2:ILE:HD11   | 2.19                     | 0.54              |
| 5:AE:45:PRO:HD2   | 12:BF:37:PRO:HG3  | 1.89                     | 0.54              |
| 3:AG:187:ILE:HD11 | 3:AG:193:ILE:HD13 | 1.90                     | 0.54              |
| 3:AH:62:LEU:HD23  | 12:BD:83:PRO:HG2  | 1.90                     | 0.54              |
| 3:AI:188:GLY:O    | 3:AI:190:ASN:N    | 2.40                     | 0.54              |
| 3:AI:205:THR:HB   | 3:AI:208:LEU:HD12 | 1.89                     | 0.54              |
| 6:AT:264:ALA:HB2  | 6:AT:389:VAL:HG13 | 1.89                     | 0.54              |
| 6:AV:409:MET:HE2  | 6:AV:409:MET:HA   | 1.89                     | 0.54              |
| 6:AW:264:ALA:HB2  | 6:AW:389:VAL:HG13 | 1.89                     | 0.54              |
| 6:AW:409:MET:HE2  | 6:AW:409:MET:HA   | 1.89                     | 0.54              |
| 6:Ad:264:ALA:HB2  | 6:Ad:389:VAL:HG13 | 1.89                     | 0.54              |
| 9:Au:75:ARG:HD2   | 9:Au:84:PRO:HD2   | 1.89                     | 0.54              |
| 9:Ay:230:ASP:OD2  | 9:Ay:230:ASP:N    | 2.40                     | 0.54              |
| 2:s:273:CYS:CB    | 2:t:264:MET:O     | 2.42                     | 0.54              |
| 3:O:78:GLU:HG2    | 3:AJ:121:GLN:NE2  | 2.23                     | 0.54              |
| 3:2:231:VAL:O     | 3:2:235:GLN:HG3   | 2.08                     | 0.54              |
| 4:ZP:74:ASP:O     | 4:ZP:359:GLY:N    | 2.40                     | 0.54              |
| 4:ZP:93:PHE:HB3   | 4:ZP:333:VAL:HG13 | 1.90                     | 0.54              |
| 4:ZQ:102:LEU:HD21 | 4:ZQ:106:ARG:HA   | 1.90                     | 0.54              |
| 4:ZT:83:PHE:HB2   | 4:ZT:95:SER:O     | 2.08                     | 0.54              |
| 4:Zc:84:ARG:HD2   | 4:Zc:345:LEU:HD21 | 1.90                     | 0.54              |
| 4:Zc:382:TYR:CE1  | 4:Zh:395:ILE:HD11 | 2.42                     | 0.54              |
| 5:AC:18:GLN:NE2   | 5:AC:41:LEU:HG    | 2.22                     | 0.54              |
| 5:AC:72:ASP:CG    | 3:AN:9:LYS:NZ     | 2.66                     | 0.54              |
| 5:AE:180:ARG:HG3  | 5:AE:180:ARG:NH1  | 2.21                     | 0.54              |
| 6:AR:409:MET:HA   | 6:AR:409:MET:HE2  | 1.89                     | 0.54              |
| 6:Ad:409:MET:HE2  | 6:Ad:409:MET:HA   | 1.89                     | 0.54              |
| 6:Ah:282:TYR:HB3  | 6:Ai:292:THR:HG21 | 1.90                     | 0.54              |
| 6:Ah:409:MET:HE2  | 6:Ah:409:MET:HA   | 1.89                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:A9:115:LYS:HE2  | 12:BE:4:LEU:HD21  | 1.90                     | 0.54              |
| 11:A9:117:GLN:HE22 | 12:BD:125:MET:HG3 | 1.73                     | 0.54              |
| 6:WK:143:THR:OG1   | 6:WL:156:HIS:NE2  | 1.94                     | 0.54              |
| 2:c:208:ARG:O      | 2:c:212:SER:OG    | 2.16                     | 0.54              |
| 3:0:116:ARG:NH1    | 3:0:220:GLU:OE2   | 2.41                     | 0.54              |
| 3:3:128:LEU:HD12   | 3:3:140:ILE:HB    | 1.90                     | 0.54              |
| 3:6:175:LEU:HD21   | 3:6:214:LEU:HD21  | 1.89                     | 0.54              |
| 3:ZC:151:ILE:HG12  | 3:ZC:157:VAL:HG22 | 1.90                     | 0.54              |
| 4:ZH:399:LEU:O     | 4:ZH:400:VAL:C    | 2.51                     | 0.54              |
| 4:Za:10:LEU:HD21   | 4:Zf:399:LEU:HD11 | 1.90                     | 0.54              |
| 3:AF:140:ILE:HG23  | 3:AF:170:VAL:HG11 | 1.90                     | 0.54              |
| 3:AG:19:MET:HE1    | 3:AG:233:MET:HG2  | 1.90                     | 0.54              |
| 3:AG:153:ARG:HH12  | 3:AM:108:PRO:HG2  | 1.72                     | 0.54              |
| 3:AL:2:ILE:CG2     | 3:AL:254:LEU:HD11 | 2.37                     | 0.54              |
| 3:AM:254:LEU:O     | 3:AM:258:THR:HG23 | 2.08                     | 0.54              |
| 6:AR:292:THR:HG21  | 6:Aa:282:TYR:HB3  | 1.90                     | 0.54              |
| 6:AS:409:MET:HE2   | 6:AS:409:MET:HA   | 1.89                     | 0.54              |
| 6:Ac:282:TYR:HB3   | 6:Ad:292:THR:HG21 | 1.90                     | 0.54              |
| 6:Ag:264:ALA:HB2   | 6:Ag:389:VAL:HG13 | 1.89                     | 0.54              |
| 7:As:58:VAL:HB     | 9:Ay:207:LEU:HD21 | 1.89                     | 0.54              |
| 9:Aw:148:ALA:HB1   | 6:WB:165:PHE:HA   | 1.90                     | 0.54              |
| 10:A4:86:ILE:HD11  | 11:A9:133:VAL:CG2 | 2.38                     | 0.54              |
| 12:BE:57:GLN:O     | 12:BE:59:THR:N    | 2.40                     | 0.54              |
| 6:BW:282:TYR:HB3   | 6:BX:292:THR:HG21 | 1.90                     | 0.54              |
| 2:a:110:MET:O      | 2:b:84:VAL:CG2    | 2.54                     | 0.53              |
| 2:e:80:GLN:NE2     | 3:AL:106:MET:HE2  | 2.22                     | 0.53              |
| 2:l:78:ASN:ND2     | 5:AE:154:THR:HG21 | 2.22                     | 0.53              |
| 3:ZB:40:VAL:O      | 3:ZB:75:VAL:N     | 2.41                     | 0.53              |
| 3:ZE:208:LEU:O     | 3:ZE:210:GLY:N    | 2.40                     | 0.53              |
| 4:ZR:373:VAL:CG1   | 4:ZX:7:VAL:HG22   | 2.38                     | 0.53              |
| 4:ZU:180:LYS:HZ1   | 4:ZU:274:ASN:C    | 2.16                     | 0.53              |
| 4:Ze:99:GLN:HE22   | 4:Ze:111:MET:HG2  | 1.73                     | 0.53              |
| 4:Zf:397:ASN:O     | 4:Zf:398:THR:C    | 2.51                     | 0.53              |
| 5:AB:46:VAL:HG12   | 11:A7:93:PRO:HB2  | 1.89                     | 0.53              |
| 5:AB:53:THR:HB     | 11:A7:92:GLN:HE21 | 1.73                     | 0.53              |
| 5:AB:213:PRO:CD    | 3:AM:2:ILE:CD1    | 2.85                     | 0.53              |
| 5:AE:131:GLU:CB    | 3:AJ:179:MET:CE   | 2.84                     | 0.53              |
| 6:AR:282:TYR:HB3   | 6:Ac:292:THR:HG21 | 1.90                     | 0.53              |
| 6:Ad:282:TYR:HB3   | 6:Ae:292:THR:HG21 | 1.90                     | 0.53              |
| 6:Af:264:ALA:HB2   | 6:Af:389:VAL:HG13 | 1.89                     | 0.53              |
| 6:Af:282:TYR:HB3   | 6:Ag:292:THR:HG21 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Af:365:ASN:ND2  | 11:A8:65:LEU:HD13 | 2.23                     | 0.53              |
| 6:Ag:282:TYR:HB3  | 6:Ah:292:THR:HG21 | 1.90                     | 0.53              |
| 6:Ai:264:ALA:HB2  | 6:Ai:389:VAL:HG13 | 1.89                     | 0.53              |
| 6:Ak:264:ALA:HB2  | 6:Ak:389:VAL:HG13 | 1.89                     | 0.53              |
| 7:As:42:THR:HG22  | 7:As:44:ILE:HG12  | 1.90                     | 0.53              |
| 9:Ax:139:LEU:HG   | 9:Ax:170:LEU:HD21 | 1.90                     | 0.53              |
| 11:A8:91:ASP:OD1  | 12:BD:19:LYS:NZ   | 2.30                     | 0.53              |
| 6:UN:126:PHE:CD1  | 6:UN:130:VAL:CG2  | 2.90                     | 0.53              |
| 6:UP:126:PHE:CD1  | 6:UP:130:VAL:CG2  | 2.90                     | 0.53              |
| 6:WK:171:SER:HB3  | 6:WK:206:PRO:HG3  | 1.89                     | 0.53              |
| 6:WK:196:HIS:CG   | 6:WL:211:THR:HG21 | 2.42                     | 0.53              |
| 6:WW:145:GLU:HG2  | 6:WW:152:SER:HA   | 1.90                     | 0.53              |
| 6:BT:282:TYR:HB3  | 6:BU:292:THR:HG21 | 1.90                     | 0.53              |
| 2:a:54:GLN:O      | 2:b:79:MET:HA     | 2.09                     | 0.53              |
| 2:i:208:ARG:O     | 2:i:212:SER:OG    | 2.16                     | 0.53              |
| 3:0:2:ILE:HG21    | 5:AD:212:LYS:CG   | 2.38                     | 0.53              |
| 3:6:52:PRO:HB3    | 3:6:65:GLY:H      | 1.73                     | 0.53              |
| 3:ZB:120:PHE:HB3  | 3:ZB:128:LEU:HD22 | 1.90                     | 0.53              |
| 4:ZH:269:GLN:CB   | 4:ZN:286:PRO:HG2  | 2.38                     | 0.53              |
| 4:ZP:112:GLN:HG2  | 4:ZP:331:ASP:HB3  | 1.89                     | 0.53              |
| 4:ZY:16:ASN:HB2   | 4:ZY:39:PHE:HZ    | 1.72                     | 0.53              |
| 4:ZY:299:THR:HG22 | 4:ZY:314:GLN:HG3  | 1.88                     | 0.53              |
| 5:AB:70:GLN:HG2   | 3:AM:6:TRP:NE1    | 2.19                     | 0.53              |
| 5:AB:148:PRO:O    | 3:AG:210:GLY:HA2  | 2.08                     | 0.53              |
| 5:AC:115:ILE:HG22 | 5:AC:116:GLN:HG3  | 1.90                     | 0.53              |
| 5:AD:87:TRP:HB3   | 5:AD:99:TYR:HB3   | 1.90                     | 0.53              |
| 6:AW:303:GLN:NE2  | 6:BO:318:ASN:O    | 2.41                     | 0.53              |
| 6:AZ:264:ALA:HB2  | 6:AZ:389:VAL:HG13 | 1.89                     | 0.53              |
| 6:Ag:409:MET:HE2  | 6:Ag:409:MET:HA   | 1.89                     | 0.53              |
| 6:Aj:282:TYR:HB3  | 6:Ak:292:THR:HG21 | 1.90                     | 0.53              |
| 9:Ax:87:GLN:NE2   | 10:A2:98:GLU:OE2  | 2.39                     | 0.53              |
| 10:A4:10:VAL:HG12 | 6:BX:372:ILE:CD1  | 2.39                     | 0.53              |
| 10:A5:4:ILE:HD11  | 6:BS:374:HIS:HB2  | 1.90                     | 0.53              |
| 6:WF:193:ALA:HB1  | 6:WG:213:VAL:CG1  | 2.38                     | 0.53              |
| 6:WO:149:PRO:HB3  | 6:WO:184:ARG:HB3  | 1.90                     | 0.53              |
| 6:WS:145:GLU:HG2  | 6:WS:152:SER:HA   | 1.91                     | 0.53              |
| 6:BR:282:TYR:HB3  | 6:BS:292:THR:HG21 | 1.90                     | 0.53              |
| 2:a:79:MET:HA     | 2:z:54:GLN:O      | 2.09                     | 0.53              |
| 2:b:54:GLN:O      | 2:c:79:MET:HA     | 2.09                     | 0.53              |
| 2:c:54:GLN:O      | 2:d:79:MET:HA     | 2.09                     | 0.53              |
| 2:m:54:GLN:O      | 2:n:79:MET:HA     | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:t:93:TYR:OH     | 2:t:173:ARG:O     | 2.25                     | 0.53              |
| 3:1:19:MET:HB2    | 3:1:236:VAL:HG11  | 1.91                     | 0.53              |
| 3:5:174:ASN:ND2   | 3:5:203:GLU:OE2   | 2.36                     | 0.53              |
| 4:ZJ:370:LYS:CE   | 4:ZP:11:ASN:ND2   | 2.69                     | 0.53              |
| 4:ZU:293:GLN:NE2  | 4:ZU:303:ASN:HD21 | 2.07                     | 0.53              |
| 4:ZV:3:PHE:O      | 4:ZV:7:VAL:HG23   | 2.09                     | 0.53              |
| 4:ZW:33:LYS:NZ    | 4:ZW:362:GLU:OE1  | 2.42                     | 0.53              |
| 4:ZY:17:LEU:HD13  | 4:Zd:395:ILE:HD11 | 1.90                     | 0.53              |
| 4:Ze:397:ASN:O    | 4:Ze:398:THR:C    | 2.48                     | 0.53              |
| 6:Ah:264:ALA:HB2  | 6:Ah:389:VAL:HG13 | 1.89                     | 0.53              |
| 6:Ai:282:TYR:HB3  | 6:Aj:292:THR:HG21 | 1.90                     | 0.53              |
| 9:Aw:39:SER:OG    | 10:A3:49:GLN:OE1  | 2.16                     | 0.53              |
| 6:WE:196:HIS:HB3  | 6:WF:211:THR:HG21 | 1.90                     | 0.53              |
| 6:WE:200:SER:O    | 6:WF:158:ALA:HB2  | 2.09                     | 0.53              |
| 6:WU:145:GLU:HG2  | 6:WU:152:SER:HA   | 1.91                     | 0.53              |
| 2:d:54:GLN:O      | 2:e:79:MET:HA     | 2.09                     | 0.53              |
| 2:n:54:GLN:O      | 2:o:79:MET:HA     | 2.09                     | 0.53              |
| 3:0:195:THR:HG23  | 5:AD:152:PRO:CB   | 2.38                     | 0.53              |
| 3:2:238:ARG:HG3   | 3:8:254:LEU:HD13  | 1.90                     | 0.53              |
| 3:3:226:VAL:HG23  | 3:ZE:1:MET:O      | 2.08                     | 0.53              |
| 3:3:238:ARG:HH21  | 3:9:251:ASP:CG    | 2.14                     | 0.53              |
| 3:6:44:LEU:HD22   | 3:AJ:86:LEU:HD12  | 1.89                     | 0.53              |
| 3:6:57:SER:O      | 3:6:59:GLN:N      | 2.35                     | 0.53              |
| 3:9:22:ILE:HG21   | 3:9:233:MET:HG3   | 1.90                     | 0.53              |
| 3:ZD:31:THR:CG2   | 4:ZI:39:PHE:HB2   | 2.35                     | 0.53              |
| 4:ZG:150:THR:OG1  | 4:ZG:282:ASN:ND2  | 2.38                     | 0.53              |
| 4:ZH:17:LEU:HD13  | 4:ZM:395:ILE:HD11 | 1.90                     | 0.53              |
| 4:ZT:158:LEU:HB2  | 4:ZT:268:GLN:HG3  | 1.90                     | 0.53              |
| 4:Zh:5:GLN:HG2    | 4:Zh:6:ALA:N      | 2.23                     | 0.53              |
| 5:AE:45:PRO:HD3   | 12:BF:37:PRO:HG3  | 1.90                     | 0.53              |
| 3:AM:2:ILE:HG22   | 3:AM:4:SER:H      | 1.73                     | 0.53              |
| 6:AT:409:MET:HE2  | 6:AT:409:MET:HA   | 1.89                     | 0.53              |
| 6:AX:409:MET:HA   | 6:AX:409:MET:HE2  | 1.89                     | 0.53              |
| 8:At:127:ARG:O    | 8:At:131:MET:HE3  | 2.08                     | 0.53              |
| 9:Au:179:LEU:HD22 | 9:Av:84:PRO:HG3   | 1.90                     | 0.53              |
| 9:Aw:168:ARG:O    | 9:Ax:99:PHE:HZ    | 1.91                     | 0.53              |
| 10:A4:68:LEU:CD2  | 12:BE:126:MET:HE2 | 2.36                     | 0.53              |
| 11:A6:10:ARG:NH1  | 11:A6:53:MET:HE3  | 2.24                     | 0.53              |
| 6:WA:200:SER:O    | 6:WB:158:ALA:HB2  | 2.08                     | 0.53              |
| 6:WJ:190:GLN:NE2  | 6:WK:216:SER:O    | 2.42                     | 0.53              |
| 6:WP:145:GLU:HG2  | 6:WP:152:SER:HA   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WQ:212:LEU:HB3  | 6:WQ:221:THR:HG23  | 1.90                     | 0.53              |
| 6:WT:145:GLU:HG2  | 6:WT:152:SER:HA    | 1.91                     | 0.53              |
| 12:BC:68:ILE:HD11 | 6:BL:312:VAL:CG2   | 2.38                     | 0.53              |
| 6:BW:264:ALA:HB2  | 6:BW:389:VAL:HG13  | 1.89                     | 0.53              |
| 2:a:273:CYS:CB    | 2:b:264:MET:O      | 2.42                     | 0.53              |
| 3:3:145:ASN:O     | 3:3:161:GLN:NE2    | 2.42                     | 0.53              |
| 3:4:78:GLU:OE1    | 3:AN:121:GLN:NE2   | 2.41                     | 0.53              |
| 3:ZA:97:ILE:HD12  | 3:ZA:116:ARG:HG3   | 1.91                     | 0.53              |
| 4:ZH:390:LYS:HB2  | 4:ZM:402:LEU:CD2   | 2.37                     | 0.53              |
| 4:ZL:382:TYR:CE1  | 4:ZQ:395:ILE:HG23  | 2.44                     | 0.53              |
| 4:ZP:396:LEU:O    | 4:ZP:400:VAL:HG23  | 2.09                     | 0.53              |
| 4:ZS:181:LYS:HD3  | 4:Zd:129:GLN:NE2   | 2.24                     | 0.53              |
| 4:ZS:367:ASP:O    | 4:ZS:371:GLU:HG2   | 2.09                     | 0.53              |
| 4:ZV:34:SER:HB3   | 4:ZV:366:VAL:HG12  | 1.91                     | 0.53              |
| 4:ZV:387:GLN:NE2  | 4:Zb:400:VAL:O     | 2.41                     | 0.53              |
| 4:Zf:111:MET:HA   | 4:Zf:111:MET:HE3   | 1.90                     | 0.53              |
| 4:Zg:157:ASN:HB3  | 4:Zg:271:THR:HG21  | 1.90                     | 0.53              |
| 6:AZ:282:TYR:HB3  | 6:Aa:292:THR:HG21  | 1.90                     | 0.53              |
| 6:Ac:264:ALA:HB2  | 6:Ac:389:VAL:HG13  | 1.89                     | 0.53              |
| 6:Ae:282:TYR:HB3  | 6:Af:292:THR:HG21  | 1.90                     | 0.53              |
| 6:Aj:264:ALA:HB2  | 6:Aj:389:VAL:HG13  | 1.89                     | 0.53              |
| 6:AO:282:TYR:HB3  | 6:AP:292:THR:HG21  | 1.90                     | 0.53              |
| 9:Au:60:MET:CE    | 9:Av:91:GLY:HA3    | 2.38                     | 0.53              |
| 6:WB:145:GLU:HG2  | 6:WB:152:SER:HA    | 1.91                     | 0.53              |
| 6:WI:145:GLU:O    | 6:WI:147:LEU:N     | 2.41                     | 0.53              |
| 6:WQ:145:GLU:HG2  | 6:WQ:152:SER:HA    | 1.91                     | 0.53              |
| 6:WU:114:GLU:O    | 6:WU:117:ASP:N     | 2.41                     | 0.53              |
| 6:WV:193:ALA:HB1  | 6:WW:213:VAL:HG11  | 1.91                     | 0.53              |
| 12:BD:10:ALA:HB3  | 12:BD:119:LEU:HD13 | 1.90                     | 0.53              |
| 6:BU:282:TYR:HB3  | 6:BV:292:THR:HG21  | 1.90                     | 0.53              |
| 2:l:54:GLN:O      | 2:m:79:MET:HA      | 2.09                     | 0.53              |
| 2:r:54:GLN:O      | 2:s:79:MET:HA      | 2.09                     | 0.53              |
| 2:y:54:GLN:O      | 2:z:79:MET:HA      | 2.09                     | 0.53              |
| 2:y:208:ARG:O     | 2:y:212:SER:OG     | 2.16                     | 0.53              |
| 3:3:57:SER:HA     | 5:AB:140:ASP:CG    | 2.34                     | 0.53              |
| 3:ZC:28:ASN:OD1   | 4:ZH:52:VAL:CB     | 2.56                     | 0.53              |
| 3:ZD:47:GLN:N     | 3:ZD:68:ILE:O      | 2.41                     | 0.53              |
| 3:ZE:85:ASN:HD22  | 4:ZP:4:SER:HB2     | 1.73                     | 0.53              |
| 4:ZL:57:ILE:HD13  | 4:ZQ:47:LYS:HB3    | 1.89                     | 0.53              |
| 4:ZQ:112:GLN:NE2  | 4:ZQ:331:ASP:HB3   | 2.24                     | 0.53              |
| 4:ZR:200:PHE:CE2  | 4:ZR:263:PHE:HE1   | 2.26                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZT:29:THR:O     | 4:ZT:30:TYR:C     | 2.52                     | 0.53              |
| 4:Zd:397:ASN:C    | 4:Zd:399:LEU:N    | 2.63                     | 0.53              |
| 5:AA:53:THR:HB    | 12:BB:23:VAL:HG23 | 1.90                     | 0.53              |
| 5:AC:216:ALA:O    | 5:AC:220:MET:HG3  | 2.08                     | 0.53              |
| 3:AF:79:ARG:HH21  | 3:AF:186:SER:HG   | 1.56                     | 0.53              |
| 6:AV:357:SER:CB   | 6:BO:318:ASN:HD21 | 2.22                     | 0.53              |
| 6:AX:372:ILE:CG2  | 10:A3:11:ILE:CG2  | 2.87                     | 0.53              |
| 6:Ac:409:MET:HA   | 6:Ac:409:MET:HE2  | 1.89                     | 0.53              |
| 6:Ad:372:ILE:HG22 | 10:A2:11:ILE:HG21 | 1.91                     | 0.53              |
| 6:Af:409:MET:HA   | 6:Af:409:MET:HE2  | 1.89                     | 0.53              |
| 6:Ak:282:TYR:HB3  | 6:Al:292:THR:HG21 | 1.90                     | 0.53              |
| 6:Al:295:SER:HB2  | 11:A7:65:LEU:HB3  | 1.90                     | 0.53              |
| 9:Au:207:LEU:HD23 | 9:Au:209:MET:HE1  | 1.91                     | 0.53              |
| 10:A2:68:LEU:CD1  | 11:A7:118:MET:SD  | 2.96                     | 0.53              |
| 6:UP:80:ALA:HB3   | 6:UP:83:SER:HB3   | 1.91                     | 0.53              |
| 6:UP:88:VAL:HB    | 6:UP:89:PRO:HD2   | 1.90                     | 0.53              |
| 6:WS:118:GLN:O    | 6:WS:119:GLU:C    | 2.49                     | 0.53              |
| 6:WS:186:LEU:HA   | 6:WS:190:GLN:OE1  | 2.08                     | 0.53              |
| 6:WU:113:PHE:HB3  | 6:WV:134:ARG:CZ   | 2.39                     | 0.53              |
| 12:BC:47:VAL:O    | 6:BL:313:PRO:HD2  | 2.07                     | 0.53              |
| 2:c:78:ASN:HD22   | 3:AG:145:ASN:ND2  | 2.02                     | 0.53              |
| 2:r:273:CYS:CB    | 2:s:264:MET:O     | 2.42                     | 0.53              |
| 2:s:54:GLN:O      | 2:t:79:MET:HA     | 2.09                     | 0.53              |
| 3:0:1:MET:HE3     | 5:AD:29:ALA:HB1   | 1.91                     | 0.53              |
| 3:1:115:THR:HB    | 3:1:191:LEU:HD23  | 1.91                     | 0.53              |
| 3:ZB:147:LEU:HD23 | 4:ZG:352:ASN:OD1  | 2.08                     | 0.53              |
| 3:ZC:240:TYR:HE2  | 4:ZH:399:LEU:CD1  | 2.22                     | 0.53              |
| 4:ZL:355:LYS:NZ   | 4:ZR:89:ASN:HD21  | 2.06                     | 0.53              |
| 4:ZO:288:ASP:OD1  | 4:ZO:289:LEU:N    | 2.41                     | 0.53              |
| 4:ZO:374:ASN:O    | 4:ZO:377:VAL:N    | 2.42                     | 0.53              |
| 4:ZR:295:ASN:ND2  | 4:ZR:299:THR:OG1  | 2.38                     | 0.53              |
| 5:AE:42:ARG:HG3   | 5:AE:58:THR:HG23  | 1.91                     | 0.53              |
| 6:AS:282:TYR:HB3  | 6:AT:292:THR:HG21 | 1.90                     | 0.53              |
| 6:AZ:409:MET:HE2  | 6:AZ:409:MET:HA   | 1.89                     | 0.53              |
| 6:Ac:293:LEU:HD21 | 6:Ac:364:SER:HB3  | 1.91                     | 0.53              |
| 6:Aj:372:ILE:CD1  | 10:A1:11:ILE:CG2  | 2.55                     | 0.53              |
| 6:AP:282:TYR:HB3  | 6:AQ:292:THR:HG21 | 1.90                     | 0.53              |
| 10:A2:8:GLU:O     | 10:A2:11:ILE:HG13 | 2.09                     | 0.53              |
| 6:UK:207:PRO:HD2  | 6:WE:187:ASP:OD1  | 1.98                     | 0.53              |
| 6:UN:80:ALA:HB3   | 6:UN:83:SER:HB3   | 1.90                     | 0.53              |
| 6:UN:159:MET:SD   | 6:UN:159:MET:N    | 2.82                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UP:159:MET:SD   | 6:UP:159:MET:N    | 2.82                     | 0.53              |
| 6:WK:145:GLU:HG2  | 6:WK:152:SER:HA   | 1.91                     | 0.53              |
| 6:WR:145:GLU:HG2  | 6:WR:152:SER:HA   | 1.91                     | 0.53              |
| 6:WV:145:GLU:HG2  | 6:WV:152:SER:HA   | 1.91                     | 0.53              |
| 12:BE:28:LEU:HD21 | 12:BE:101:GLU:HB2 | 1.91                     | 0.53              |
| 2:e:54:GLN:O      | 2:f:79:MET:HA     | 2.09                     | 0.53              |
| 2:h:54:GLN:O      | 2:i:79:MET:HA     | 2.09                     | 0.53              |
| 2:x:54:GLN:O      | 2:y:79:MET:HA     | 2.09                     | 0.53              |
| 3:5:241:GLU:HG2   | 3:ZA:256:LYS:CE   | 2.32                     | 0.53              |
| 3:7:49:ILE:HG21   | 3:7:66:LEU:HD23   | 1.91                     | 0.53              |
| 4:ZF:84:ARG:NH1   | 4:ZF:134:PRO:HB2  | 2.23                     | 0.53              |
| 4:ZL:18:ASP:CB    | 4:ZQ:5:GLN:NE2    | 2.72                     | 0.53              |
| 4:ZO:156:ILE:HG13 | 4:ZO:276:ILE:HA   | 1.90                     | 0.53              |
| 4:ZW:112:GLN:OE1  | 4:ZW:112:GLN:N    | 2.42                     | 0.53              |
| 4:Za:24:ILE:HG21  | 4:Zf:384:SER:OG   | 2.08                     | 0.53              |
| 4:Ze:137:ILE:HG21 | 4:Ze:300:VAL:HG21 | 1.90                     | 0.53              |
| 5:AA:70:GLN:HG3   | 3:AL:3:SER:HA     | 0.62                     | 0.53              |
| 3:AF:9:LYS:CE     | 12:BF:100:GLY:HA2 | 2.35                     | 0.53              |
| 3:AK:80:LEU:O     | 3:AK:223:ASN:ND2  | 2.42                     | 0.53              |
| 6:AS:293:LEU:HD21 | 6:AS:364:SER:HB3  | 1.91                     | 0.53              |
| 6:Aa:293:LEU:HD21 | 6:Aa:364:SER:HB3  | 1.91                     | 0.53              |
| 6:Am:264:ALA:HB2  | 6:Am:389:VAL:HG13 | 1.89                     | 0.53              |
| 10:A5:87:GLN:HG2  | 12:BA:130:LEU:O   | 2.08                     | 0.53              |
| 6:UK:207:PRO:CG   | 6:WE:187:ASP:OD2  | 2.57                     | 0.53              |
| 6:WA:145:GLU:HG2  | 6:WA:152:SER:HA   | 1.91                     | 0.53              |
| 6:WF:116:LEU:HD21 | 6:WF:134:ARG:CZ   | 2.38                     | 0.53              |
| 6:WP:200:SER:O    | 6:WQ:158:ALA:HB3  | 2.09                     | 0.53              |
| 6:WU:160:PRO:HG2  | 6:WU:170:LYS:O    | 2.08                     | 0.53              |
| 6:BW:293:LEU:HD21 | 6:BW:364:SER:HB3  | 1.91                     | 0.53              |
| 2:g:54:GLN:O      | 2:h:79:MET:HA     | 2.09                     | 0.53              |
| 2:i:54:GLN:O      | 2:j:79:MET:HA     | 2.09                     | 0.53              |
| 2:q:54:GLN:O      | 2:r:79:MET:HA     | 2.09                     | 0.53              |
| 3:7:256:LYS:HD2   | 3:7:256:LYS:O     | 2.08                     | 0.53              |
| 3:ZB:122:VAL:HG23 | 4:ZG:321:ALA:O    | 2.09                     | 0.53              |
| 4:ZF:288:ASP:OD2  | 4:ZF:288:ASP:N    | 2.40                     | 0.53              |
| 4:ZI:190:GLN:OE1  | 4:ZI:192:ASN:ND2  | 2.36                     | 0.53              |
| 4:ZO:148:SER:HA   | 4:ZO:187:TYR:O    | 2.08                     | 0.53              |
| 4:ZU:328:SER:HB3  | 4:ZZ:43:PHE:CD2   | 2.43                     | 0.53              |
| 4:ZV:128:ILE:HD12 | 4:ZV:314:GLN:HB2  | 1.90                     | 0.53              |
| 4:ZY:106:ARG:HH12 | 4:ZY:141:ASN:HB3  | 1.74                     | 0.53              |
| 4:ZZ:269:GLN:CD   | 4:Zf:146:ALA:HB2  | 2.33                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AA:76:ARG:HB3   | 5:AA:79:ASP:OD1   | 2.09                     | 0.53              |
| 5:AB:137:ILE:HG12 | 5:AB:143:ILE:HG12 | 1.91                     | 0.53              |
| 5:AC:91:GLN:HB3   | 5:AC:119:PRO:HG2  | 1.89                     | 0.53              |
| 5:AD:27:ALA:HB1   | 3:AI:72:VAL:CG1   | 2.39                     | 0.53              |
| 5:AE:26:LEU:HD22  | 3:AJ:242:ILE:HG12 | 1.91                     | 0.53              |
| 5:AE:214:VAL:HG13 | 3:AK:12:LEU:CD1   | 2.38                     | 0.53              |
| 3:AN:43:ASP:N     | 3:AN:43:ASP:OD1   | 2.41                     | 0.53              |
| 6:AT:282:TYR:HB3  | 6:AU:292:THR:HG21 | 1.90                     | 0.53              |
| 6:AX:282:TYR:HB3  | 6:AY:292:THR:HG21 | 1.90                     | 0.53              |
| 6:AY:282:TYR:HB3  | 6:AZ:292:THR:HG21 | 1.91                     | 0.53              |
| 6:Ae:264:ALA:HB2  | 6:Ae:389:VAL:HG13 | 1.89                     | 0.53              |
| 6:Al:282:TYR:HB3  | 6:Am:292:THR:HG21 | 1.90                     | 0.53              |
| 11:A8:46:ALA:O    | 11:A8:50:LYS:HG3  | 2.09                     | 0.53              |
| 2:t:54:GLN:O      | 2:u:79:MET:HA     | 2.09                     | 0.53              |
| 3:3:167:PRO:HD3   | 3:ZE:196:GLN:HB3  | 1.90                     | 0.53              |
| 3:ZE:19:MET:HE3   | 4:ZJ:395:ILE:CD1  | 2.39                     | 0.53              |
| 4:ZG:217:ASP:HB3  | 4:ZG:220:ALA:HB2  | 1.90                     | 0.53              |
| 4:ZH:382:TYR:CE1  | 4:ZM:395:ILE:HG23 | 2.44                     | 0.53              |
| 4:ZJ:151:THR:OG1  | 4:ZJ:282:ASN:ND2  | 2.42                     | 0.53              |
| 4:ZO:201:VAL:HG23 | 4:ZO:209:ALA:HB3  | 1.91                     | 0.53              |
| 4:ZU:160:SER:HA   | 4:ZU:268:GLN:HE21 | 1.74                     | 0.53              |
| 4:ZX:331:ASP:O    | 4:ZX:333:VAL:HG23 | 2.08                     | 0.53              |
| 4:Zc:10:LEU:HD22  | 4:Zc:389:ILE:HD12 | 1.91                     | 0.53              |
| 5:AA:107:VAL:HG12 | 5:AA:113:LEU:HD23 | 1.91                     | 0.53              |
| 5:AC:152:PRO:HG2  | 3:AN:193:ILE:HD12 | 1.91                     | 0.53              |
| 5:AC:220:MET:HE3  | 3:AH:245:LYS:CD   | 2.38                     | 0.53              |
| 5:AE:175:ASP:OD1  | 3:AJ:67:GLN:NE2   | 2.42                     | 0.53              |
| 6:AR:293:LEU:HD21 | 6:AR:364:SER:HB3  | 1.91                     | 0.53              |
| 6:Ao:282:TYR:HB3  | 6:Ap:292:THR:HG21 | 1.90                     | 0.53              |
| 6:AQ:282:TYR:HB3  | 6:BR:292:THR:HG21 | 1.90                     | 0.53              |
| 9:Au:153:LEU:HD23 | 6:WR:165:PHE:CE2  | 2.44                     | 0.53              |
| 9:Aw:153:LEU:HD22 | 9:Ax:99:PHE:HB3   | 1.90                     | 0.53              |
| 9:Ax:153:LEU:HD21 | 6:WG:165:PHE:CE2  | 2.44                     | 0.53              |
| 9:Ax:214:PRO:HD2  | 9:Ay:211:MET:O    | 2.09                     | 0.53              |
| 10:A5:61:LEU:CD2  | 11:A0:50:LYS:HZ3  | 2.22                     | 0.53              |
| 6:UJ:127:SER:O    | 6:UJ:131:ASN:CG   | 2.52                     | 0.53              |
| 6:UN:98:LEU:CD1   | 6:UN:146:THR:HG1  | 2.22                     | 0.53              |
| 6:UO:80:ALA:HB3   | 6:UO:83:SER:HB3   | 1.91                     | 0.53              |
| 6:WD:168:GLU:CD   | 6:WD:170:LYS:NZ   | 2.67                     | 0.53              |
| 6:WO:145:GLU:HG2  | 6:WO:152:SER:HA   | 1.91                     | 0.53              |
| 6:WT:161:LYS:HB3  | 6:WT:162:PRO:HD2  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WV:142:ARG:O    | 6:WV:146:THR:HG23 | 2.09                     | 0.53              |
| 6:BU:293:LEU:HD21 | 6:BU:364:SER:HB3  | 1.91                     | 0.53              |
| 6:BV:282:TYR:HB3  | 6:BW:292:THR:HG21 | 1.90                     | 0.53              |
| 2:j:54:GLN:O      | 2:k:79:MET:HA     | 2.09                     | 0.52              |
| 3:1:257:LEU:CD2   | 5:AE:213:PRO:HB2  | 2.39                     | 0.52              |
| 3:1:260:LEU:HD21  | 5:AE:221:ILE:CD1  | 2.39                     | 0.52              |
| 3:6:1:MET:HB2     | 3:AJ:29:VAL:CG1   | 2.40                     | 0.52              |
| 3:8:257:LEU:HD21  | 3:AL:227:ALA:HA   | 1.90                     | 0.52              |
| 3:ZC:5:LEU:O      | 3:ZC:9:LYS:HG3    | 2.09                     | 0.52              |
| 3:ZD:158:SER:HB3  | 3:ZD:167:PRO:HB2  | 1.91                     | 0.52              |
| 3:ZE:167:PRO:CG   | 4:ZP:338:GLN:NE2  | 2.71                     | 0.52              |
| 4:ZH:10:LEU:HD21  | 4:ZM:399:LEU:HD11 | 1.90                     | 0.52              |
| 4:ZR:44:ALA:HB3   | 4:ZR:50:LEU:HD12  | 1.91                     | 0.52              |
| 4:ZU:77:ILE:HG13  | 4:ZU:96:ARG:HH21  | 1.75                     | 0.52              |
| 4:ZX:18:ASP:HB3   | 4:Zc:5:GLN:HE22   | 1.74                     | 0.52              |
| 4:ZZ:33:LYS:NZ    | 4:ZZ:362:GLU:OE1  | 2.42                     | 0.52              |
| 4:Zh:2:SER:C      | 4:Zh:392:GLN:HE22 | 2.17                     | 0.52              |
| 3:AF:19:MET:HE1   | 3:AF:233:MET:HE2  | 1.90                     | 0.52              |
| 3:AG:199:GLY:O    | 3:AG:200:ALA:C    | 2.52                     | 0.52              |
| 3:AH:50:ARG:HD2   | 6:BM:328:ILE:HD13 | 1.91                     | 0.52              |
| 3:AH:127:GLN:H    | 3:AH:141:THR:HG23 | 1.74                     | 0.52              |
| 3:AN:3:SER:O      | 3:AN:7:ILE:HG13   | 2.09                     | 0.52              |
| 6:AU:293:LEU:HD21 | 6:AU:364:SER:HB3  | 1.91                     | 0.52              |
| 6:AZ:293:LEU:HD21 | 6:AZ:364:SER:HB3  | 1.91                     | 0.52              |
| 7:Ab:54:LYS:CD    | 9:Av:207:LEU:HD23 | 2.39                     | 0.52              |
| 7:Ab:89:GLY:CA    | 6:WS:165:PHE:CE1  | 2.89                     | 0.52              |
| 6:Ae:409:MET:HE2  | 6:Ae:409:MET:HA   | 1.89                     | 0.52              |
| 8:At:227:MET:SD   | 8:At:228:LEU:N    | 2.82                     | 0.52              |
| 6:UL:159:MET:SD   | 6:UL:159:MET:N    | 2.82                     | 0.52              |
| 6:WC:145:GLU:HG2  | 6:WC:152:SER:HA   | 1.91                     | 0.52              |
| 6:WP:166:VAL:HA   | 6:WP:169:GLN:HB2  | 1.91                     | 0.52              |
| 6:BV:293:LEU:HD21 | 6:BV:364:SER:HB3  | 1.91                     | 0.52              |
| 2:f:54:GLN:O      | 2:g:79:MET:HA     | 2.09                     | 0.52              |
| 2:o:54:GLN:O      | 2:p:79:MET:HA     | 2.09                     | 0.52              |
| 4:ZK:146:ALA:HB2  | 4:ZK:286:PRO:HD3  | 1.91                     | 0.52              |
| 4:ZN:269:GLN:HE21 | 4:ZT:146:ALA:HB3  | 1.73                     | 0.52              |
| 4:ZR:83:PHE:HB2   | 4:ZR:95:SER:O     | 2.10                     | 0.52              |
| 4:ZT:196:MET:HA   | 4:ZT:196:MET:HE3  | 1.90                     | 0.52              |
| 4:Za:188:ASP:OD1  | 4:Za:192:ASN:N    | 2.42                     | 0.52              |
| 4:Zb:233:ASN:HD21 | 4:Zb:237:ILE:HB   | 1.74                     | 0.52              |
| 5:AA:213:PRO:HG3  | 3:AL:1:MET:CE     | 2.38                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AE:173:ARG:CD   | 3:AJ:46:TYR:CE1   | 2.92                     | 0.52              |
| 6:AV:293:LEU:HD21 | 6:AV:364:SER:HB3  | 1.91                     | 0.52              |
| 6:AW:282:TYR:HB3  | 6:AX:292:THR:HG21 | 1.90                     | 0.52              |
| 6:AX:293:LEU:HD21 | 6:AX:364:SER:HB3  | 1.91                     | 0.52              |
| 6:Ae:293:LEU:HD21 | 6:Ae:364:SER:HB3  | 1.91                     | 0.52              |
| 9:Av:59:LEU:O     | 9:Av:65:THR:OG1   | 2.21                     | 0.52              |
| 9:Ay:144:GLU:O    | 9:Ay:145:ALA:C    | 2.53                     | 0.52              |
| 6:UI:80:ALA:HB3   | 6:UI:83:SER:HB3   | 1.91                     | 0.52              |
| 6:UJ:80:ALA:HB3   | 6:UJ:83:SER:HB3   | 1.91                     | 0.52              |
| 6:UK:159:MET:N    | 6:UK:159:MET:SD   | 2.82                     | 0.52              |
| 6:UL:88:VAL:HB    | 6:UL:89:PRO:HD2   | 1.90                     | 0.52              |
| 6:WU:186:LEU:HA   | 6:WU:190:GLN:OE1  | 2.10                     | 0.52              |
| 6:BT:293:LEU:HD21 | 6:BT:364:SER:HB3  | 1.91                     | 0.52              |
| 6:BX:293:LEU:HD21 | 6:BX:364:SER:HB3  | 1.91                     | 0.52              |
| 2:j:273:CYS:CB    | 2:k:264:MET:O     | 2.42                     | 0.52              |
| 2:k:54:GLN:O      | 2:l:79:MET:HA     | 2.09                     | 0.52              |
| 2:w:54:GLN:O      | 2:x:79:MET:HA     | 2.09                     | 0.52              |
| 3:1:79:ARG:NH2    | 3:1:184:LEU:O     | 2.43                     | 0.52              |
| 3:3:242:ILE:HD12  | 3:9:1:MET:HE1     | 1.90                     | 0.52              |
| 4:ZF:54:VAL:O     | 4:ZF:55:ALA:C     | 2.52                     | 0.52              |
| 4:ZG:382:TYR:HE1  | 4:ZL:399:LEU:HD11 | 1.74                     | 0.52              |
| 4:ZL:26:ASN:ND2   | 4:ZQ:52:VAL:HG22  | 2.24                     | 0.52              |
| 4:ZS:369:SER:HA   | 4:Zd:399:LEU:CD1  | 2.40                     | 0.52              |
| 4:ZU:159:ASN:N    | 4:ZU:274:ASN:OD1  | 2.32                     | 0.52              |
| 4:ZV:180:LYS:HD3  | 4:ZV:274:ASN:HB3  | 1.91                     | 0.52              |
| 4:ZV:379:GLN:NE2  | 4:Za:394:GLN:OE1  | 2.42                     | 0.52              |
| 4:ZX:42:MET:HG2   | 4:ZX:53:LYS:HE3   | 1.91                     | 0.52              |
| 4:Zd:281:GLN:NE2  | 4:Zd:283:GLY:O    | 2.39                     | 0.52              |
| 4:Zd:397:ASN:O    | 4:Zd:399:LEU:N    | 2.43                     | 0.52              |
| 4:Ze:165:PRO:HG2  | 4:Ze:201:VAL:HG13 | 1.91                     | 0.52              |
| 6:AT:293:LEU:HD21 | 6:AT:364:SER:HB3  | 1.91                     | 0.52              |
| 6:AU:409:MET:HA   | 6:AU:409:MET:HE2  | 1.89                     | 0.52              |
| 9:Aw:232:TRP:O    | 9:Aw:236:MET:HG3  | 2.09                     | 0.52              |
| 9:Ax:143:ARG:NH1  | 6:WD:165:PHE:CE1  | 2.77                     | 0.52              |
| 9:Ay:66:ARG:HG2   | 9:Ay:243:PHE:CZ   | 2.44                     | 0.52              |
| 9:Ay:68:ILE:HG23  | 9:Ay:69:ILE:N     | 2.24                     | 0.52              |
| 6:UK:88:VAL:HB    | 6:UK:89:PRO:HD2   | 1.90                     | 0.52              |
| 6:UL:80:ALA:HB3   | 6:UL:83:SER:HB3   | 1.90                     | 0.52              |
| 6:UN:127:SER:O    | 6:UN:131:ASN:CG   | 2.52                     | 0.52              |
| 6:WM:145:GLU:HG2  | 6:WM:152:SER:HA   | 1.91                     | 0.52              |
| 6:WQ:145:GLU:O    | 6:WQ:147:LEU:N    | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WQ:168:GLU:O    | 6:WQ:169:GLN:C    | 2.52                     | 0.52              |
| 12:BC:47:VAL:O    | 6:BL:313:PRO:CD   | 2.57                     | 0.52              |
| 2:o:208:ARG:O     | 2:o:212:SER:OG    | 2.16                     | 0.52              |
| 3:2:1:MET:HB3     | 3:AF:29:VAL:CG1   | 2.39                     | 0.52              |
| 3:2:208:LEU:O     | 3:2:210:GLY:N     | 2.42                     | 0.52              |
| 3:3:238:ARG:CZ    | 3:9:251:ASP:OD2   | 2.57                     | 0.52              |
| 4:ZG:109:VAL:HG12 | 4:ZG:115:GLN:HA   | 1.90                     | 0.52              |
| 4:ZU:170:PHE:HE2  | 4:ZU:223:PRO:HG2  | 1.73                     | 0.52              |
| 4:ZW:181:LYS:HZ3  | 4:Zh:129:GLN:HE21 | 1.55                     | 0.52              |
| 4:ZY:230:LEU:HD21 | 4:ZY:263:PHE:HD2  | 1.74                     | 0.52              |
| 5:AC:21:VAL:CG2   | 3:AH:68:ILE:CG2   | 2.71                     | 0.52              |
| 5:AD:241:GLU:CD   | 11:A9:106:ARG:NH2 | 2.66                     | 0.52              |
| 5:AE:115:ILE:HD12 | 5:AE:120:VAL:HG22 | 1.91                     | 0.52              |
| 3:AJ:143:PRO:HG2  | 3:AJ:161:GLN:HE22 | 1.73                     | 0.52              |
| 6:AV:282:TYR:HB3  | 6:AW:292:THR:HG21 | 1.90                     | 0.52              |
| 9:Aw:80:THR:O     | 9:Aw:80:THR:OG1   | 2.26                     | 0.52              |
| 9:Ax:180:LYS:O    | 9:Ax:184:GLN:HG3  | 2.09                     | 0.52              |
| 10:Az:77:LYS:O    | 10:Az:80:VAL:N    | 2.42                     | 0.52              |
| 6:UL:127:SER:O    | 6:UL:131:ASN:CG   | 2.52                     | 0.52              |
| 12:BF:120:ASN:O   | 12:BF:123:LYS:HG2 | 2.08                     | 0.52              |
| 6:BS:293:LEU:HD21 | 6:BS:364:SER:HB3  | 1.91                     | 0.52              |
| 2:n:80:GLN:CD     | 3:AJ:137:GLN:HG3  | 2.34                     | 0.52              |
| 2:x:196:MET:SD    | 2:x:247:THR:HG22  | 2.50                     | 0.52              |
| 3:0:127:GLN:HA    | 3:0:140:ILE:O     | 2.10                     | 0.52              |
| 3:1:6:TRP:CG      | 5:AE:70:GLN:HB2   | 2.44                     | 0.52              |
| 3:1:242:ILE:HG22  | 3:AK:26:LEU:HD13  | 1.92                     | 0.52              |
| 3:4:260:LEU:HD13  | 3:AH:234:ILE:HD11 | 1.90                     | 0.52              |
| 3:5:1:MET:HE1     | 3:AN:242:ILE:HG13 | 1.91                     | 0.52              |
| 3:ZE:240:TYR:CE2  | 4:ZJ:399:LEU:HD11 | 2.44                     | 0.52              |
| 4:ZJ:306:ASN:O    | 4:ZJ:307:GLU:HG2  | 2.10                     | 0.52              |
| 4:ZK:170:PHE:HE2  | 4:ZK:223:PRO:HG2  | 1.74                     | 0.52              |
| 4:ZQ:373:VAL:CG1  | 4:ZW:7:VAL:HG22   | 2.39                     | 0.52              |
| 4:ZX:319:ASN:OD1  | 4:ZX:320:PHE:N    | 2.42                     | 0.52              |
| 4:ZZ:14:ALA:HB2   | 4:ZZ:382:TYR:HE2  | 1.73                     | 0.52              |
| 4:Za:287:GLY:N    | 4:Za:306:ASN:HD22 | 2.07                     | 0.52              |
| 6:AY:365:ASN:CG   | 11:A9:72:HIS:HD2  | 2.16                     | 0.52              |
| 6:Am:282:TYR:HB3  | 6:An:292:THR:HG21 | 1.90                     | 0.52              |
| 9:Av:74:LEU:HD22  | 9:Av:235:LEU:HD22 | 1.91                     | 0.52              |
| 9:Ax:40:LEU:HD22  | 11:A9:8:ALA:HB3   | 1.92                     | 0.52              |
| 9:Ay:138:MET:HE1  | 9:Ay:171:LEU:HA   | 1.90                     | 0.52              |
| 11:A6:29:ASN:ND2  | 11:A6:41:ARG:O    | 2.36                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UI:88:VAL:HB    | 6:UI:89:PRO:HD2   | 1.90                     | 0.52              |
| 6:UM:127:SER:O    | 6:UM:131:ASN:CG   | 2.52                     | 0.52              |
| 6:UN:88:VAL:HB    | 6:UN:89:PRO:HD2   | 1.90                     | 0.52              |
| 12:BB:23:VAL:HG21 | 12:BB:47:VAL:HG13 | 1.91                     | 0.52              |
| 6:WN:145:GLU:HG2  | 6:WN:152:SER:HA   | 1.90                     | 0.52              |
| 6:BS:282:TYR:HB3  | 6:BT:292:THR:HG21 | 1.90                     | 0.52              |
| 2:b:196:MET:SD    | 2:b:247:THR:HG22  | 2.50                     | 0.52              |
| 2:d:196:MET:SD    | 2:d:247:THR:HG22  | 2.50                     | 0.52              |
| 2:e:62:LEU:HD22   | 2:e:81:LEU:HD11   | 1.91                     | 0.52              |
| 2:f:196:MET:SD    | 2:f:247:THR:HG22  | 2.50                     | 0.52              |
| 2:l:208:ARG:O     | 2:l:212:SER:OG    | 2.16                     | 0.52              |
| 2:u:208:ARG:O     | 2:u:212:SER:OG    | 2.16                     | 0.52              |
| 2:z:196:MET:SD    | 2:z:247:THR:HG22  | 2.50                     | 0.52              |
| 3:2:236:VAL:O     | 3:2:237:GLN:C     | 2.53                     | 0.52              |
| 3:2:237:GLN:O     | 3:2:241:GLU:HG3   | 2.09                     | 0.52              |
| 3:4:85:ASN:HA     | 4:ZF:50:LEU:HD22  | 1.91                     | 0.52              |
| 3:4:130:THR:OG1   | 3:4:131:ALA:N     | 2.42                     | 0.52              |
| 3:5:20:ASP:OD1    | 3:ZA:4:SER:N      | 2.42                     | 0.52              |
| 4:ZN:212:THR:HG21 | 4:ZN:246:ILE:HD11 | 1.91                     | 0.52              |
| 4:ZO:178:TYR:HA   | 4:ZO:201:VAL:HG12 | 1.92                     | 0.52              |
| 4:ZP:208:TRP:NE1  | 4:ZP:268:GLN:OE1  | 2.36                     | 0.52              |
| 4:ZR:162:ASP:OD2  | 4:ZR:274:ASN:ND2  | 2.42                     | 0.52              |
| 4:ZS:307:GLU:N    | 4:ZS:307:GLU:OE2  | 2.43                     | 0.52              |
| 4:ZT:10:LEU:HD21  | 4:ZY:399:LEU:HD21 | 1.92                     | 0.52              |
| 4:ZU:382:TYR:CZ   | 4:ZZ:395:ILE:HG23 | 2.44                     | 0.52              |
| 4:ZY:17:LEU:HG    | 4:ZY:378:ALA:HB1  | 1.91                     | 0.52              |
| 4:Zg:85:LEU:HD13  | 4:Zg:114:MET:HB3  | 1.91                     | 0.52              |
| 4:Zg:111:MET:HE2  | 4:Zg:111:MET:N    | 2.25                     | 0.52              |
| 5:AA:79:ASP:HB3   | 5:AA:206:LEU:HD13 | 1.92                     | 0.52              |
| 5:AD:35:ARG:HH11  | 5:AD:101:ARG:HG3  | 1.74                     | 0.52              |
| 3:AI:185:GLU:HB3  | 3:AI:193:ILE:HG13 | 1.92                     | 0.52              |
| 3:AL:79:ARG:HH22  | 3:AL:184:LEU:HB2  | 1.74                     | 0.52              |
| 6:AS:292:THR:HG21 | 6:BX:282:TYR:HB3  | 1.90                     | 0.52              |
| 6:AY:293:LEU:HD21 | 6:AY:364:SER:HB3  | 1.92                     | 0.52              |
| 6:Ad:293:LEU:HD21 | 6:Ad:364:SER:HB3  | 1.92                     | 0.52              |
| 6:Af:293:LEU:HD21 | 6:Af:364:SER:HB3  | 1.91                     | 0.52              |
| 7:Ar:85:PRO:CG    | 9:Ax:241:GLN:HB3  | 2.39                     | 0.52              |
| 9:Av:205:MET:HE3  | 9:Aw:209:MET:HA   | 1.91                     | 0.52              |
| 11:A6:50:LYS:O    | 11:A6:54:VAL:HG22 | 2.09                     | 0.52              |
| 6:WD:145:GLU:HG2  | 6:WD:152:SER:HA   | 1.91                     | 0.52              |
| 6:WJ:128:GLU:HG3  | 6:WK:126:PHE:CD2  | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WL:145:GLU:HG2  | 6:WL:152:SER:HA   | 1.91                     | 0.52              |
| 6:WT:187:ASP:OD1  | 6:WT:190:GLN:N    | 2.39                     | 0.52              |
| 6:WV:120:LYS:HZ3  | 6:WV:123:ILE:CD1  | 2.17                     | 0.52              |
| 12:BD:68:ILE:HD11 | 6:BN:312:VAL:HG22 | 1.83                     | 0.52              |
| 1:S:106:PHE:CE1   | 1:T:126:ALA:HB2   | 2.45                     | 0.52              |
| 2:b:273:CYS:CB    | 2:c:264:MET:O     | 2.42                     | 0.52              |
| 2:f:62:LEU:HD22   | 2:f:81:LEU:HD11   | 1.92                     | 0.52              |
| 2:g:62:LEU:HD22   | 2:g:81:LEU:HD11   | 1.91                     | 0.52              |
| 2:n:62:LEU:HD22   | 2:n:81:LEU:HD11   | 1.92                     | 0.52              |
| 2:v:196:MET:SD    | 2:v:247:THR:HG22  | 2.50                     | 0.52              |
| 3:1:16:GLN:OE1    | 3:1:16:GLN:HA     | 2.10                     | 0.52              |
| 3:8:227:ALA:HB1   | 4:ZJ:399:LEU:HD22 | 1.92                     | 0.52              |
| 3:ZA:76:ALA:HA    | 4:ZF:47:LYS:HZ3   | 1.71                     | 0.52              |
| 3:ZB:57:SER:HA    | 3:AJ:154:ASP:HB2  | 1.91                     | 0.52              |
| 4:ZG:208:TRP:NE1  | 4:ZG:268:GLN:OE1  | 2.40                     | 0.52              |
| 4:ZJ:231:LYS:NZ   | 4:ZJ:239:GLU:OE1  | 2.38                     | 0.52              |
| 4:ZK:103:ASP:OD1  | 4:ZK:107:ASN:N    | 2.40                     | 0.52              |
| 4:ZO:2:SER:OG     | 4:ZO:3:PHE:N      | 2.37                     | 0.52              |
| 4:ZP:380:ARG:NE   | 4:ZV:393:ASP:OD2  | 2.43                     | 0.52              |
| 4:ZU:144:MET:HE3  | 4:ZU:306:ASN:HD21 | 1.73                     | 0.52              |
| 4:ZW:210:VAL:O    | 4:ZW:227:SER:OG   | 2.22                     | 0.52              |
| 5:AC:229:MET:HB3  | 12:BD:28:LEU:HD21 | 1.92                     | 0.52              |
| 6:AT:235:LEU:HB3  | 6:AU:244:ARG:HH22 | 1.75                     | 0.52              |
| 6:AW:293:LEU:HD21 | 6:AW:364:SER:HB3  | 1.91                     | 0.52              |
| 7:Ab:37:ILE:CD1   | 7:Aq:44:ILE:HD11  | 2.35                     | 0.52              |
| 6:Ah:235:LEU:HB3  | 6:Ai:244:ARG:HH22 | 1.75                     | 0.52              |
| 9:Au:67:ILE:H     | 9:Au:67:ILE:HD12  | 1.75                     | 0.52              |
| 6:UJ:88:VAL:HB    | 6:UJ:89:PRO:HD2   | 1.90                     | 0.52              |
| 6:BU:235:LEU:HB3  | 6:BV:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:G:106:PHE:CE1   | 1:H:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:H:106:PHE:CE1   | 1:I:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:M:106:PHE:CE1   | 1:N:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:N:106:PHE:CE1   | 1:O:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:Q:106:PHE:CE1   | 1:R:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:T:106:PHE:CE1   | 1:U:126:ALA:HB2   | 2.45                     | 0.52              |
| 2:f:208:ARG:O     | 2:f:212:SER:OG    | 2.16                     | 0.52              |
| 2:m:62:LEU:HD22   | 2:m:81:LEU:HD11   | 1.92                     | 0.52              |
| 2:o:62:LEU:HD22   | 2:o:81:LEU:HD11   | 1.92                     | 0.52              |
| 2:p:54:GLN:O      | 2:q:79:MET:HA     | 2.09                     | 0.52              |
| 2:q:273:CYS:CB    | 2:r:264:MET:O     | 2.42                     | 0.52              |
| 2:u:54:GLN:O      | 2:v:79:MET:HA     | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:0:83:GLN:NE2    | 3:0:97:ILE:O      | 2.20                     | 0.52              |
| 3:1:42:GLU:HB3    | 3:1:75:VAL:HG21   | 1.91                     | 0.52              |
| 3:ZC:98:LYS:HG3   | 3:ZC:98:LYS:O     | 2.10                     | 0.52              |
| 4:ZN:102:LEU:O    | 4:ZS:322:ASN:ND2  | 2.43                     | 0.52              |
| 4:ZO:268:GLN:NE2  | 4:ZU:190:GLN:HE22 | 2.07                     | 0.52              |
| 4:ZS:118:GLY:HA2  | 4:ZS:316:VAL:HG12 | 1.92                     | 0.52              |
| 5:AA:102:ASN:HD22 | 5:AA:116:GLN:HE21 | 1.57                     | 0.52              |
| 5:AD:234:ILE:CG2  | 3:AI:260:LEU:HD21 | 2.40                     | 0.52              |
| 5:AE:214:VAL:HG13 | 3:AK:12:LEU:HD13  | 1.92                     | 0.52              |
| 3:AH:242:ILE:HD11 | 3:AN:258:THR:HG22 | 1.92                     | 0.52              |
| 6:Am:235:LEU:HB3  | 6:An:244:ARG:HH22 | 1.75                     | 0.52              |
| 6:An:235:LEU:HB3  | 6:Ao:244:ARG:HH22 | 1.75                     | 0.52              |
| 6:An:282:TYR:HB3  | 6:Ao:292:THR:HG21 | 1.90                     | 0.52              |
| 6:AO:235:LEU:HB3  | 6:AP:244:ARG:HH22 | 1.75                     | 0.52              |
| 7:As:35:ILE:HG21  | 7:As:50:SER:HA    | 1.92                     | 0.52              |
| 9:Aw:58:LEU:O     | 9:Aw:62:THR:OG1   | 2.23                     | 0.52              |
| 6:UI:159:MET:N    | 6:UI:159:MET:SD   | 2.82                     | 0.52              |
| 6:UK:80:ALA:HB3   | 6:UK:83:SER:HB3   | 1.90                     | 0.52              |
| 6:UK:127:SER:O    | 6:UK:131:ASN:CG   | 2.52                     | 0.52              |
| 6:UM:80:ALA:HB3   | 6:UM:83:SER:HB3   | 1.91                     | 0.52              |
| 6:WD:168:GLU:OE1  | 6:WD:170:LYS:NZ   | 2.42                     | 0.52              |
| 6:WF:197:LEU:HA   | 6:WG:175:SER:OG   | 2.10                     | 0.52              |
| 6:WP:145:GLU:O    | 6:WP:147:LEU:N    | 2.42                     | 0.52              |
| 1:A:126:ALA:HB2   | 1:Z:106:PHE:CE1   | 2.45                     | 0.52              |
| 1:I:106:PHE:CE1   | 1:J:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:R:106:PHE:CE1   | 1:S:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:R:219:MET:SD    | 1:S:212:TYR:CD1   | 3.03                     | 0.52              |
| 1:X:106:PHE:CE1   | 1:Y:126:ALA:HB2   | 2.45                     | 0.52              |
| 2:d:62:LEU:HD22   | 2:d:81:LEU:HD11   | 1.92                     | 0.52              |
| 2:v:54:GLN:O      | 2:w:79:MET:HA     | 2.09                     | 0.52              |
| 3:2:151:ILE:HG12  | 3:2:157:VAL:HG22  | 1.91                     | 0.52              |
| 3:9:106:MET:HE2   | 3:9:137:GLN:HB2   | 1.91                     | 0.52              |
| 4:ZP:104:GLU:HG2  | 4:ZU:338:GLN:O    | 2.09                     | 0.52              |
| 4:ZT:281:GLN:NE2  | 4:ZT:283:GLY:O    | 2.35                     | 0.52              |
| 4:ZW:93:PHE:HB3   | 4:ZW:333:VAL:HG13 | 1.92                     | 0.52              |
| 4:ZY:18:ASP:HB3   | 4:Zd:5:GLN:HE22   | 1.74                     | 0.52              |
| 4:ZY:125:PRO:HD2  | 4:ZY:125:PRO:O    | 2.08                     | 0.52              |
| 4:ZY:188:ASP:OD1  | 4:ZY:194:HIS:NE2  | 2.39                     | 0.52              |
| 4:Zf:317:LEU:HD21 | 4:Zf:356:LEU:HD11 | 1.91                     | 0.52              |
| 5:AB:214:VAL:HG22 | 3:AM:257:LEU:CD2  | 2.38                     | 0.52              |
| 5:AE:49:LEU:HD23  | 11:A0:90:PRO:HD2  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AH:91:ASN:HB3   | 3:AH:94:ASP:OD2   | 2.09                     | 0.52              |
| 6:Ag:293:LEU:HD21 | 6:Ag:364:SER:HB3  | 1.92                     | 0.52              |
| 9:Au:199:VAL:O    | 9:Au:203:VAL:HG23 | 2.09                     | 0.52              |
| 9:Ax:48:ILE:CD1   | 10:A4:89:ARG:HH12 | 2.23                     | 0.52              |
| 9:Ay:138:MET:HE2  | 9:Ay:170:LEU:HG   | 1.92                     | 0.52              |
| 11:A0:41:ARG:HG3  | 12:BE:59:THR:HG21 | 1.92                     | 0.52              |
| 6:UI:127:SER:O    | 6:UI:131:ASN:CG   | 2.52                     | 0.52              |
| 6:UM:88:VAL:HB    | 6:UM:89:PRO:HD2   | 1.90                     | 0.52              |
| 6:UO:88:VAL:HB    | 6:UO:89:PRO:HD2   | 1.90                     | 0.52              |
| 6:UO:127:SER:O    | 6:UO:131:ASN:CG   | 2.52                     | 0.52              |
| 6:UP:127:SER:O    | 6:UP:131:ASN:CG   | 2.53                     | 0.52              |
| 6:WS:190:GLN:HG2  | 6:WT:217:GLY:HA3  | 1.91                     | 0.52              |
| 12:BF:72:ALA:HB3  | 12:BF:95:ASN:HD22 | 1.74                     | 0.52              |
| 6:BO:325:GLU:OE1  | 6:BO:325:GLU:N    | 2.42                     | 0.52              |
| 6:BR:293:LEU:HD21 | 6:BR:364:SER:HB3  | 1.91                     | 0.52              |
| 6:BW:235:LEU:HB3  | 6:BX:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:H:219:MET:SD    | 1:I:212:TYR:CD1   | 3.03                     | 0.52              |
| 1:P:106:PHE:CE1   | 1:Q:126:ALA:HB2   | 2.45                     | 0.52              |
| 1:U:219:MET:SD    | 1:V:212:TYR:CD1   | 3.03                     | 0.52              |
| 1:W:219:MET:SD    | 1:X:212:TYR:CD1   | 3.03                     | 0.52              |
| 1:Y:106:PHE:CE1   | 1:Z:126:ALA:HB2   | 2.45                     | 0.52              |
| 2:c:62:LEU:HD22   | 2:c:81:LEU:HD11   | 1.91                     | 0.52              |
| 2:h:62:LEU:HD22   | 2:h:81:LEU:HD11   | 1.91                     | 0.52              |
| 2:h:196:MET:SD    | 2:h:247:THR:HG22  | 2.50                     | 0.52              |
| 3:2:227:ALA:HA    | 3:ZD:257:LEU:HD21 | 1.92                     | 0.52              |
| 3:3:9:LYS:HE3     | 3:AL:228:GLU:HG3  | 1.91                     | 0.52              |
| 3:3:42:GLU:OE1    | 3:AM:189:GLU:HB3  | 2.10                     | 0.52              |
| 3:5:43:ASP:OD1    | 3:5:43:ASP:N      | 2.43                     | 0.52              |
| 3:ZA:40:VAL:HG23  | 3:ZA:75:VAL:HB    | 1.92                     | 0.52              |
| 3:ZB:31:THR:CG2   | 4:ZG:39:PHE:HB2   | 2.27                     | 0.52              |
| 3:ZB:56:SER:O     | 3:AJ:152:GLY:C    | 2.52                     | 0.52              |
| 3:ZB:85:ASN:ND2   | 4:ZM:50:LEU:HG    | 2.24                     | 0.52              |
| 3:ZE:237:GLN:HB2  | 4:ZJ:391:THR:HG23 | 1.92                     | 0.52              |
| 4:ZH:268:GLN:HG2  | 4:ZN:190:GLN:OE1  | 2.10                     | 0.52              |
| 4:ZN:102:LEU:O    | 4:ZS:322:ASN:HB2  | 2.09                     | 0.52              |
| 4:ZQ:331:ASP:N    | 4:ZV:41:ASP:O     | 2.26                     | 0.52              |
| 4:ZS:151:THR:OG1  | 4:ZS:282:ASN:ND2  | 2.43                     | 0.52              |
| 5:AA:213:PRO:HB2  | 3:AL:257:LEU:CD2  | 2.40                     | 0.52              |
| 5:AB:109:PRO:CG   | 3:AG:197:SER:HA   | 2.40                     | 0.52              |
| 5:AC:27:ALA:O     | 3:AH:72:VAL:CG1   | 2.55                     | 0.52              |
| 5:AC:123:GLU:HG3  | 5:AC:160:ARG:HB3  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AI:260:LEU:CD2  | 12:BD:106:MET:SD  | 2.98                     | 0.52              |
| 6:Aj:372:ILE:HG22 | 10:A1:11:ILE:HG21 | 1.83                     | 0.52              |
| 6:Ak:235:LEU:HB3  | 6:Al:244:ARG:HH22 | 1.75                     | 0.52              |
| 6:AQ:293:LEU:HD21 | 6:AQ:364:SER:HB3  | 1.91                     | 0.52              |
| 7:Ar:4:GLU:C      | 7:Ar:6:VAL:N      | 2.67                     | 0.52              |
| 9:Av:83:ALA:HB1   | 9:Av:84:PRO:HD2   | 1.92                     | 0.52              |
| 6:WD:149:PRO:HG2  | 6:WD:190:GLN:NE2  | 2.23                     | 0.52              |
| 6:WV:186:LEU:HA   | 6:WV:190:GLN:OE1  | 2.10                     | 0.52              |
| 6:BR:235:LEU:HB3  | 6:BS:244:ARG:HH22 | 1.75                     | 0.52              |
| 1:L:106:PHE:CE1   | 1:M:126:ALA:HB2   | 2.45                     | 0.51              |
| 2:i:196:MET:SD    | 2:i:247:THR:HG22  | 2.50                     | 0.51              |
| 2:k:196:MET:SD    | 2:k:247:THR:HG22  | 2.50                     | 0.51              |
| 2:l:62:LEU:HD22   | 2:l:81:LEU:HD11   | 1.92                     | 0.51              |
| 2:t:196:MET:SD    | 2:t:247:THR:HG22  | 2.50                     | 0.51              |
| 3:0:86:LEU:HD12   | 3:ZB:44:LEU:HD22  | 1.92                     | 0.51              |
| 3:2:242:ILE:HG22  | 3:AL:26:LEU:HD13  | 1.92                     | 0.51              |
| 3:4:7:ILE:HG23    | 3:4:71:GLY:HA2    | 1.92                     | 0.51              |
| 3:6:210:GLY:O     | 3:6:211:ALA:C     | 2.53                     | 0.51              |
| 3:ZB:25:ASN:HD21  | 3:ZB:37:GLN:H     | 1.57                     | 0.51              |
| 3:ZB:130:THR:HG22 | 3:ZB:131:ALA:H    | 1.75                     | 0.51              |
| 3:ZE:128:LEU:HD13 | 3:ZE:140:ILE:HB   | 1.92                     | 0.51              |
| 4:ZQ:30:TYR:HD1   | 4:ZQ:363:ALA:HA   | 1.75                     | 0.51              |
| 4:ZQ:183:THR:OG1  | 4:Zb:131:GLY:O    | 2.28                     | 0.51              |
| 4:ZQ:200:PHE:HE2  | 4:ZQ:263:PHE:HE2  | 1.57                     | 0.51              |
| 4:ZT:165:PRO:HG2  | 4:ZT:201:VAL:HG13 | 1.92                     | 0.51              |
| 4:Za:234:GLU:O    | 4:Zg:190:GLN:HG3  | 2.09                     | 0.51              |
| 5:AB:238:ASP:HB2  | 12:BB:106:MET:HE3 | 1.92                     | 0.51              |
| 5:AE:35:ARG:O     | 5:AE:173:ARG:NH2  | 2.43                     | 0.51              |
| 3:AH:35:LYS:HD2   | 3:AH:81:HIS:HA    | 1.91                     | 0.51              |
| 3:AH:195:THR:O    | 3:AH:196:GLN:C    | 2.53                     | 0.51              |
| 3:AI:62:LEU:HG    | 12:BE:84:LEU:HD23 | 1.91                     | 0.51              |
| 3:AJ:98:LYS:HG3   | 3:AJ:215:TYR:HE2  | 1.75                     | 0.51              |
| 3:AK:107:LEU:HD12 | 3:AK:111:THR:HG23 | 1.92                     | 0.51              |
| 3:AM:116:ARG:NH2  | 3:AM:220:GLU:OE1  | 2.42                     | 0.51              |
| 6:AW:235:LEU:HB3  | 6:AX:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:AZ:235:LEU:HB3  | 6:Aa:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:Ae:235:LEU:HB3  | 6:Af:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:Ae:370:ARG:NE   | 10:A2:7:ILE:HD11  | 2.23                     | 0.51              |
| 6:Aj:235:LEU:HB3  | 6:Ak:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:Al:293:LEU:HD21 | 6:Al:364:SER:HB3  | 1.91                     | 0.51              |
| 6:Ao:278:THR:HG22 | 10:Az:7:ILE:HG21  | 1.81                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Ap:282:TYR:HB3  | 6:AO:292:THR:HG21 | 1.90                     | 0.51              |
| 7:Ar:40:ALA:CB    | 7:As:44:ILE:CD1   | 2.88                     | 0.51              |
| 9:Au:148:ALA:HA   | 6:WP:164:LEU:HD13 | 1.91                     | 0.51              |
| 6:WG:145:GLU:HG2  | 6:WG:152:SER:HA   | 1.91                     | 0.51              |
| 6:BS:235:LEU:HB3  | 6:BT:244:ARG:HH22 | 1.75                     | 0.51              |
| 1:A:106:PHE:CE1   | 1:B:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:F:106:PHE:CE1   | 1:G:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:J:106:PHE:CE1   | 1:K:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:O:106:PHE:CE1   | 1:P:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:U:106:PHE:CE1   | 1:V:126:ALA:HB2   | 2.45                     | 0.51              |
| 2:g:196:MET:SD    | 2:g:247:THR:HG22  | 2.50                     | 0.51              |
| 2:j:196:MET:SD    | 2:j:247:THR:HG22  | 2.50                     | 0.51              |
| 2:m:196:MET:SD    | 2:m:247:THR:HG22  | 2.50                     | 0.51              |
| 2:p:62:LEU:HD22   | 2:p:81:LEU:HD11   | 1.92                     | 0.51              |
| 2:x:51:GLN:HG3    | 3:AH:125:ASN:ND2  | 2.25                     | 0.51              |
| 3:O:2:ILE:CG2     | 5:AD:212:LYS:CA   | 2.83                     | 0.51              |
| 3:ZE:238:ARG:NH1  | 3:ZE:241:GLU:OE1  | 2.43                     | 0.51              |
| 4:ZI:75:VAL:O     | 4:ZI:98:GLY:HA3   | 2.10                     | 0.51              |
| 4:ZI:367:ASP:O    | 4:ZI:371:GLU:HG2  | 2.10                     | 0.51              |
| 4:ZJ:101:LYS:HB2  | 4:ZO:324:GLU:OE2  | 2.10                     | 0.51              |
| 4:ZL:57:ILE:HD13  | 4:ZQ:47:LYS:CB    | 2.39                     | 0.51              |
| 4:ZU:156:ILE:HG13 | 4:ZU:276:ILE:HA   | 1.91                     | 0.51              |
| 4:Za:116:LEU:HD21 | 4:Za:315:ILE:HD13 | 1.92                     | 0.51              |
| 4:Zb:95:SER:HB2   | 4:Zb:333:VAL:HG22 | 1.92                     | 0.51              |
| 4:Zd:180:LYS:HB3  | 4:Zd:200:PHE:HB2  | 1.90                     | 0.51              |
| 5:AC:208:GLY:HA3  | 3:AN:6:TRP:CZ3    | 2.44                     | 0.51              |
| 5:AD:59:ALA:CB    | 3:AI:66:LEU:HD11  | 2.40                     | 0.51              |
| 3:AM:4:SER:HB2    | 3:AM:250:THR:CG2  | 2.40                     | 0.51              |
| 3:AM:205:THR:OG1  | 3:AM:208:LEU:HB2  | 2.11                     | 0.51              |
| 6:AS:244:ARG:HH22 | 6:BX:235:LEU:HB3  | 1.75                     | 0.51              |
| 6:Ah:293:LEU:HD21 | 6:Ah:364:SER:HB3  | 1.91                     | 0.51              |
| 6:Ao:235:LEU:HB3  | 6:Ap:244:ARG:HH22 | 1.75                     | 0.51              |
| 8:At:130:ASP:O    | 8:At:134:MET:HG2  | 2.10                     | 0.51              |
| 9:Av:52:THR:HG22  | 10:A1:91:LYS:HE2  | 1.91                     | 0.51              |
| 6:WF:125:GLN:O    | 6:WF:126:PHE:C    | 2.53                     | 0.51              |
| 6:WJ:141:ALA:O    | 6:WJ:145:GLU:HG3  | 2.09                     | 0.51              |
| 1:A:212:TYR:CD1   | 1:Z:219:MET:SD    | 3.03                     | 0.51              |
| 1:J:62:TYR:CD1    | 2:h:129:VAL:HG11  | 2.37                     | 0.51              |
| 1:P:219:MET:SD    | 1:Q:212:TYR:CD1   | 3.03                     | 0.51              |
| 1:T:219:MET:SD    | 1:U:212:TYR:CD1   | 3.03                     | 0.51              |
| 2:l:196:MET:SD    | 2:l:247:THR:HG22  | 2.50                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:v:62:LEU:HD22   | 2:v:81:LEU:HD11   | 1.92                     | 0.51              |
| 3:4:56:SER:C      | 5:AC:138:ALA:CB   | 2.70                     | 0.51              |
| 3:ZA:167:PRO:HD3  | 4:ZL:338:GLN:HB3  | 1.93                     | 0.51              |
| 4:ZI:154:MET:HG3  | 4:ZI:279:THR:HG22 | 1.91                     | 0.51              |
| 4:ZO:157:ASN:HD22 | 4:ZU:143:LEU:CD2  | 2.23                     | 0.51              |
| 4:ZO:199:TYR:O    | 4:ZO:210:VAL:HA   | 2.11                     | 0.51              |
| 4:ZV:211:TYR:CE2  | 4:ZV:226:ALA:HA   | 2.45                     | 0.51              |
| 4:ZX:290:VAL:HA   | 4:Zc:352:ASN:ND2  | 2.26                     | 0.51              |
| 4:ZZ:210:VAL:HB   | 4:ZZ:228:THR:HG22 | 1.91                     | 0.51              |
| 4:Zf:397:ASN:O    | 4:Zf:400:VAL:N    | 2.43                     | 0.51              |
| 4:Zg:317:LEU:HD11 | 4:Zg:356:LEU:HD21 | 1.92                     | 0.51              |
| 5:AD:34:PHE:CE1   | 3:AI:46:TYR:OH    | 2.63                     | 0.51              |
| 5:AD:243:ARG:NH2  | 12:BE:113:GLN:CB  | 2.73                     | 0.51              |
| 5:AE:26:LEU:HD21  | 3:AJ:242:ILE:HG12 | 1.92                     | 0.51              |
| 5:AE:50:SER:HB3   | 11:A0:91:ASP:O    | 2.10                     | 0.51              |
| 3:AM:129:VAL:HG12 | 3:AM:135:GLN:HA   | 1.91                     | 0.51              |
| 6:AR:244:ARG:HH22 | 6:Aa:235:LEU:HB3  | 1.75                     | 0.51              |
| 6:AU:282:TYR:HB3  | 6:AV:292:THR:HG21 | 1.91                     | 0.51              |
| 6:Ai:293:LEU:HD21 | 6:Ai:364:SER:HB3  | 1.91                     | 0.51              |
| 6:Ao:293:LEU:HD21 | 6:Ao:364:SER:HB3  | 1.91                     | 0.51              |
| 6:Ap:235:LEU:HB3  | 6:AO:244:ARG:HH22 | 1.75                     | 0.51              |
| 7:Ar:13:ALA:HB1   | 9:Ax:195:ILE:HD11 | 1.93                     | 0.51              |
| 9:Av:193:PHE:HB3  | 9:Av:222:LYS:HD3  | 1.92                     | 0.51              |
| 6:UM:159:MET:N    | 6:UM:159:MET:SD   | 2.82                     | 0.51              |
| 6:WQ:125:GLN:O    | 6:WQ:128:GLU:N    | 2.43                     | 0.51              |
| 6:WR:165:PHE:C    | 6:WR:167:ARG:H    | 2.18                     | 0.51              |
| 12:BD:20:ARG:NH2  | 12:BD:107:SER:HB2 | 2.24                     | 0.51              |
| 12:BE:23:VAL:HG21 | 12:BE:47:VAL:HG13 | 1.91                     | 0.51              |
| 1:B:106:PHE:CE1   | 1:C:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:K:219:MET:SD    | 1:L:212:TYR:CD1   | 3.03                     | 0.51              |
| 1:U:65:LEU:CG     | 2:t:65:MET:HG3    | 2.39                     | 0.51              |
| 1:W:106:PHE:CE1   | 1:X:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:X:219:MET:SD    | 1:Y:212:TYR:CD1   | 3.03                     | 0.51              |
| 2:n:196:MET:SD    | 2:n:247:THR:HG22  | 2.50                     | 0.51              |
| 2:o:196:MET:SD    | 2:o:247:THR:HG22  | 2.50                     | 0.51              |
| 2:u:62:LEU:HD22   | 2:u:81:LEU:HD11   | 1.92                     | 0.51              |
| 2:y:62:LEU:HD22   | 2:y:81:LEU:HD11   | 1.91                     | 0.51              |
| 2:z:93:TYR:OH     | 2:z:173:ARG:O     | 2.25                     | 0.51              |
| 3:1:260:LEU:HD21  | 5:AE:221:ILE:HD11 | 1.92                     | 0.51              |
| 3:5:9:LYS:HE3     | 3:AN:228:GLU:HG3  | 1.92                     | 0.51              |
| 3:9:46:TYR:HA     | 3:9:69:GLY:HA2    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:ZC:34:PHE:HB3   | 3:ZC:222:SER:HB3   | 1.91                     | 0.51              |
| 3:ZC:128:LEU:HD12 | 3:ZC:140:ILE:HB    | 1.92                     | 0.51              |
| 3:ZE:57:SER:HA    | 3:AM:154:ASP:HB3   | 1.92                     | 0.51              |
| 4:ZF:162:ASP:OD2  | 4:ZF:274:ASN:ND2   | 2.30                     | 0.51              |
| 4:ZG:264:LEU:HD12 | 4:ZG:265:ASN:H     | 1.75                     | 0.51              |
| 4:ZH:112:GLN:HG2  | 4:ZH:331:ASP:HB3   | 1.93                     | 0.51              |
| 4:ZK:322:ASN:OD1  | 4:ZK:325:GLY:N     | 2.43                     | 0.51              |
| 4:ZW:210:VAL:HB   | 4:ZW:228:THR:HG22  | 1.93                     | 0.51              |
| 5:AA:70:GLN:CG    | 3:AL:3:SER:CB      | 2.89                     | 0.51              |
| 5:AC:27:ALA:HB1   | 3:AH:72:VAL:HG12   | 1.92                     | 0.51              |
| 3:AN:21:VAL:HG21  | 3:AN:39:ALA:HB2    | 1.91                     | 0.51              |
| 6:Af:235:LEU:HB3  | 6:Ag:244:ARG:HH22  | 1.75                     | 0.51              |
| 6:Am:256:ILE:HG13 | 6:Am:257:VAL:N     | 2.26                     | 0.51              |
| 7:Ar:6:VAL:HG22   | 9:Ax:187:PHE:HZ    | 1.75                     | 0.51              |
| 10:Az:89:ARG:HH12 | 10:A5:104:VAL:HG22 | 1.76                     | 0.51              |
| 6:UO:159:MET:N    | 6:UO:159:MET:SD    | 2.82                     | 0.51              |
| 6:WC:197:LEU:CD1  | 6:WD:175:SER:OG    | 2.58                     | 0.51              |
| 6:WD:142:ARG:O    | 6:WD:146:THR:HG23  | 2.10                     | 0.51              |
| 6:WI:145:GLU:HG2  | 6:WI:152:SER:HA    | 1.91                     | 0.51              |
| 6:WL:145:GLU:O    | 6:WL:146:THR:C     | 2.53                     | 0.51              |
| 6:WR:190:GLN:NE2  | 6:WS:216:SER:O     | 2.43                     | 0.51              |
| 6:BV:235:LEU:HB3  | 6:BW:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:D:106:PHE:CE1   | 1:E:126:ALA:HB2    | 2.45                     | 0.51              |
| 1:D:219:MET:SD    | 1:E:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:E:106:PHE:CE1   | 1:F:126:ALA:HB2    | 2.45                     | 0.51              |
| 1:E:219:MET:SD    | 1:F:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:G:219:MET:SD    | 1:H:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:S:219:MET:SD    | 1:T:212:TYR:CD1    | 3.03                     | 0.51              |
| 2:b:62:LEU:HD22   | 2:b:81:LEU:HD11    | 1.92                     | 0.51              |
| 2:d:93:TYR:OH     | 2:d:173:ARG:O      | 2.25                     | 0.51              |
| 2:e:196:MET:SD    | 2:e:247:THR:HG22   | 2.50                     | 0.51              |
| 2:j:51:GLN:HG3    | 3:6:59:GLN:NE2     | 2.24                     | 0.51              |
| 2:k:62:LEU:HD22   | 2:k:81:LEU:HD11    | 1.92                     | 0.51              |
| 2:p:196:MET:SD    | 2:p:247:THR:HG22   | 2.50                     | 0.51              |
| 2:q:62:LEU:HD22   | 2:q:81:LEU:HD11    | 1.92                     | 0.51              |
| 2:u:21:ARG:HB2    | 2:u:243:GLU:HA     | 1.93                     | 0.51              |
| 2:w:21:ARG:HB2    | 2:w:243:GLU:HA     | 1.93                     | 0.51              |
| 2:x:62:LEU:HD22   | 2:x:81:LEU:HD11    | 1.91                     | 0.51              |
| 3:0:251:ASP:OD1   | 3:AI:238:ARG:NE    | 2.43                     | 0.51              |
| 3:2:218:TYR:OH    | 3:ZD:73:ARG:HG3    | 2.11                     | 0.51              |
| 3:4:50:ARG:NH1    | 3:AN:75:VAL:HG13   | 2.26                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:5:49:ILE:HG22   | 3:5:50:ARG:HG3     | 1.93                     | 0.51              |
| 3:9:155:GLY:HA2   | 3:9:214:LEU:HD12   | 1.92                     | 0.51              |
| 3:ZD:151:ILE:HG23 | 3:ZD:157:VAL:HG22  | 1.93                     | 0.51              |
| 4:ZH:235:ASN:OD1  | 4:ZN:189:SER:OG    | 2.26                     | 0.51              |
| 4:ZP:139:ILE:HA   | 4:ZP:312:LEU:HD13  | 1.91                     | 0.51              |
| 4:ZP:331:ASP:HA   | 4:ZU:40:ALA:HB1    | 1.91                     | 0.51              |
| 4:ZR:200:PHE:HE2  | 4:ZR:263:PHE:HE1   | 1.58                     | 0.51              |
| 4:ZU:183:THR:HB   | 4:Zf:132:ALA:CA    | 2.32                     | 0.51              |
| 4:Zg:95:SER:OG    | 4:Zg:332:ASN:O     | 2.19                     | 0.51              |
| 4:Zh:3:PHE:O      | 4:Zh:7:VAL:HG23    | 2.11                     | 0.51              |
| 5:AC:247:LEU:HD13 | 12:BD:119:LEU:HD23 | 1.92                     | 0.51              |
| 5:AD:135:ILE:HG23 | 5:AD:143:ILE:HG23  | 1.92                     | 0.51              |
| 3:AG:79:ARG:NH2   | 3:AG:186:SER:OG    | 2.44                     | 0.51              |
| 6:AX:235:LEU:HB3  | 6:AY:244:ARG:HH22  | 1.75                     | 0.51              |
| 6:AP:235:LEU:HB3  | 6:AQ:244:ARG:HH22  | 1.75                     | 0.51              |
| 7:Ar:77:VAL:HG12  | 9:Ax:229:VAL:HG11  | 1.91                     | 0.51              |
| 10:A5:83:GLN:HG3  | 12:BA:127:LEU:HD11 | 1.92                     | 0.51              |
| 11:A8:67:LEU:HA   | 11:A8:72:HIS:HE2   | 1.74                     | 0.51              |
| 6:UI:204:GLY:O    | 6:UI:206:PRO:HD3   | 2.11                     | 0.51              |
| 6:UK:204:GLY:O    | 6:UK:206:PRO:HD3   | 2.11                     | 0.51              |
| 6:UO:204:GLY:O    | 6:UO:206:PRO:HD3   | 2.11                     | 0.51              |
| 12:BA:22:ASN:HB2  | 6:BG:315:ALA:CB    | 2.35                     | 0.51              |
| 12:BA:131:THR:O   | 12:BA:131:THR:HG22 | 2.09                     | 0.51              |
| 6:WD:149:PRO:CG   | 6:WD:190:GLN:HE22  | 2.23                     | 0.51              |
| 6:WF:125:GLN:O    | 6:WF:128:GLU:N     | 2.43                     | 0.51              |
| 6:WQ:125:GLN:O    | 6:WQ:126:PHE:C     | 2.53                     | 0.51              |
| 6:WR:111:VAL:HB   | 6:WR:114:GLU:HB3   | 1.91                     | 0.51              |
| 6:BT:235:LEU:HB3  | 6:BU:244:ARG:HH22  | 1.75                     | 0.51              |
| 1:I:219:MET:SD    | 1:J:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:L:219:MET:SD    | 1:M:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:Y:219:MET:SD    | 1:Z:212:TYR:CD1    | 3.03                     | 0.51              |
| 2:i:62:LEU:HD22   | 2:i:81:LEU:HD11    | 1.92                     | 0.51              |
| 2:q:196:MET:SD    | 2:q:247:THR:HG22   | 2.50                     | 0.51              |
| 2:u:196:MET:SD    | 2:u:247:THR:HG22   | 2.50                     | 0.51              |
| 2:v:21:ARG:HB2    | 2:v:243:GLU:HA     | 1.93                     | 0.51              |
| 2:w:62:LEU:HD22   | 2:w:81:LEU:HD11    | 1.92                     | 0.51              |
| 3:4:121:GLN:NE2   | 3:9:78:GLU:OE1     | 2.43                     | 0.51              |
| 3:4:231:VAL:HG11  | 3:ZA:9:LYS:CG      | 2.41                     | 0.51              |
| 3:ZE:240:TYR:CE2  | 4:ZJ:399:LEU:CD1   | 2.93                     | 0.51              |
| 4:ZL:93:PHE:CD2   | 4:ZL:114:MET:HE1   | 2.45                     | 0.51              |
| 4:ZM:206:ASN:ND2  | 4:ZM:233:ASN:O     | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZS:5:GLN:HG3    | 4:ZS:50:LEU:O     | 2.11                     | 0.51              |
| 4:ZT:188:ASP:HA   | 4:ZT:257:ALA:HB2  | 1.93                     | 0.51              |
| 4:ZV:18:ASP:HB3   | 4:Za:5:GLN:HE22   | 1.75                     | 0.51              |
| 4:ZV:65:THR:HG21  | 4:Zg:4:SER:CB     | 2.40                     | 0.51              |
| 4:ZZ:204:LYS:HG3  | 4:ZZ:205:ASP:H    | 1.76                     | 0.51              |
| 4:Za:112:GLN:NE2  | 4:Za:331:ASP:O    | 2.43                     | 0.51              |
| 3:AF:62:LEU:HD23  | 12:BB:83:PRO:HG2  | 1.92                     | 0.51              |
| 6:AS:235:LEU:HB3  | 6:AT:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:AU:256:ILE:HG13 | 6:AU:257:VAL:N    | 2.26                     | 0.51              |
| 6:Ac:235:LEU:HB3  | 6:Ad:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:Am:293:LEU:HD21 | 6:Am:364:SER:HB3  | 1.91                     | 0.51              |
| 6:AP:293:LEU:HD21 | 6:AP:364:SER:HB3  | 1.92                     | 0.51              |
| 8:At:24:LEU:HB3   | 10:Az:89:ARG:NH2  | 2.26                     | 0.51              |
| 6:WF:116:LEU:CD2  | 6:WF:134:ARG:HD3  | 2.41                     | 0.51              |
| 1:B:219:MET:SD    | 1:C:212:TYR:CD1   | 3.03                     | 0.51              |
| 1:C:106:PHE:CE1   | 1:D:126:ALA:HB2   | 2.45                     | 0.51              |
| 2:s:196:MET:SD    | 2:s:247:THR:HG22  | 2.50                     | 0.51              |
| 2:t:62:LEU:HD22   | 2:t:81:LEU:HD11   | 1.92                     | 0.51              |
| 2:w:196:MET:SD    | 2:w:247:THR:HG22  | 2.50                     | 0.51              |
| 2:y:196:MET:SD    | 2:y:247:THR:HG22  | 2.50                     | 0.51              |
| 2:z:62:LEU:HD22   | 2:z:81:LEU:HD11   | 1.92                     | 0.51              |
| 3:4:56:SER:HA     | 5:AC:138:ALA:CB   | 2.41                     | 0.51              |
| 3:4:151:ILE:HG12  | 3:4:157:VAL:HG22  | 1.93                     | 0.51              |
| 3:7:37:GLN:HB3    | 3:7:77:THR:HG22   | 1.93                     | 0.51              |
| 3:ZE:115:THR:HB   | 3:ZE:191:LEU:HD23 | 1.93                     | 0.51              |
| 4:ZL:27:SER:O     | 4:ZL:364:SER:OG   | 2.27                     | 0.51              |
| 4:ZM:80:ASN:OD1   | 4:ZM:81:GLY:N     | 2.43                     | 0.51              |
| 4:ZO:129:GLN:O    | 4:ZO:129:GLN:HG3  | 2.11                     | 0.51              |
| 4:ZS:180:LYS:HB2  | 4:ZS:274:ASN:HD22 | 1.76                     | 0.51              |
| 4:ZU:150:THR:HG23 | 4:ZU:151:THR:HG23 | 1.93                     | 0.51              |
| 4:ZU:270:ASN:OD1  | 4:Za:191:GLY:HA3  | 2.11                     | 0.51              |
| 4:Za:332:ASN:N    | 4:Zf:41:ASP:OD1   | 2.33                     | 0.51              |
| 4:Za:376:ILE:CG2  | 4:Zg:393:ASP:OD2  | 2.59                     | 0.51              |
| 4:Zf:139:ILE:HA   | 4:Zf:312:LEU:HD13 | 1.91                     | 0.51              |
| 5:AC:58:THR:OG1   | 6:BL:320:PRO:HG2  | 2.10                     | 0.51              |
| 3:AH:155:GLY:O    | 3:AH:172:GLN:HA   | 2.11                     | 0.51              |
| 6:AV:235:LEU:HB3  | 6:AW:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:AV:256:ILE:HG13 | 6:AV:257:VAL:N    | 2.26                     | 0.51              |
| 6:Ac:256:ILE:HG13 | 6:Ac:257:VAL:N    | 2.26                     | 0.51              |
| 6:Ag:235:LEU:HB3  | 6:Ah:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:Aj:293:LEU:HD21 | 6:Aj:364:SER:HB3  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AO:293:LEU:HD21 | 6:AO:364:SER:HB3  | 1.91                     | 0.51              |
| 9:Ax:73:LEU:HD13  | 9:Ax:186:GLY:HA3  | 1.92                     | 0.51              |
| 10:A4:59:PHE:CD2  | 11:A9:118:MET:HE2 | 2.46                     | 0.51              |
| 10:A5:57:GLU:HB2  | 11:A0:11:PHE:CE2  | 2.46                     | 0.51              |
| 11:A0:91:ASP:OD2  | 12:BF:19:LYS:HE2  | 2.11                     | 0.51              |
| 6:UL:204:GLY:O    | 6:UL:206:PRO:HD3  | 2.11                     | 0.51              |
| 6:UM:204:GLY:O    | 6:UM:206:PRO:HD3  | 2.11                     | 0.51              |
| 6:WC:197:LEU:HA   | 6:WD:175:SER:OG   | 2.11                     | 0.51              |
| 6:WH:145:GLU:HG2  | 6:WH:152:SER:HA   | 1.91                     | 0.51              |
| 6:WN:200:SER:HB2  | 6:WO:173:SER:HB2  | 1.92                     | 0.51              |
| 6:WU:114:GLU:O    | 6:WU:115:LEU:C    | 2.54                     | 0.51              |
| 6:WV:200:SER:OG   | 6:WW:175:SER:HB2  | 2.11                     | 0.51              |
| 1:K:106:PHE:CE1   | 1:L:126:ALA:HB2   | 2.45                     | 0.51              |
| 1:V:106:PHE:CE1   | 1:W:126:ALA:HB2   | 2.45                     | 0.51              |
| 2:a:80:GLN:NE2    | 3:8:58:GLU:CG     | 2.45                     | 0.51              |
| 2:o:21:ARG:HB2    | 2:o:243:GLU:HA    | 1.93                     | 0.51              |
| 2:p:273:CYS:CB    | 2:q:264:MET:O     | 2.42                     | 0.51              |
| 2:t:21:ARG:HB2    | 2:t:243:GLU:HA    | 1.93                     | 0.51              |
| 3:0:9:LYS:HZ1     | 5:AD:72:ASP:HA    | 1.76                     | 0.51              |
| 3:7:244:SER:HB2   | 3:ZC:260:LEU:HD21 | 1.92                     | 0.51              |
| 3:ZC:122:VAL:O    | 4:ZH:322:ASN:ND2  | 2.44                     | 0.51              |
| 4:ZL:355:LYS:HZ1  | 4:ZR:89:ASN:HD21  | 1.59                     | 0.51              |
| 4:ZO:102:LEU:HD21 | 4:ZO:106:ARG:HD2  | 1.93                     | 0.51              |
| 4:ZP:24:ILE:HG22  | 4:ZU:385:ASN:OD1  | 2.10                     | 0.51              |
| 4:ZQ:104:GLU:OE2  | 4:ZV:339:ALA:HA   | 2.11                     | 0.51              |
| 4:ZQ:367:ASP:O    | 4:ZQ:371:GLU:HG2  | 2.10                     | 0.51              |
| 4:ZS:93:PHE:HB3   | 4:ZS:333:VAL:HG13 | 1.93                     | 0.51              |
| 4:Zb:86:VAL:HG13  | 4:Zb:115:GLN:HB2  | 1.92                     | 0.51              |
| 4:Zc:146:ALA:HB2  | 4:Zc:286:PRO:HD3  | 1.92                     | 0.51              |
| 5:AA:26:LEU:CD1   | 3:AF:242:ILE:HG23 | 2.33                     | 0.51              |
| 5:AA:235:THR:OG1  | 3:AF:260:LEU:CD1  | 2.59                     | 0.51              |
| 5:AB:89:VAL:HG12  | 5:AB:121:ILE:HB   | 1.91                     | 0.51              |
| 5:AB:172:GLN:HB2  | 5:AB:182:THR:HG22 | 1.93                     | 0.51              |
| 5:AB:214:VAL:CG2  | 3:AM:257:LEU:HD22 | 2.40                     | 0.51              |
| 3:AK:9:LYS:C      | 3:AK:11:GLY:N     | 2.68                     | 0.51              |
| 6:Ad:235:LEU:HB3  | 6:Ae:244:ARG:HH22 | 1.75                     | 0.51              |
| 6:Ae:256:ILE:HG13 | 6:Ae:257:VAL:N    | 2.26                     | 0.51              |
| 6:Aj:256:ILE:HG13 | 6:Aj:257:VAL:N    | 2.26                     | 0.51              |
| 6:Al:294:ARG:HD2  | 11:A7:68:THR:HG21 | 1.92                     | 0.51              |
| 6:Ap:256:ILE:HG13 | 6:Ap:257:VAL:N    | 2.26                     | 0.51              |
| 8:At:88:MET:HG2   | 8:At:146:LEU:HD11 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:Aw:48:ILE:CD1   | 11:A8:134:LEU:HD23 | 2.40                     | 0.51              |
| 9:Ay:66:ARG:HB2   | 9:Ay:182:ALA:HB2   | 1.92                     | 0.51              |
| 6:UN:204:GLY:O    | 6:UN:206:PRO:HD3   | 2.11                     | 0.51              |
| 6:WD:197:LEU:HA   | 6:WE:175:SER:CB    | 2.40                     | 0.51              |
| 6:WN:203:ALA:HB1  | 6:WO:160:PRO:HB3   | 1.93                     | 0.51              |
| 1:N:219:MET:SD    | 1:O:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:O:219:MET:SD    | 1:P:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:Q:219:MET:SD    | 1:R:212:TYR:CD1    | 3.03                     | 0.51              |
| 1:V:219:MET:SD    | 1:W:212:TYR:CD1    | 3.03                     | 0.51              |
| 2:a:196:MET:SD    | 2:a:247:THR:HG22   | 2.50                     | 0.51              |
| 2:c:196:MET:SD    | 2:c:247:THR:HG22   | 2.50                     | 0.51              |
| 2:c:273:CYS:CB    | 2:d:264:MET:O      | 2.42                     | 0.51              |
| 2:n:21:ARG:HB2    | 2:n:243:GLU:HA     | 1.93                     | 0.51              |
| 2:r:196:MET:SD    | 2:r:247:THR:HG22   | 2.50                     | 0.51              |
| 2:x:21:ARG:HB2    | 2:x:243:GLU:HA     | 1.93                     | 0.51              |
| 3:6:106:MET:HE3   | 3:6:137:GLN:HG3    | 1.93                     | 0.51              |
| 3:6:115:THR:HB    | 3:6:191:LEU:HD23   | 1.93                     | 0.51              |
| 3:7:1:MET:HB3     | 3:AK:29:VAL:HG11   | 1.91                     | 0.51              |
| 3:8:57:SER:OG     | 3:AG:154:ASP:CG    | 2.54                     | 0.51              |
| 3:8:194:GLU:OE1   | 3:8:201:PRO:HD3    | 2.10                     | 0.51              |
| 3:9:85:ASN:HB3    | 4:ZK:4:SER:HB3     | 1.93                     | 0.51              |
| 3:ZD:42:GLU:OE2   | 3:ZD:73:ARG:NE     | 2.35                     | 0.51              |
| 3:ZE:77:THR:OG1   | 4:ZJ:47:LYS:HA     | 2.10                     | 0.51              |
| 4:ZF:139:ILE:HG12 | 4:ZF:312:LEU:HD22  | 1.92                     | 0.51              |
| 4:ZG:30:TYR:HD1   | 4:ZG:363:ALA:HA    | 1.75                     | 0.51              |
| 4:ZG:157:ASN:ND2  | 4:ZM:143:LEU:HD13  | 2.26                     | 0.51              |
| 4:ZM:203:THR:OG1  | 4:ZM:207:GLU:OE1   | 2.23                     | 0.51              |
| 4:ZN:17:LEU:HD13  | 4:ZS:395:ILE:HD11  | 1.93                     | 0.51              |
| 4:ZR:114:MET:HE1  | 4:ZR:333:VAL:HG11  | 1.93                     | 0.51              |
| 4:ZS:102:LEU:HD21 | 4:ZS:106:ARG:HD3   | 1.93                     | 0.51              |
| 4:ZU:33:LYS:NZ    | 4:ZU:362:GLU:OE1   | 2.40                     | 0.51              |
| 4:ZV:184:VAL:HG13 | 4:ZV:196:MET:HB2   | 1.93                     | 0.51              |
| 4:ZV:269:GLN:CB   | 4:Zb:286:PRO:HG2   | 2.40                     | 0.51              |
| 4:Zd:349:GLY:HA3  | 4:Zd:355:LYS:HD3   | 1.92                     | 0.51              |
| 4:Zh:284:TYR:HB2  | 4:Zh:306:ASN:HD22  | 1.76                     | 0.51              |
| 6:AR:235:LEU:HB3  | 6:Ac:244:ARG:HH22  | 1.75                     | 0.51              |
| 6:AS:256:ILE:HG13 | 6:AS:257:VAL:N     | 2.26                     | 0.51              |
| 6:Ag:297:GLN:CB   | 11:A8:73:ILE:HD13  | 2.35                     | 0.51              |
| 6:Ai:235:LEU:HB3  | 6:Aj:244:ARG:HH22  | 1.75                     | 0.51              |
| 6:Ak:256:ILE:HG13 | 6:Ak:257:VAL:N     | 2.26                     | 0.51              |
| 6:Ap:303:GLN:OE1  | 6:BI:320:PRO:HG2   | 2.10                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:Aw:38:TRP:HA    | 10:A3:46:SER:OG    | 2.11                     | 0.51              |
| 9:Aw:40:LEU:HG    | 11:A8:130:MET:HE1  | 1.93                     | 0.51              |
| 11:A7:67:LEU:HG   | 11:A7:72:HIS:HB3   | 1.92                     | 0.51              |
| 6:UP:129:GLN:O    | 6:UP:133:GLN:N     | 2.29                     | 0.51              |
| 12:BB:7:PHE:HZ    | 12:BB:123:LYS:HB2  | 1.76                     | 0.51              |
| 12:BC:4:LEU:HD13  | 12:BC:126:MET:HE1  | 1.91                     | 0.51              |
| 1:L:62:TYR:HD1    | 2:j:129:VAL:HG11   | 1.62                     | 0.51              |
| 2:a:62:LEU:HD22   | 2:a:81:LEU:HD11    | 1.92                     | 0.51              |
| 2:b:21:ARG:HB2    | 2:b:243:GLU:HA     | 1.93                     | 0.51              |
| 2:b:80:GLN:OE1    | 3:AG:170:VAL:C     | 2.53                     | 0.51              |
| 2:j:62:LEU:HD22   | 2:j:81:LEU:HD11    | 1.92                     | 0.51              |
| 2:r:62:LEU:HD22   | 2:r:81:LEU:HD11    | 1.92                     | 0.51              |
| 3:0:120:PHE:HB3   | 3:0:128:LEU:HD22   | 1.92                     | 0.51              |
| 3:2:254:LEU:HD13  | 3:AK:238:ARG:HG3   | 1.93                     | 0.51              |
| 3:4:73:ARG:HH22   | 3:9:50:ARG:HH12    | 1.59                     | 0.51              |
| 3:5:7:ILE:HG23    | 3:5:71:GLY:HA2     | 1.93                     | 0.51              |
| 3:6:35:LYS:NZ     | 3:6:220:GLU:OE2    | 2.39                     | 0.51              |
| 3:ZC:174:ASN:ND2  | 3:ZC:203:GLU:OE2   | 2.42                     | 0.51              |
| 4:ZG:390:LYS:HG2  | 4:ZG:394:GLN:HE21  | 1.76                     | 0.51              |
| 4:ZJ:109:VAL:HG12 | 4:ZJ:115:GLN:HG3   | 1.93                     | 0.51              |
| 4:ZK:348:ALA:HB2  | 4:ZK:356:LEU:HD13  | 1.93                     | 0.51              |
| 4:ZO:373:VAL:O    | 4:ZO:374:ASN:C     | 2.54                     | 0.51              |
| 4:ZT:18:ASP:O     | 4:ZY:5:GLN:OE1     | 2.27                     | 0.51              |
| 4:ZV:211:TYR:HE2  | 4:ZV:226:ALA:HA    | 1.75                     | 0.51              |
| 4:Za:109:VAL:HG12 | 4:Za:115:GLN:HA    | 1.92                     | 0.51              |
| 4:Zc:188:ASP:OD1  | 4:Zc:192:ASN:N     | 2.44                     | 0.51              |
| 4:Zh:392:GLN:HA   | 4:Zh:395:ILE:HG22  | 1.93                     | 0.51              |
| 5:AA:9:MET:CB     | 12:BA:103:VAL:HG21 | 2.41                     | 0.51              |
| 5:AC:231:MET:CE   | 3:AH:260:LEU:HD22  | 2.40                     | 0.51              |
| 3:AI:241:GLU:HG2  | 3:AN:256:LYS:HG2   | 1.93                     | 0.51              |
| 6:AV:278:THR:CG2  | 10:A3:21:ALA:CB    | 2.74                     | 0.51              |
| 6:AX:278:THR:HG22 | 10:A3:7:ILE:HG21   | 1.91                     | 0.51              |
| 6:AY:235:LEU:HB3  | 6:AZ:244:ARG:HH22  | 1.75                     | 0.51              |
| 6:Aa:256:ILE:HG13 | 6:Aa:257:VAL:N     | 2.26                     | 0.51              |
| 6:Ak:293:LEU:HD21 | 6:Ak:364:SER:HB3   | 1.91                     | 0.51              |
| 6:Ak:370:ARG:HE   | 10:A1:7:ILE:CD1    | 2.24                     | 0.51              |
| 6:An:256:ILE:HG13 | 6:An:257:VAL:N     | 2.26                     | 0.51              |
| 6:Ap:293:LEU:HD21 | 6:Ap:364:SER:HB3   | 1.92                     | 0.51              |
| 7:As:89:GLY:O     | 9:Ay:143:ARG:NE    | 2.44                     | 0.51              |
| 9:Ay:38:TRP:HZ2   | 10:A5:39:HIS:CD2   | 2.29                     | 0.51              |
| 10:A5:11:ILE:HG22 | 6:BR:372:ILE:CG2   | 2.41                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:A8:128:LYS:CE  | 12:BC:134:GLN:HE21 | 2.24                     | 0.51              |
| 6:WB:190:GLN:NE2  | 6:WC:216:SER:O     | 2.44                     | 0.51              |
| 6:WM:132:TYR:CD1  | 6:WN:130:VAL:HG22  | 2.45                     | 0.51              |
| 1:J:219:MET:SD    | 1:K:212:TYR:CD1    | 3.03                     | 0.50              |
| 1:V:65:LEU:CG     | 2:u:65:MET:HG3     | 2.39                     | 0.50              |
| 2:c:21:ARG:HB2    | 2:c:243:GLU:HA     | 1.93                     | 0.50              |
| 2:p:21:ARG:HB2    | 2:p:243:GLU:HA     | 1.93                     | 0.50              |
| 3:3:122:VAL:O     | 3:8:180:ASN:ND2    | 2.42                     | 0.50              |
| 3:4:184:LEU:HB3   | 3:4:192:TYR:HB3    | 1.93                     | 0.50              |
| 3:6:137:GLN:HA    | 3:6:138:PRO:O      | 2.11                     | 0.50              |
| 3:8:42:GLU:CB     | 3:8:75:VAL:HG23    | 2.40                     | 0.50              |
| 3:ZA:50:ARG:CB    | 3:ZA:66:LEU:H      | 2.23                     | 0.50              |
| 3:ZB:175:LEU:HD21 | 3:ZB:214:LEU:HD21  | 1.93                     | 0.50              |
| 4:ZJ:34:SER:HB3   | 4:ZJ:366:VAL:HG22  | 1.92                     | 0.50              |
| 4:ZK:27:SER:HA    | 4:ZK:366:VAL:HG21  | 1.93                     | 0.50              |
| 4:ZQ:71:ARG:HG2   | 4:ZQ:73:LEU:H      | 1.76                     | 0.50              |
| 4:ZS:139:ILE:HA   | 4:ZS:312:LEU:HD23  | 1.93                     | 0.50              |
| 4:Za:41:ASP:N     | 4:Za:41:ASP:OD1    | 2.44                     | 0.50              |
| 4:Zc:382:TYR:CE2  | 4:Zh:395:ILE:HD11  | 2.46                     | 0.50              |
| 5:AC:28:ASN:CG    | 3:AH:72:VAL:HB     | 2.36                     | 0.50              |
| 6:AS:295:SER:HB2  | 11:A0:65:LEU:CB    | 2.39                     | 0.50              |
| 6:AU:235:LEU:HB3  | 6:AV:244:ARG:HH22  | 1.75                     | 0.50              |
| 6:AX:372:ILE:CB   | 10:A3:11:ILE:HG22  | 2.40                     | 0.50              |
| 6:AY:256:ILE:HG13 | 6:AY:257:VAL:N     | 2.26                     | 0.50              |
| 6:UP:204:GLY:O    | 6:UP:206:PRO:HD3   | 2.11                     | 0.50              |
| 12:BB:37:PRO:HA   | 6:BI:328:ILE:O     | 2.11                     | 0.50              |
| 6:WB:187:ASP:OD1  | 6:WB:190:GLN:N     | 2.41                     | 0.50              |
| 6:WK:200:SER:CA   | 6:WL:173:SER:OG    | 2.59                     | 0.50              |
| 6:WR:115:LEU:HD22 | 6:WR:134:ARG:HH11  | 1.75                     | 0.50              |
| 6:WV:196:HIS:HB3  | 6:WW:211:THR:HG21  | 1.93                     | 0.50              |
| 6:WW:145:GLU:C    | 6:WW:147:LEU:H     | 2.19                     | 0.50              |
| 6:BL:320:PRO:C    | 6:BM:328:ILE:HD11  | 2.35                     | 0.50              |
| 1:M:219:MET:SD    | 1:N:212:TYR:CD1    | 3.03                     | 0.50              |
| 2:a:21:ARG:HB2    | 2:a:243:GLU:HA     | 1.93                     | 0.50              |
| 2:m:21:ARG:HB2    | 2:m:243:GLU:HA     | 1.93                     | 0.50              |
| 2:s:21:ARG:HB2    | 2:s:243:GLU:HA     | 1.93                     | 0.50              |
| 2:s:62:LEU:HD22   | 2:s:81:LEU:HD11    | 1.92                     | 0.50              |
| 3:0:6:TRP:CE3     | 5:AD:72:ASP:HB3    | 2.46                     | 0.50              |
| 3:0:185:GLU:HB3   | 3:0:193:ILE:HG13   | 1.93                     | 0.50              |
| 3:1:142:ILE:HD11  | 3:1:149:ILE:HD12   | 1.93                     | 0.50              |
| 3:3:180:ASN:OD1   | 3:3:182:THR:OG1    | 2.24                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:7:17:THR:O      | 3:7:18:ASN:C      | 2.54                     | 0.50              |
| 3:7:54:ALA:O      | 3:7:55:GLN:C      | 2.53                     | 0.50              |
| 3:ZB:104:GLN:HG2  | 3:ZB:137:GLN:HB3  | 1.93                     | 0.50              |
| 3:ZD:137:GLN:HA   | 3:ZD:139:ALA:N    | 2.23                     | 0.50              |
| 4:ZM:17:LEU:HD13  | 4:ZR:395:ILE:HD11 | 1.92                     | 0.50              |
| 4:ZM:144:MET:HE3  | 4:ZM:306:ASN:HD21 | 1.76                     | 0.50              |
| 4:ZV:95:SER:OG    | 4:ZV:333:VAL:HG23 | 2.11                     | 0.50              |
| 4:Zd:317:LEU:HD11 | 4:Zd:356:LEU:HD21 | 1.93                     | 0.50              |
| 4:Zf:314:GLN:NE2  | 4:Zf:347:THR:OG1  | 2.44                     | 0.50              |
| 4:Zf:381:ASN:O    | 4:Zf:385:ASN:ND2  | 2.44                     | 0.50              |
| 4:Zg:83:PHE:HB2   | 4:Zg:95:SER:O     | 2.11                     | 0.50              |
| 3:AL:2:ILE:HG23   | 3:AL:254:LEU:HD11 | 1.91                     | 0.50              |
| 6:AW:256:ILE:HG13 | 6:AW:257:VAL:N    | 2.26                     | 0.50              |
| 6:Al:256:ILE:HG13 | 6:Al:257:VAL:N    | 2.26                     | 0.50              |
| 6:AQ:235:LEU:HB3  | 6:BR:244:ARG:HH22 | 1.75                     | 0.50              |
| 7:As:58:VAL:O     | 7:As:62:ILE:HD12  | 2.12                     | 0.50              |
| 8:At:205:ASN:HB3  | 9:Au:209:MET:HG3  | 1.92                     | 0.50              |
| 9:Av:75:ARG:NH2   | 9:Av:84:PRO:O     | 2.44                     | 0.50              |
| 9:Ax:204:LEU:HD11 | 9:Ax:217:ILE:HD12 | 1.93                     | 0.50              |
| 6:UO:129:GLN:O    | 6:UO:133:GLN:N    | 2.29                     | 0.50              |
| 6:UP:162:PRO:O    | 6:UP:163:SER:C    | 2.55                     | 0.50              |
| 6:BV:256:ILE:HG13 | 6:BV:257:VAL:N    | 2.26                     | 0.50              |
| 6:BX:256:ILE:HG13 | 6:BX:257:VAL:N    | 2.26                     | 0.50              |
| 1:A:219:MET:SD    | 1:B:212:TYR:CD1   | 3.03                     | 0.50              |
| 3:0:242:ILE:HG21  | 3:AJ:26:LEU:HD22  | 1.92                     | 0.50              |
| 3:ZB:5:LEU:O      | 3:ZB:9:LYS:HG3    | 2.11                     | 0.50              |
| 3:ZB:151:ILE:HG23 | 3:ZB:157:VAL:HG22 | 1.93                     | 0.50              |
| 3:ZC:167:PRO:HG2  | 4:ZN:338:GLN:HB2  | 1.93                     | 0.50              |
| 4:ZI:17:LEU:HD13  | 4:ZN:395:ILE:CD1  | 2.40                     | 0.50              |
| 4:ZK:248:THR:HG1  | 4:ZK:257:ALA:N    | 2.09                     | 0.50              |
| 4:ZM:374:ASN:O    | 4:ZM:377:VAL:N    | 2.43                     | 0.50              |
| 4:ZO:380:ARG:HD2  | 4:ZU:396:LEU:HB3  | 1.93                     | 0.50              |
| 4:ZP:22:ASN:N     | 4:ZU:5:GLN:NE2    | 2.59                     | 0.50              |
| 4:ZW:17:LEU:CD1   | 4:Zb:395:ILE:HD11 | 2.41                     | 0.50              |
| 5:AB:229:MET:HG2  | 12:BC:102:MET:SD  | 2.51                     | 0.50              |
| 5:AC:49:LEU:HG    | 6:BM:322:PRO:CD   | 2.41                     | 0.50              |
| 5:AD:234:ILE:CG2  | 3:AI:260:LEU:HD11 | 2.41                     | 0.50              |
| 3:AF:82:SER:OG    | 3:AF:223:ASN:ND2  | 2.36                     | 0.50              |
| 3:AG:20:ASP:OD1   | 3:AL:4:SER:OG     | 2.28                     | 0.50              |
| 3:AJ:176:THR:HA   | 3:AJ:203:GLU:HA   | 1.93                     | 0.50              |
| 6:AX:256:ILE:HG13 | 6:AX:257:VAL:N    | 2.26                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:Ay:143:ARG:NE   | 9:Ay:180:LYS:HE2   | 2.27                     | 0.50              |
| 6:U1:98:LEU:HD22  | 6:U1:147:LEU:CD2   | 2.39                     | 0.50              |
| 6:UL:162:PRO:O    | 6:UL:163:SER:C     | 2.55                     | 0.50              |
| 12:BB:54:ALA:HB3  | 12:BB:55:PRO:HD3   | 1.92                     | 0.50              |
| 1:C:219:MET:SD    | 1:D:212:TYR:CD1    | 3.03                     | 0.50              |
| 1:F:219:MET:SD    | 1:G:212:TYR:CD1    | 3.03                     | 0.50              |
| 2:b:80:GLN:OE1    | 3:AG:170:VAL:CA    | 2.59                     | 0.50              |
| 2:q:21:ARG:HB2    | 2:q:243:GLU:HA     | 1.93                     | 0.50              |
| 2:w:54:GLN:OE1    | 3:AH:141:THR:CG2   | 2.60                     | 0.50              |
| 3:0:231:VAL:O     | 3:0:235:GLN:HG3    | 2.12                     | 0.50              |
| 3:1:248:SER:O     | 3:1:252:GLN:HG3    | 2.11                     | 0.50              |
| 3:4:255:GLN:HE21  | 3:4:259:GLN:NE2    | 2.10                     | 0.50              |
| 3:7:164:GLN:HE22  | 3:7:166:ALA:HB3    | 1.76                     | 0.50              |
| 3:ZA:235:GLN:NE2  | 4:ZG:3:PHE:CG      | 2.79                     | 0.50              |
| 3:ZC:88:GLN:HE21  | 4:ZN:53:LYS:HB2    | 1.74                     | 0.50              |
| 4:ZF:157:ASN:HD22 | 4:ZL:143:LEU:HD13  | 1.76                     | 0.50              |
| 4:ZQ:268:GLN:HG2  | 4:ZW:190:GLN:NE2   | 2.26                     | 0.50              |
| 4:ZU:157:ASN:ND2  | 4:Za:143:LEU:CD2   | 2.74                     | 0.50              |
| 4:ZV:314:GLN:NE2  | 4:ZV:347:THR:OG1   | 2.44                     | 0.50              |
| 4:ZX:387:GLN:HG3  | 4:Zd:400:VAL:HB    | 1.93                     | 0.50              |
| 4:Zb:109:VAL:HG12 | 4:Zb:115:GLN:HA    | 1.92                     | 0.50              |
| 4:Zb:322:ASN:OD1  | 4:Zb:325:GLY:N     | 2.45                     | 0.50              |
| 4:Ze:362:GLU:OE1  | 4:Ze:362:GLU:N     | 2.38                     | 0.50              |
| 5:AA:217:MET:HE2  | 3:AL:258:THR:HA    | 1.94                     | 0.50              |
| 5:AE:229:MET:CE   | 3:AK:257:LEU:HD23  | 2.39                     | 0.50              |
| 3:AH:142:ILE:HG21 | 3:AH:149:ILE:HG12  | 1.93                     | 0.50              |
| 6:Ah:256:ILE:HG13 | 6:Ah:257:VAL:N     | 2.26                     | 0.50              |
| 9:Au:232:TRP:NE1  | 9:Au:236:MET:HE3   | 2.27                     | 0.50              |
| 9:Ay:84:PRO:O     | 9:Ay:85:PRO:C      | 2.54                     | 0.50              |
| 9:Ay:167:MET:HG3  | 9:Ay:171:LEU:HG    | 1.93                     | 0.50              |
| 10:A4:86:ILE:HD11 | 11:A9:133:VAL:HG22 | 1.92                     | 0.50              |
| 6:U1:162:PRO:O    | 6:U1:163:SER:C     | 2.55                     | 0.50              |
| 6:WJ:139:GLU:HB3  | 6:WK:156:HIS:HE1   | 1.76                     | 0.50              |
| 6:WK:160:PRO:HB3  | 6:WK:170:LYS:HB2   | 1.93                     | 0.50              |
| 6:WQ:163:SER:HB3  | 6:WQ:166:VAL:HG23  | 1.94                     | 0.50              |
| 6:WT:162:PRO:O    | 6:WT:163:SER:HB3   | 2.11                     | 0.50              |
| 1:B:65:LEU:CG     | 2:a:65:MET:HG3     | 2.39                     | 0.50              |
| 3:0:6:TRP:CZ2     | 3:AI:235:GLN:NE2   | 2.78                     | 0.50              |
| 3:1:44:LEU:HD13   | 5:AE:71:LEU:HD12   | 1.93                     | 0.50              |
| 3:3:45:LEU:HD22   | 3:AG:98:LYS:HG3    | 1.93                     | 0.50              |
| 3:4:32:ASN:HD21   | 3:9:38:ARG:NH2     | 2.10                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:108:PRO:HG2   | 3:AM:153:ARG:HH21 | 1.76                     | 0.50              |
| 3:ZB:56:SER:C     | 3:AJ:153:ARG:H    | 2.19                     | 0.50              |
| 4:ZG:300:VAL:HG13 | 4:ZG:312:LEU:HB2  | 1.93                     | 0.50              |
| 4:ZH:84:ARG:HD2   | 4:ZH:345:LEU:HD21 | 1.93                     | 0.50              |
| 4:ZH:319:ASN:HB2  | 4:ZH:353:PHE:CE1  | 2.47                     | 0.50              |
| 4:ZN:233:ASN:HD21 | 4:ZN:237:ILE:HB   | 1.77                     | 0.50              |
| 4:ZU:183:THR:OG1  | 4:Zf:132:ALA:HA   | 2.10                     | 0.50              |
| 4:Zc:382:TYR:CZ   | 4:Zh:395:ILE:HD11 | 2.47                     | 0.50              |
| 4:Zf:319:ASN:OD1  | 4:Zf:320:PHE:N    | 2.44                     | 0.50              |
| 5:AB:71:LEU:CD2   | 3:AM:70:THR:HG21  | 2.35                     | 0.50              |
| 3:AF:47:GLN:HE22  | 12:BA:73:PRO:CB   | 2.24                     | 0.50              |
| 3:AM:2:ILE:HG13   | 3:AM:254:LEU:HD21 | 1.93                     | 0.50              |
| 6:Ae:372:ILE:HG22 | 10:A2:4:ILE:HG13  | 1.92                     | 0.50              |
| 6:An:293:LEU:HD21 | 6:An:364:SER:HB3  | 1.91                     | 0.50              |
| 6:AQ:256:ILE:HG13 | 6:AQ:257:VAL:N    | 2.26                     | 0.50              |
| 9:Ax:59:LEU:O     | 9:Ax:65:THR:OG1   | 2.28                     | 0.50              |
| 11:A0:46:ALA:O    | 11:A0:50:LYS:HG2  | 2.11                     | 0.50              |
| 6:WI:193:ALA:HB1  | 6:WJ:213:VAL:HG21 | 1.93                     | 0.50              |
| 6:WP:128:GLU:CG   | 6:WQ:126:PHE:CE2  | 2.93                     | 0.50              |
| 2:d:21:ARG:HB2    | 2:d:243:GLU:HA    | 1.93                     | 0.50              |
| 2:y:21:ARG:HB2    | 2:y:243:GLU:HA    | 1.93                     | 0.50              |
| 3:0:150:THR:OG1   | 3:0:158:SER:OG    | 2.29                     | 0.50              |
| 3:0:163:GLY:HA2   | 3:ZB:111:THR:HG21 | 1.93                     | 0.50              |
| 3:3:180:ASN:HB3   | 3:3:198:SER:HA    | 1.93                     | 0.50              |
| 3:ZB:240:TYR:CE2  | 4:ZG:399:LEU:HD11 | 2.47                     | 0.50              |
| 3:ZE:59:GLN:HG2   | 3:ZE:60:THR:HG23  | 1.92                     | 0.50              |
| 4:ZL:42:MET:HG2   | 4:ZL:53:LYS:HD3   | 1.93                     | 0.50              |
| 4:ZP:6:ALA:HB1    | 4:ZP:389:ILE:HG13 | 1.94                     | 0.50              |
| 5:AC:235:THR:OG1  | 3:AH:260:LEU:HD12 | 2.10                     | 0.50              |
| 5:AD:129:VAL:HG11 | 5:AD:135:ILE:HD11 | 1.92                     | 0.50              |
| 5:AE:101:ARG:NH1  | 5:AE:207:GLU:OE1  | 2.45                     | 0.50              |
| 3:AI:164:GLN:C    | 3:AI:166:ALA:H    | 2.19                     | 0.50              |
| 6:Af:297:GLN:HE22 | 11:A8:76:GLN:N    | 2.08                     | 0.50              |
| 6:Al:235:LEU:HB3  | 6:Am:244:ARG:HH22 | 1.75                     | 0.50              |
| 11:A8:92:GLN:NE2  | 12:BD:22:ASN:HD22 | 2.10                     | 0.50              |
| 6:WC:181:GLU:O    | 6:WC:182:PRO:C    | 2.53                     | 0.50              |
| 6:WF:116:LEU:HD22 | 6:WF:131:ASN:HA   | 1.94                     | 0.50              |
| 6:WG:115:LEU:HG   | 6:WG:116:LEU:N    | 2.25                     | 0.50              |
| 12:BC:68:ILE:HD11 | 6:BL:312:VAL:HG22 | 1.93                     | 0.50              |
| 1:K:65:LEU:CG     | 2:j:65:MET:HG3    | 2.39                     | 0.50              |
| 1:L:65:LEU:CG     | 2:k:65:MET:HG3    | 2.39                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:a:208:ARG:O     | 2:a:212:SER:OG     | 2.16                     | 0.50              |
| 2:d:273:CYS:CB    | 2:e:264:MET:O      | 2.42                     | 0.50              |
| 3:0:19:MET:HB2    | 3:0:236:VAL:HG11   | 1.94                     | 0.50              |
| 3:3:151:ILE:HG12  | 3:3:157:VAL:HG22   | 1.93                     | 0.50              |
| 3:5:56:SER:H      | 3:5:61:THR:HA      | 1.77                     | 0.50              |
| 3:5:173:LEU:HD23  | 3:5:214:LEU:HD13   | 1.93                     | 0.50              |
| 3:5:235:GLN:HG3   | 3:ZB:5:LEU:CD2     | 2.41                     | 0.50              |
| 3:9:175:LEU:HD13  | 3:9:206:PRO:HG3    | 1.93                     | 0.50              |
| 3:ZA:218:TYR:OH   | 4:ZL:53:LYS:HB2    | 2.11                     | 0.50              |
| 3:ZC:231:VAL:HG11 | 4:ZI:7:VAL:HG22    | 1.94                     | 0.50              |
| 4:ZF:99:GLN:HG2   | 4:ZF:111:MET:HE2   | 1.93                     | 0.50              |
| 4:ZG:160:SER:HA   | 4:ZG:268:GLN:HE21  | 1.76                     | 0.50              |
| 4:ZH:210:VAL:O    | 4:ZH:227:SER:N     | 2.45                     | 0.50              |
| 4:ZT:337:THR:OG1  | 4:ZT:338:GLN:N     | 2.45                     | 0.50              |
| 4:ZU:379:GLN:NE2  | 4:ZZ:391:THR:HA    | 2.25                     | 0.50              |
| 4:ZW:269:GLN:OE1  | 4:Zc:286:PRO:CG    | 2.60                     | 0.50              |
| 4:Za:102:LEU:O    | 4:Zf:322:ASN:CB    | 2.58                     | 0.50              |
| 4:Za:102:LEU:O    | 4:Zf:322:ASN:CG    | 2.55                     | 0.50              |
| 5:AC:50:SER:HB3   | 11:A8:91:ASP:O     | 2.12                     | 0.50              |
| 5:AC:231:MET:HE1  | 3:AH:260:LEU:HD22  | 1.93                     | 0.50              |
| 5:AE:248:LEU:HD13 | 12:BE:118:VAL:HG23 | 1.93                     | 0.50              |
| 3:AL:184:LEU:HB3  | 3:AL:192:TYR:HB3   | 1.94                     | 0.50              |
| 6:AW:299:ASN:HD22 | 11:A9:55:ARG:HH22  | 1.56                     | 0.50              |
| 10:Az:80:VAL:HG11 | 11:A6:5:LEU:HD11   | 1.93                     | 0.50              |
| 10:A4:83:GLN:HG3  | 11:A0:131:MET:SD   | 2.52                     | 0.50              |
| 10:A5:55:GLN:HG2  | 10:A5:71:VAL:HG22  | 1.94                     | 0.50              |
| 6:UJ:253:GLY:O    | 6:UJ:255:PRO:HD3   | 2.11                     | 0.50              |
| 6:WM:197:LEU:HA   | 6:WN:175:SER:CB    | 2.42                     | 0.50              |
| 6:WQ:190:GLN:HG2  | 6:WR:216:SER:O     | 2.11                     | 0.50              |
| 6:BS:256:ILE:HG13 | 6:BS:257:VAL:N     | 2.26                     | 0.50              |
| 2:h:21:ARG:HB2    | 2:h:243:GLU:HA     | 1.93                     | 0.50              |
| 2:i:21:ARG:HB2    | 2:i:243:GLU:HA     | 1.93                     | 0.50              |
| 2:k:273:CYS:CB    | 2:l:264:MET:O      | 2.42                     | 0.50              |
| 3:3:31:THR:HG22   | 3:8:41:PHE:O       | 2.12                     | 0.50              |
| 3:3:31:THR:HG22   | 3:8:41:PHE:C       | 2.37                     | 0.50              |
| 3:5:5:LEU:HD21    | 3:AN:234:ILE:HG22  | 1.93                     | 0.50              |
| 3:7:52:PRO:HB3    | 3:7:65:GLY:H       | 1.77                     | 0.50              |
| 3:ZC:10:THR:HG23  | 3:ZC:71:GLY:HA3    | 1.94                     | 0.50              |
| 3:ZD:40:VAL:HG23  | 3:ZD:75:VAL:HB     | 1.94                     | 0.50              |
| 4:ZI:374:ASN:O    | 4:ZI:375:MET:C     | 2.54                     | 0.50              |
| 4:ZJ:171:SER:O    | 4:ZJ:177:SER:OG    | 2.28                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZM:165:PRO:HG2  | 4:ZM:201:VAL:HG13  | 1.92                     | 0.50              |
| 4:ZP:234:GLU:OE1  | 4:ZV:255:THR:N     | 2.42                     | 0.50              |
| 4:ZQ:74:ASP:HB3   | 4:ZQ:361:LEU:HG    | 1.93                     | 0.50              |
| 4:ZW:18:ASP:HB3   | 4:Zb:5:GLN:HE22    | 1.76                     | 0.50              |
| 4:Za:348:ALA:HB1  | 4:Za:355:LYS:HA    | 1.94                     | 0.50              |
| 4:Zb:293:GLN:NE2  | 4:Zb:303:ASN:OD1   | 2.45                     | 0.50              |
| 4:Zd:389:ILE:O    | 4:Zd:390:LYS:C     | 2.55                     | 0.50              |
| 4:Zh:77:ILE:HD13  | 4:Zh:96:ARG:HD2    | 1.92                     | 0.50              |
| 5:AB:9:MET:HG3    | 12:BB:103:VAL:CG2  | 2.40                     | 0.50              |
| 5:AD:51:LEU:HD12  | 12:BE:19:LYS:HD2   | 1.94                     | 0.50              |
| 5:AE:54:ARG:NH1   | 12:BF:22:ASN:HD21  | 2.10                     | 0.50              |
| 6:Af:256:ILE:HG13 | 6:Af:257:VAL:N     | 2.26                     | 0.50              |
| 6:Ag:256:ILE:HG13 | 6:Ag:257:VAL:N     | 2.26                     | 0.50              |
| 6:Ao:256:ILE:HG13 | 6:Ao:257:VAL:N     | 2.26                     | 0.50              |
| 6:AP:256:ILE:HG13 | 6:AP:257:VAL:N     | 2.26                     | 0.50              |
| 8:At:229:MET:O    | 8:At:233:MET:HG2   | 2.12                     | 0.50              |
| 10:A4:53:ARG:O    | 10:A4:57:GLU:HG2   | 2.11                     | 0.50              |
| 11:A6:17:ASN:HD22 | 11:A6:57:ARG:NH1   | 2.10                     | 0.50              |
| 11:A6:133:VAL:C   | 11:A6:135:GLN:H    | 2.19                     | 0.50              |
| 11:A8:128:LYS:HE2 | 12:BC:134:GLN:HE21 | 1.76                     | 0.50              |
| 6:UN:162:PRO:O    | 6:UN:163:SER:C     | 2.55                     | 0.50              |
| 6:UP:98:LEU:HD22  | 6:UP:147:LEU:CD2   | 2.39                     | 0.50              |
| 6:WB:114:GLU:O    | 6:WB:115:LEU:C     | 2.55                     | 0.50              |
| 6:WH:193:ALA:CB   | 6:WI:213:VAL:CG1   | 2.88                     | 0.50              |
| 6:WQ:147:LEU:O    | 6:WQ:148:GLY:C     | 2.54                     | 0.50              |
| 6:WT:160:PRO:HD3  | 6:WT:172:PRO:CA    | 2.38                     | 0.50              |
| 1:M:65:LEU:CG     | 2:l:65:MET:HG3     | 2.39                     | 0.50              |
| 2:h:208:ARG:O     | 2:h:212:SER:OG     | 2.16                     | 0.50              |
| 2:m:80:GLN:OE1    | 3:AJ:203:GLU:N     | 2.45                     | 0.50              |
| 2:r:21:ARG:HB2    | 2:r:243:GLU:HA     | 1.93                     | 0.50              |
| 2:r:78:ASN:OD1    | 3:ZA:58:GLU:OE1    | 2.29                     | 0.50              |
| 2:z:21:ARG:HB2    | 2:z:243:GLU:HA     | 1.93                     | 0.50              |
| 3:1:180:ASN:ND2   | 3:AK:122:VAL:O     | 2.45                     | 0.50              |
| 3:2:58:GLU:CG     | 5:AA:160:ARG:HH11  | 2.11                     | 0.50              |
| 3:5:1:MET:HA      | 3:AI:29:VAL:HG22   | 1.94                     | 0.50              |
| 3:5:20:ASP:OD1    | 3:ZA:4:SER:HB3     | 2.12                     | 0.50              |
| 3:5:111:THR:HG21  | 3:AI:163:GLY:HA2   | 1.93                     | 0.50              |
| 3:5:205:THR:HB    | 3:5:208:LEU:HD23   | 1.94                     | 0.50              |
| 3:ZE:93:LYS:NZ    | 3:ZE:122:VAL:HG23  | 2.27                     | 0.50              |
| 4:ZF:52:VAL:HG22  | 4:ZF:53:LYS:N      | 2.27                     | 0.50              |
| 4:ZG:107:ASN:HD22 | 4:ZG:138:THR:HG22  | 1.77                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZO:65:THR:HG22  | 4:ZZ:50:LEU:HD22   | 1.93                     | 0.50              |
| 4:ZQ:156:ILE:HG22 | 4:ZQ:276:ILE:HG23  | 1.93                     | 0.50              |
| 4:ZQ:157:ASN:HD21 | 4:ZW:143:LEU:HD23  | 1.77                     | 0.50              |
| 4:ZS:116:LEU:HD21 | 4:ZS:315:ILE:HD13  | 1.94                     | 0.50              |
| 4:ZT:196:MET:SD   | 4:ZT:248:THR:HG22  | 2.51                     | 0.50              |
| 4:Za:24:ILE:HD13  | 4:Zf:384:SER:HG    | 1.76                     | 0.50              |
| 4:Za:106:ARG:NH1  | 4:Zf:321:ALA:CB    | 2.75                     | 0.50              |
| 4:Zg:144:MET:HE2  | 4:Zg:310:GLN:HE21  | 1.76                     | 0.50              |
| 5:AB:248:LEU:HD13 | 12:BB:118:VAL:HG23 | 1.92                     | 0.50              |
| 9:Au:224:MET:O    | 9:Au:228:LEU:HB2   | 2.12                     | 0.50              |
| 9:Av:82:SER:HA    | 10:Az:103:GLN:HE21 | 1.77                     | 0.50              |
| 6:UJ:73:MET:HE3   | 6:UJ:99:ARG:CD     | 2.41                     | 0.50              |
| 6:WA:112:GLY:O    | 6:WA:115:LEU:HB3   | 2.12                     | 0.50              |
| 6:WA:213:VAL:CG2  | 6:WW:193:ALA:HB1   | 2.42                     | 0.50              |
| 6:BU:256:ILE:HG13 | 6:BU:257:VAL:N     | 2.26                     | 0.50              |
| 1:H:62:TYR:HD1    | 2:f:129:VAL:HG11   | 1.62                     | 0.49              |
| 1:W:65:LEU:CG     | 2:v:65:MET:HG3     | 2.39                     | 0.49              |
| 2:o:273:CYS:CB    | 2:p:264:MET:O      | 2.42                     | 0.49              |
| 3:0:51:GLN:NE2    | 3:0:65:GLY:HA3     | 2.27                     | 0.49              |
| 3:2:70:THR:HG22   | 3:2:71:GLY:H       | 1.77                     | 0.49              |
| 3:2:231:VAL:HG11  | 3:8:9:LYS:CG       | 2.39                     | 0.49              |
| 3:5:241:GLU:HB3   | 3:ZB:258:THR:HG21  | 1.94                     | 0.49              |
| 3:7:1:MET:HB3     | 3:AK:29:VAL:CG1    | 2.42                     | 0.49              |
| 3:8:34:PHE:HB3    | 3:8:222:SER:HB3    | 1.94                     | 0.49              |
| 4:ZH:175:ALA:HA   | 4:ZH:178:TYR:CZ    | 2.47                     | 0.49              |
| 4:ZL:379:GLN:HG3  | 4:ZQ:391:THR:HG23  | 1.94                     | 0.49              |
| 4:ZT:233:ASN:HD21 | 4:ZT:237:ILE:HB    | 1.77                     | 0.49              |
| 4:ZT:379:GLN:NE2  | 4:ZY:394:GLN:HB2   | 2.27                     | 0.49              |
| 4:ZU:285:LYS:O    | 4:ZU:306:ASN:ND2   | 2.42                     | 0.49              |
| 4:ZV:269:GLN:HB3  | 4:Zb:286:PRO:HG2   | 1.94                     | 0.49              |
| 4:Zb:154:MET:HE3  | 4:Zb:156:ILE:HB    | 1.93                     | 0.49              |
| 4:Zb:288:ASP:O    | 4:Zb:305:SER:N     | 2.45                     | 0.49              |
| 5:AA:71:LEU:HG    | 3:AL:70:THR:HG21   | 1.94                     | 0.49              |
| 3:AI:36:ARG:NH2   | 3:AI:229:GLU:OE2   | 2.45                     | 0.49              |
| 6:Af:294:ARG:HG2  | 11:A8:66:THR:OG1   | 2.11                     | 0.49              |
| 6:Ai:256:ILE:HG13 | 6:Ai:257:VAL:N     | 2.26                     | 0.49              |
| 6:Al:294:ARG:HD2  | 6:Al:367:GLU:OE1   | 2.12                     | 0.49              |
| 6:Am:294:ARG:HD2  | 6:Am:367:GLU:OE1   | 2.12                     | 0.49              |
| 7:Aq:9:MET:O      | 7:Aq:12:GLU:HG2    | 2.12                     | 0.49              |
| 7:As:2:THR:HG23   | 7:As:5:SER:H       | 1.76                     | 0.49              |
| 8:At:145:TRP:HA   | 6:WJ:164:LEU:HD11  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Aw:105:ILE:HG22 | 10:A2:32:VAL:HB   | 1.94                     | 0.49              |
| 6:UK:162:PRO:O    | 6:UK:163:SER:C    | 2.55                     | 0.49              |
| 6:UM:98:LEU:HD22  | 6:UM:147:LEU:CD2  | 2.39                     | 0.49              |
| 6:UN:69:GLN:HE22  | 6:WS:182:PRO:HG2  | 1.77                     | 0.49              |
| 6:WA:132:TYR:HB2  | 6:WB:126:PHE:HZ   | 1.76                     | 0.49              |
| 6:WD:197:LEU:CD1  | 6:WE:175:SER:OG   | 2.59                     | 0.49              |
| 6:WO:142:ARG:O    | 6:WO:146:THR:HG23 | 2.11                     | 0.49              |
| 6:WP:163:SER:C    | 6:WP:165:PHE:H    | 2.18                     | 0.49              |
| 6:WS:197:LEU:HA   | 6:WT:175:SER:OG   | 2.11                     | 0.49              |
| 12:BD:106:MET:O   | 12:BD:110:ARG:HG2 | 2.12                     | 0.49              |
| 6:BT:256:ILE:HG13 | 6:BT:257:VAL:N    | 2.26                     | 0.49              |
| 6:BV:294:ARG:HD2  | 6:BV:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:BW:256:ILE:HG13 | 6:BW:257:VAL:N    | 2.26                     | 0.49              |
| 6:BW:294:ARG:HD2  | 6:BW:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:35:THR:CG2    | 1:Z:166:GLU:HB2   | 2.30                     | 0.49              |
| 1:C:65:LEU:CG     | 2:b:65:MET:HG3    | 2.39                     | 0.49              |
| 1:D:102:THR:HG23  | 1:E:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:I:102:THR:HG23  | 1:J:130:ASN:ND2   | 2.27                     | 0.49              |
| 1:K:102:THR:HG23  | 1:L:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:L:88:ALA:HB1    | 1:N:171:ILE:CD1   | 2.43                     | 0.49              |
| 1:M:88:ALA:HB1    | 1:O:171:ILE:CD1   | 2.43                     | 0.49              |
| 2:j:21:ARG:HB2    | 2:j:243:GLU:HA    | 1.93                     | 0.49              |
| 2:l:21:ARG:HB2    | 2:l:243:GLU:HA    | 1.93                     | 0.49              |
| 3:4:126:GLY:CA    | 3:9:179:MET:HE3   | 2.42                     | 0.49              |
| 3:ZA:56:SER:O     | 3:AI:153:ARG:N    | 2.45                     | 0.49              |
| 4:ZP:96:ARG:NH2   | 4:ZP:362:GLU:OE2  | 2.39                     | 0.49              |
| 4:ZS:322:ASN:OD1  | 4:ZS:325:GLY:N    | 2.45                     | 0.49              |
| 4:ZX:195:ASP:OD2  | 4:ZX:216:SER:OG   | 2.30                     | 0.49              |
| 4:ZX:208:TRP:NE1  | 4:ZX:268:GLN:OE1  | 2.36                     | 0.49              |
| 4:Zb:114:MET:HE1  | 4:Zb:333:VAL:HG11 | 1.94                     | 0.49              |
| 4:Zc:382:TYR:CD1  | 4:Zh:395:ILE:CD1  | 2.95                     | 0.49              |
| 5:AA:202:MET:SD   | 3:AL:44:LEU:CD2   | 3.00                     | 0.49              |
| 5:AB:71:LEU:HB3   | 3:AM:70:THR:HG22  | 1.94                     | 0.49              |
| 3:AI:189:GLU:O    | 3:AI:191:LEU:HG   | 2.11                     | 0.49              |
| 3:AM:17:THR:C     | 3:AM:19:MET:N     | 2.69                     | 0.49              |
| 7:Ab:74:LEU:C     | 7:Ab:76:TYR:N     | 2.68                     | 0.49              |
| 6:Al:294:ARG:CD   | 11:A7:68:THR:HG21 | 2.42                     | 0.49              |
| 6:AP:294:ARG:HD2  | 6:AP:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:AQ:276:GLU:CD   | 10:A5:11:ILE:HD11 | 2.38                     | 0.49              |
| 7:Aq:85:PRO:HB3   | 9:Aw:242:SER:CA   | 2.43                     | 0.49              |
| 7:As:11:THR:O     | 7:As:15:LYS:HG3   | 2.11                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:As:81:PHE:CZ    | 9:Ay:189:ILE:HD13  | 2.47                     | 0.49              |
| 9:Au:101:MET:HE1  | 9:Au:137:PHE:CZ    | 2.47                     | 0.49              |
| 9:Ay:64:PHE:CE1   | 9:Ay:94:LEU:HD22   | 2.47                     | 0.49              |
| 10:A1:55:GLN:HG2  | 10:A1:71:VAL:HG22  | 1.95                     | 0.49              |
| 10:A4:84:MET:O    | 10:A4:88:VAL:HG23  | 2.11                     | 0.49              |
| 11:A7:96:ASP:OD1  | 11:A7:96:ASP:N     | 2.39                     | 0.49              |
| 6:UJ:159:MET:N    | 6:UJ:159:MET:SD    | 2.82                     | 0.49              |
| 6:BX:294:ARG:HD2  | 6:BX:367:GLU:OE1   | 2.12                     | 0.49              |
| 1:A:88:ALA:HB1    | 1:C:171:ILE:CD1    | 2.43                     | 0.49              |
| 1:B:88:ALA:HB1    | 1:D:171:ILE:CD1    | 2.43                     | 0.49              |
| 1:O:88:ALA:HB1    | 1:Q:171:ILE:CD1    | 2.43                     | 0.49              |
| 2:g:21:ARG:HB2    | 2:g:243:GLU:HA     | 1.93                     | 0.49              |
| 2:n:346:MET:HE3   | 2:p:142:LEU:CD1    | 2.42                     | 0.49              |
| 3:4:73:ARG:HH12   | 3:9:50:ARG:NH1     | 2.11                     | 0.49              |
| 3:9:252:GLN:O     | 3:9:256:LYS:HG2    | 2.12                     | 0.49              |
| 3:ZB:31:THR:HG22  | 4:ZG:39:PHE:HB3    | 1.89                     | 0.49              |
| 3:ZC:77:THR:O     | 3:ZC:77:THR:OG1    | 2.28                     | 0.49              |
| 4:ZI:373:VAL:HG23 | 4:ZT:399:LEU:CD2   | 2.42                     | 0.49              |
| 4:ZJ:237:ILE:H    | 4:ZJ:237:ILE:HD12  | 1.77                     | 0.49              |
| 4:ZL:30:TYR:HD1   | 4:ZL:363:ALA:HA    | 1.77                     | 0.49              |
| 4:ZN:139:ILE:HA   | 4:ZN:312:LEU:HD22  | 1.93                     | 0.49              |
| 4:ZO:268:GLN:OE1  | 4:ZU:190:GLN:NE2   | 2.46                     | 0.49              |
| 4:ZQ:160:SER:O    | 4:ZW:252:ASN:ND2   | 2.45                     | 0.49              |
| 4:ZY:150:THR:OG1  | 4:ZY:282:ASN:ND2   | 2.35                     | 0.49              |
| 5:AC:229:MET:HA   | 12:BD:102:MET:CE   | 2.42                     | 0.49              |
| 5:AD:46:VAL:HG12  | 11:A9:93:PRO:HB2   | 1.94                     | 0.49              |
| 5:AD:91:GLN:HB2   | 5:AD:121:ILE:HD11  | 1.94                     | 0.49              |
| 6:AR:256:ILE:HG13 | 6:AR:257:VAL:N     | 2.26                     | 0.49              |
| 6:AT:256:ILE:HG13 | 6:AT:257:VAL:N     | 2.26                     | 0.49              |
| 6:Ad:256:ILE:HG13 | 6:Ad:257:VAL:N     | 2.26                     | 0.49              |
| 6:AO:256:ILE:HG13 | 6:AO:257:VAL:N     | 2.26                     | 0.49              |
| 9:Au:143:ARG:HH21 | 9:Au:180:LYS:HB3   | 1.77                     | 0.49              |
| 9:Au:159:LEU:O    | 6:WP:164:LEU:O     | 2.30                     | 0.49              |
| 9:Au:211:MET:SD   | 9:Av:211:MET:HE3   | 2.53                     | 0.49              |
| 9:Av:48:ILE:CD1   | 11:A7:134:LEU:HD23 | 2.43                     | 0.49              |
| 10:A3:99:VAL:O    | 10:A3:102:MET:HG2  | 2.13                     | 0.49              |
| 11:A7:87:TYR:CE2  | 6:BK:320:PRO:HB3   | 2.47                     | 0.49              |
| 6:UJ:103:GLN:HB3  | 6:WD:182:PRO:HA    | 1.91                     | 0.49              |
| 6:UM:162:PRO:O    | 6:UM:163:SER:C     | 2.55                     | 0.49              |
| 6:WB:187:ASP:OD1  | 6:WB:190:GLN:HG3   | 2.12                     | 0.49              |
| 6:WC:143:THR:OG1  | 6:WD:154:ARG:HG2   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WH:202:VAL:HB   | 6:WH:205:LEU:HB2  | 1.95                     | 0.49              |
| 6:WK:132:TYR:CB   | 6:WL:126:PHE:HZ   | 2.19                     | 0.49              |
| 6:WN:202:VAL:HB   | 6:WN:205:LEU:HB2  | 1.94                     | 0.49              |
| 6:WO:200:SER:HG   | 6:WP:175:SER:HB2  | 1.69                     | 0.49              |
| 6:WT:206:PRO:O    | 6:WT:207:PRO:C    | 2.56                     | 0.49              |
| 1:B:171:ILE:CD1   | 1:Z:88:ALA:HB1    | 2.43                     | 0.49              |
| 1:C:88:ALA:HB1    | 1:E:171:ILE:CD1   | 2.43                     | 0.49              |
| 1:F:102:THR:HG23  | 1:G:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:N:65:LEU:CG     | 2:m:65:MET:HG3    | 2.39                     | 0.49              |
| 1:N:88:ALA:HB1    | 1:P:171:ILE:CD1   | 2.43                     | 0.49              |
| 3:1:194:GLU:O     | 5:AE:152:PRO:HG2  | 2.12                     | 0.49              |
| 3:6:46:TYR:HA     | 3:6:69:GLY:HA2    | 1.93                     | 0.49              |
| 3:ZA:50:ARG:HB2   | 3:ZA:66:LEU:CB    | 2.41                     | 0.49              |
| 3:ZA:91:ASN:C     | 3:ZA:93:LYS:H     | 2.21                     | 0.49              |
| 3:ZB:163:GLY:O    | 3:ZB:165:ALA:N    | 2.46                     | 0.49              |
| 4:ZH:270:ASN:CB   | 4:ZN:191:GLY:C    | 2.85                     | 0.49              |
| 4:ZK:372:LEU:O    | 4:ZK:373:VAL:C    | 2.56                     | 0.49              |
| 4:ZO:236:GLY:CA   | 4:ZO:268:GLN:H    | 2.21                     | 0.49              |
| 4:ZV:270:ASN:OD1  | 4:Zb:285:LYS:NZ   | 2.29                     | 0.49              |
| 4:ZZ:208:TRP:NE1  | 4:ZZ:268:GLN:OE1  | 2.38                     | 0.49              |
| 4:Zb:373:VAL:O    | 4:Zb:377:VAL:HG23 | 2.12                     | 0.49              |
| 4:Zh:391:THR:O    | 4:Zh:395:ILE:HG22 | 2.13                     | 0.49              |
| 5:AB:5:ILE:CD1    | 12:BB:106:MET:HE2 | 2.39                     | 0.49              |
| 5:AC:213:PRO:HG3  | 3:AN:1:MET:HB2    | 1.93                     | 0.49              |
| 3:AF:122:VAL:O    | 3:AK:180:ASN:ND2  | 2.46                     | 0.49              |
| 3:AH:129:VAL:HG12 | 3:AH:135:GLN:HA   | 1.93                     | 0.49              |
| 3:AJ:2:ILE:HD11   | 12:BE:32:ASP:OD1  | 2.08                     | 0.49              |
| 6:AS:372:ILE:CG2  | 10:A4:4:ILE:HG12  | 2.43                     | 0.49              |
| 6:AY:372:ILE:CG2  | 10:A3:4:ILE:HG12  | 2.43                     | 0.49              |
| 6:AZ:256:ILE:HG13 | 6:AZ:257:VAL:N    | 2.26                     | 0.49              |
| 6:Aa:294:ARG:HD2  | 6:Aa:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:Ak:294:ARG:HD2  | 6:Ak:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:AQ:294:ARG:HD2  | 6:AQ:367:GLU:OE1  | 2.13                     | 0.49              |
| 6:UK:73:MET:HE1   | 6:UK:99:ARG:HD2   | 1.95                     | 0.49              |
| 6:UN:208:GLY:CA   | 6:WR:187:ASP:OD1  | 2.60                     | 0.49              |
| 12:BB:86:ASP:OD1  | 12:BB:86:ASP:N    | 2.41                     | 0.49              |
| 6:WD:167:ARG:HH21 | 6:WD:168:GLU:HA   | 1.77                     | 0.49              |
| 6:WF:116:LEU:HD21 | 6:WF:134:ARG:HD3  | 1.92                     | 0.49              |
| 6:WI:206:PRO:O    | 6:WI:207:PRO:C    | 2.56                     | 0.49              |
| 6:WL:202:VAL:HB   | 6:WL:205:LEU:HB2  | 1.95                     | 0.49              |
| 6:WQ:142:ARG:O    | 6:WQ:146:THR:HG23 | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WR:206:PRO:O    | 6:WR:207:PRO:C    | 2.56                     | 0.49              |
| 6:BR:256:ILE:HG13 | 6:BR:257:VAL:N    | 2.26                     | 0.49              |
| 6:BU:294:ARG:HD2  | 6:BU:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:102:THR:HG23  | 1:C:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:K:88:ALA:HB1    | 1:M:171:ILE:CD1   | 2.43                     | 0.49              |
| 1:P:88:ALA:HB1    | 1:R:171:ILE:CD1   | 2.43                     | 0.49              |
| 1:S:102:THR:HG23  | 1:T:130:ASN:ND2   | 2.27                     | 0.49              |
| 1:Y:102:THR:HG23  | 1:Z:130:ASN:ND2   | 2.28                     | 0.49              |
| 2:e:21:ARG:HB2    | 2:e:243:GLU:HA    | 1.93                     | 0.49              |
| 3:2:235:GLN:HG2   | 3:8:5:LEU:HD21    | 1.94                     | 0.49              |
| 3:4:238:ARG:CZ    | 3:ZA:251:ASP:OD2  | 2.59                     | 0.49              |
| 4:ZH:397:ASN:OD1  | 4:ZH:401:ASN:ND2  | 2.45                     | 0.49              |
| 4:ZK:109:VAL:HG12 | 4:ZK:115:GLN:HA   | 1.93                     | 0.49              |
| 4:ZK:228:THR:HB   | 4:ZK:244:VAL:HG11 | 1.95                     | 0.49              |
| 4:ZR:180:LYS:NZ   | 4:ZR:181:LYS:O    | 2.45                     | 0.49              |
| 4:ZT:396:LEU:O    | 4:ZT:400:VAL:HG23 | 2.12                     | 0.49              |
| 4:ZU:104:GLU:OE2  | 4:ZU:104:GLU:N    | 2.31                     | 0.49              |
| 4:ZY:27:SER:O     | 4:ZY:364:SER:OG   | 2.30                     | 0.49              |
| 4:Zb:24:ILE:O     | 4:Zb:27:SER:OG    | 2.31                     | 0.49              |
| 4:Zc:317:LEU:HD21 | 4:Zc:356:LEU:HD21 | 1.95                     | 0.49              |
| 4:Zd:397:ASN:O    | 4:Zd:398:THR:C    | 2.53                     | 0.49              |
| 5:AA:46:VAL:HA    | 6:BI:326:ALA:HB2  | 1.95                     | 0.49              |
| 5:AA:228:GLU:HB2  | 3:AG:258:THR:HB   | 1.93                     | 0.49              |
| 5:AB:221:ILE:HG21 | 3:AH:251:ASP:OD2  | 2.12                     | 0.49              |
| 5:AB:243:ARG:O    | 5:AB:246:GLN:N    | 2.45                     | 0.49              |
| 5:AC:174:SER:OG   | 5:AC:176:ASP:OD1  | 2.29                     | 0.49              |
| 5:AE:226:ARG:O    | 5:AE:230:GLN:HG2  | 2.13                     | 0.49              |
| 3:AF:185:GLU:HB3  | 3:AF:193:ILE:HG23 | 1.95                     | 0.49              |
| 3:AG:233:MET:HE1  | 3:AL:245:LYS:HG3  | 1.94                     | 0.49              |
| 3:AI:62:LEU:CG    | 12:BE:84:LEU:HD23 | 2.41                     | 0.49              |
| 3:AM:19:MET:HB2   | 3:AM:236:VAL:HG11 | 1.93                     | 0.49              |
| 6:AO:294:ARG:HD2  | 6:AO:367:GLU:OE1  | 2.12                     | 0.49              |
| 9:Ay:65:THR:O     | 9:Ay:68:ILE:HG22  | 2.12                     | 0.49              |
| 10:A3:48:ARG:NH2  | 11:A9:6:ASP:OD2   | 2.45                     | 0.49              |
| 11:A9:31:ALA:HB1  | 12:BD:13:ALA:HB2  | 1.94                     | 0.49              |
| 11:A0:32:ASN:HD21 | 12:BE:61:GLY:C    | 2.20                     | 0.49              |
| 6:UK:98:LEU:HD22  | 6:UK:147:LEU:CD2  | 2.39                     | 0.49              |
| 6:UN:73:MET:HE1   | 6:UN:99:ARG:HD2   | 1.95                     | 0.49              |
| 6:UO:103:GLN:CG   | 6:WU:182:PRO:HB3  | 2.42                     | 0.49              |
| 6:WB:202:VAL:HB   | 6:WB:205:LEU:HB2  | 1.94                     | 0.49              |
| 6:WV:206:PRO:O    | 6:WV:207:PRO:C    | 2.56                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:BT:294:ARG:HD2  | 6:BT:367:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:102:THR:HG23  | 1:B:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:A:171:ILE:CD1   | 1:Y:88:ALA:HB1    | 2.43                     | 0.49              |
| 1:D:88:ALA:HB1    | 1:F:171:ILE:CD1   | 2.43                     | 0.49              |
| 1:K:166:GLU:HB2   | 1:L:35:THR:CG2    | 2.30                     | 0.49              |
| 1:M:102:THR:HG23  | 1:N:130:ASN:ND2   | 2.28                     | 0.49              |
| 2:e:273:CYS:CB    | 2:f:264:MET:O     | 2.42                     | 0.49              |
| 2:s:219:ARG:NH1   | 2:t:94:PRO:HB2    | 2.28                     | 0.49              |
| 3:2:248:SER:HB2   | 3:7:260:LEU:CD2   | 2.42                     | 0.49              |
| 3:ZA:76:ALA:CA    | 4:ZF:47:LYS:HD3   | 2.42                     | 0.49              |
| 4:ZL:84:ARG:HH12  | 4:ZL:92:VAL:HG22  | 1.77                     | 0.49              |
| 4:ZN:156:ILE:HD12 | 4:ZN:276:ILE:HG13 | 1.94                     | 0.49              |
| 4:ZP:159:ASN:OD1  | 4:ZP:161:THR:N    | 2.46                     | 0.49              |
| 4:ZX:380:ARG:HH12 | 4:Zd:397:ASN:ND2  | 2.11                     | 0.49              |
| 4:ZZ:373:VAL:HG21 | 4:Zf:10:LEU:CD2   | 2.42                     | 0.49              |
| 4:Za:171:SER:O    | 4:Za:177:SER:OG   | 2.28                     | 0.49              |
| 4:Zh:386:ALA:O    | 4:Zh:389:ILE:HG22 | 2.13                     | 0.49              |
| 5:AA:16:LEU:HD21  | 3:AF:253:MET:HE3  | 1.94                     | 0.49              |
| 5:AC:89:VAL:HG12  | 5:AC:121:ILE:HB   | 1.94                     | 0.49              |
| 5:AD:54:ARG:NH1   | 12:BE:22:ASN:ND2  | 2.61                     | 0.49              |
| 5:AE:225:ARG:HD2  | 3:AK:254:LEU:CB   | 2.42                     | 0.49              |
| 3:AG:62:LEU:HG    | 12:BC:84:LEU:HD11 | 1.94                     | 0.49              |
| 3:AJ:123:ASP:OD2  | 3:AJ:127:GLN:HB2  | 2.13                     | 0.49              |
| 3:AM:8:ALA:O      | 3:AM:11:GLY:N     | 2.45                     | 0.49              |
| 6:AR:294:ARG:HD2  | 6:AR:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:AV:355:PRO:CB   | 6:BO:319:GLN:CD   | 2.86                     | 0.49              |
| 6:Ad:294:ARG:HD2  | 6:Ad:367:GLU:OE1  | 2.12                     | 0.49              |
| 9:Aw:65:THR:O     | 9:Aw:68:ILE:HG22  | 2.12                     | 0.49              |
| 9:Ay:84:PRO:HG2   | 9:Ay:89:LEU:HD11  | 1.94                     | 0.49              |
| 11:A0:66:THR:HG23 | 6:BX:365:ASN:ND2  | 2.27                     | 0.49              |
| 6:UP:73:MET:HE1   | 6:UP:99:ARG:HD2   | 1.95                     | 0.49              |
| 6:WA:206:PRO:O    | 6:WA:207:PRO:C    | 2.56                     | 0.49              |
| 6:WL:206:PRO:O    | 6:WL:207:PRO:C    | 2.56                     | 0.49              |
| 6:WO:206:PRO:O    | 6:WO:207:PRO:C    | 2.56                     | 0.49              |
| 6:WP:206:PRO:O    | 6:WP:207:PRO:C    | 2.56                     | 0.49              |
| 6:BS:294:ARG:HD2  | 6:BS:367:GLU:OE1  | 2.13                     | 0.49              |
| 1:N:102:THR:HG23  | 1:O:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:T:102:THR:HG23  | 1:U:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:W:102:THR:HG23  | 1:X:130:ASN:ND2   | 2.28                     | 0.49              |
| 2:a:219:ARG:NH1   | 2:b:94:PRO:HB2    | 2.28                     | 0.49              |
| 2:f:273:CYS:CB    | 2:g:264:MET:O     | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:52:THR:HB     | 2:g:59:THR:HG23   | 1.95                     | 0.49              |
| 2:x:219:ARG:NH1   | 2:y:94:PRO:HB2    | 2.28                     | 0.49              |
| 2:y:219:ARG:NH1   | 2:z:94:PRO:HB2    | 2.28                     | 0.49              |
| 3:0:47:GLN:HE22   | 5:AD:67:THR:CG2   | 2.25                     | 0.49              |
| 3:5:215:TYR:HB3   | 3:5:218:TYR:HD2   | 1.78                     | 0.49              |
| 3:6:55:GLN:O      | 5:AE:138:ALA:CB   | 2.46                     | 0.49              |
| 3:6:230:LEU:HA    | 3:6:233:MET:HG3   | 1.95                     | 0.49              |
| 3:7:34:PHE:HB3    | 3:7:222:SER:HB3   | 1.95                     | 0.49              |
| 3:8:185:GLU:HG3   | 3:ZD:67:GLN:NE2   | 2.28                     | 0.49              |
| 3:ZD:27:ALA:C     | 4:ZI:52:VAL:HG22  | 2.36                     | 0.49              |
| 3:ZD:167:PRO:HG3  | 4:ZO:338:GLN:OE1  | 2.13                     | 0.49              |
| 3:ZD:189:GLU:OE1  | 4:ZI:53:LYS:HE2   | 2.13                     | 0.49              |
| 3:ZE:144:ALA:O    | 4:ZJ:352:ASN:ND2  | 2.46                     | 0.49              |
| 4:ZG:159:ASN:ND2  | 4:ZG:272:GLY:O    | 2.45                     | 0.49              |
| 4:ZH:144:MET:HE3  | 4:ZH:306:ASN:HD21 | 1.77                     | 0.49              |
| 4:ZJ:373:VAL:HG11 | 4:ZP:7:VAL:HG22   | 1.95                     | 0.49              |
| 4:ZL:18:ASP:CG    | 4:ZQ:5:GLN:NE2    | 2.70                     | 0.49              |
| 4:ZL:18:ASP:CG    | 4:ZQ:5:GLN:HE21   | 2.21                     | 0.49              |
| 4:ZL:372:LEU:HD21 | 4:ZQ:384:SER:CB   | 2.42                     | 0.49              |
| 4:ZO:80:ASN:OD1   | 4:ZO:81:GLY:N     | 2.45                     | 0.49              |
| 4:ZR:261:LEU:HD21 | 4:ZR:263:PHE:HE2  | 1.78                     | 0.49              |
| 4:ZW:104:GLU:HG2  | 4:ZW:105:ASN:OD1  | 2.13                     | 0.49              |
| 4:Zf:126:PRO:HB2  | 4:Zf:311:VAL:HG12 | 1.94                     | 0.49              |
| 5:AA:52:ALA:HA    | 11:A6:93:PRO:CG   | 2.43                     | 0.49              |
| 5:AC:221:ILE:CG2  | 3:AI:251:ASP:OD2  | 2.60                     | 0.49              |
| 5:AD:173:ARG:HD2  | 3:AI:67:GLN:NE2   | 2.28                     | 0.49              |
| 5:AE:60:SER:HB2   | 3:AJ:65:GLY:O     | 2.12                     | 0.49              |
| 3:AG:7:ILE:O      | 3:AG:10:THR:N     | 2.46                     | 0.49              |
| 3:AJ:19:MET:HG2   | 3:AJ:236:VAL:HG11 | 1.93                     | 0.49              |
| 6:AS:294:ARG:HD2  | 6:AS:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:AZ:236:LYS:CE   | 6:UP:167:ARG:NH1  | 2.76                     | 0.49              |
| 6:Ac:294:ARG:HD2  | 6:Ac:367:GLU:OE1  | 2.13                     | 0.49              |
| 6:Ap:294:ARG:HD2  | 6:Ap:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:UJ:162:PRO:O    | 6:UJ:163:SER:C    | 2.55                     | 0.49              |
| 6:UK:73:MET:HE3   | 6:UK:99:ARG:CD    | 2.41                     | 0.49              |
| 6:UO:162:PRO:O    | 6:UO:163:SER:C    | 2.55                     | 0.49              |
| 12:BA:128:LYS:O   | 12:BA:129:THR:C   | 2.55                     | 0.49              |
| 6:WD:200:SER:O    | 6:WE:158:ALA:HB3  | 2.10                     | 0.49              |
| 6:WH:206:PRO:O    | 6:WH:207:PRO:C    | 2.55                     | 0.49              |
| 6:WK:202:VAL:HB   | 6:WK:205:LEU:HB2  | 1.95                     | 0.49              |
| 6:WQ:202:VAL:HB   | 6:WQ:205:LEU:HB2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WU:202:VAL:HB   | 6:WU:205:LEU:HB2   | 1.95                     | 0.49              |
| 12:BD:10:ALA:O    | 12:BD:14:LEU:HG    | 2.12                     | 0.49              |
| 12:BD:51:VAL:O    | 12:BD:52:ASP:C     | 2.56                     | 0.49              |
| 6:BR:294:ARG:HD2  | 6:BR:367:GLU:OE1   | 2.13                     | 0.49              |
| 1:J:88:ALA:HB1    | 1:L:171:ILE:CD1    | 2.43                     | 0.49              |
| 1:P:102:THR:HG23  | 1:Q:130:ASN:ND2    | 2.27                     | 0.49              |
| 1:Q:88:ALA:HB1    | 1:S:171:ILE:CD1    | 2.43                     | 0.49              |
| 1:X:88:ALA:HB1    | 1:Z:171:ILE:CD1    | 2.43                     | 0.49              |
| 2:a:94:PRO:HB2    | 2:z:219:ARG:NH1    | 2.28                     | 0.49              |
| 2:f:52:THR:HB     | 2:f:59:THR:HG23    | 1.95                     | 0.49              |
| 2:t:219:ARG:NH1   | 2:u:94:PRO:HB2     | 2.28                     | 0.49              |
| 2:y:78:ASN:ND2    | 3:AM:202:ASN:OD1   | 2.45                     | 0.49              |
| 3:3:1:MET:HB2     | 3:AG:226:VAL:CG2   | 2.43                     | 0.49              |
| 3:6:248:SER:OG    | 3:ZB:260:LEU:HD22  | 2.12                     | 0.49              |
| 3:ZA:56:SER:HB2   | 3:AI:153:ARG:HB2   | 1.94                     | 0.49              |
| 4:ZF:65:THR:HA    | 4:ZQ:50:LEU:HD11   | 1.95                     | 0.49              |
| 4:ZK:25:ALA:HB1   | 4:ZP:52:VAL:CG1    | 2.43                     | 0.49              |
| 4:ZK:175:ALA:HA   | 4:ZK:178:TYR:CZ    | 2.47                     | 0.49              |
| 4:ZO:14:ALA:HB2   | 4:ZO:382:TYR:HE2   | 1.77                     | 0.49              |
| 4:ZP:83:PHE:HB2   | 4:ZP:95:SER:O      | 2.13                     | 0.49              |
| 4:ZR:199:TYR:HB2  | 4:ZR:211:TYR:HB2   | 1.95                     | 0.49              |
| 4:ZT:106:ARG:HH22 | 4:ZT:289:LEU:CD2   | 2.26                     | 0.49              |
| 4:Zd:171:SER:O    | 4:Zd:177:SER:OG    | 2.30                     | 0.49              |
| 5:AA:51:LEU:O     | 5:AA:53:THR:N      | 2.46                     | 0.49              |
| 5:AB:220:MET:SD   | 3:AG:246:ALA:HB2   | 2.53                     | 0.49              |
| 5:AC:152:PRO:CG   | 3:AN:193:ILE:HD12  | 2.42                     | 0.49              |
| 5:AC:232:LYS:HB3  | 12:BD:102:MET:HE1  | 1.95                     | 0.49              |
| 3:AH:248:SER:HB2  | 3:AM:260:LEU:HD13  | 1.95                     | 0.49              |
| 6:AZ:294:ARG:HD2  | 6:AZ:367:GLU:OE1   | 2.13                     | 0.49              |
| 6:Ad:266:VAL:HG22 | 6:Ad:387:VAL:HG22  | 1.95                     | 0.49              |
| 6:Ae:294:ARG:HD2  | 6:Ae:367:GLU:OE1   | 2.12                     | 0.49              |
| 6:An:294:ARG:HD2  | 6:An:367:GLU:OE1   | 2.13                     | 0.49              |
| 7:As:33:LEU:HB2   | 8:At:216:ILE:HD12  | 1.95                     | 0.49              |
| 9:Aw:48:ILE:HD11  | 11:A8:134:LEU:CD2  | 2.42                     | 0.49              |
| 9:Ax:41:SER:HB3   | 10:A4:82:MET:HE2   | 1.95                     | 0.49              |
| 9:Ax:211:MET:O    | 9:Ay:211:MET:HE2   | 2.12                     | 0.49              |
| 11:A9:67:LEU:HD21 | 11:A9:74:PRO:HB3   | 1.94                     | 0.49              |
| 11:A9:102:MET:HB3 | 11:A9:106:ARG:HH21 | 1.77                     | 0.49              |
| 6:WC:128:GLU:HG2  | 6:WC:129:GLN:N     | 2.28                     | 0.49              |
| 6:WD:145:GLU:O    | 6:WD:147:LEU:N     | 2.46                     | 0.49              |
| 6:WI:197:LEU:HD13 | 6:WJ:175:SER:OG    | 2.09                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WN:206:PRO:O    | 6:WN:207:PRO:C    | 2.56                     | 0.49              |
| 6:BU:266:VAL:HG22 | 6:BU:387:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:62:TYR:CE1    | 2:y:129:VAL:HG13  | 2.47                     | 0.49              |
| 1:G:102:THR:HG23  | 1:H:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:R:166:GLU:HB2   | 1:S:35:THR:CG2    | 2.30                     | 0.49              |
| 2:b:219:ARG:NH1   | 2:c:94:PRO:HB2    | 2.28                     | 0.49              |
| 2:n:273:CYS:CB    | 2:o:264:MET:O     | 2.42                     | 0.49              |
| 2:r:78:ASN:CG     | 3:ZA:58:GLU:OE1   | 2.56                     | 0.49              |
| 2:r:219:ARG:NH1   | 2:s:94:PRO:HB2    | 2.28                     | 0.49              |
| 2:u:219:ARG:NH1   | 2:v:94:PRO:HB2    | 2.28                     | 0.49              |
| 2:w:219:ARG:NH1   | 2:x:94:PRO:HB2    | 2.28                     | 0.49              |
| 3:4:44:LEU:HB3    | 3:4:70:THR:HB     | 1.95                     | 0.49              |
| 3:4:123:ASP:OD1   | 3:4:127:GLN:N     | 2.45                     | 0.49              |
| 3:5:55:GLN:O      | 5:AD:138:ALA:HB1  | 2.11                     | 0.49              |
| 4:ZM:160:SER:O    | 4:ZM:202:LYS:NZ   | 2.41                     | 0.49              |
| 4:ZQ:379:GLN:NE2  | 4:ZV:394:GLN:HE22 | 2.10                     | 0.49              |
| 4:ZT:24:ILE:HD12  | 4:ZY:388:THR:OG1  | 2.13                     | 0.49              |
| 4:ZY:270:ASN:HB3  | 4:Ze:286:PRO:HD2  | 1.94                     | 0.49              |
| 4:Za:17:LEU:HD22  | 4:Zf:391:THR:HG21 | 1.93                     | 0.49              |
| 4:Zg:159:ASN:ND2  | 4:Zg:161:THR:OG1  | 2.44                     | 0.49              |
| 5:AB:241:GLU:HG2  | 12:BB:110:ARG:HB3 | 1.94                     | 0.49              |
| 5:AC:70:GLN:NE2   | 3:AN:6:TRP:CZ3    | 2.81                     | 0.49              |
| 3:AI:129:VAL:HG12 | 3:AI:135:GLN:HA   | 1.94                     | 0.49              |
| 3:AM:129:VAL:HA   | 3:AM:136:VAL:HG23 | 1.95                     | 0.49              |
| 6:AY:294:ARG:HD2  | 6:AY:367:GLU:OE1  | 2.13                     | 0.49              |
| 6:Ae:266:VAL:HG22 | 6:Ae:387:VAL:HG22 | 1.95                     | 0.49              |
| 6:AP:266:VAL:HG22 | 6:AP:387:VAL:HG22 | 1.95                     | 0.49              |
| 8:At:93:ALA:HB2   | 9:Au:88:VAL:HG21  | 1.94                     | 0.49              |
| 6:UJ:256:PRO:HD2  | 6:WC:187:ASP:HB3  | 1.94                     | 0.49              |
| 6:UK:80:ALA:CB    | 6:UK:83:SER:HB3   | 2.43                     | 0.49              |
| 6:UL:80:ALA:CB    | 6:UL:83:SER:HB3   | 2.43                     | 0.49              |
| 6:WE:112:GLY:O    | 6:WE:115:LEU:HB3  | 2.12                     | 0.49              |
| 6:WE:202:VAL:HB   | 6:WE:205:LEU:HB2  | 1.95                     | 0.49              |
| 6:WE:206:PRO:O    | 6:WE:207:PRO:C    | 2.56                     | 0.49              |
| 6:WG:206:PRO:O    | 6:WG:207:PRO:C    | 2.56                     | 0.49              |
| 6:WI:202:VAL:HB   | 6:WI:205:LEU:HB2  | 1.94                     | 0.49              |
| 6:WJ:206:PRO:O    | 6:WJ:207:PRO:C    | 2.56                     | 0.49              |
| 6:WK:206:PRO:O    | 6:WK:207:PRO:C    | 2.56                     | 0.49              |
| 6:WM:145:GLU:O    | 6:WM:146:THR:C    | 2.54                     | 0.49              |
| 6:WQ:206:PRO:O    | 6:WQ:207:PRO:C    | 2.56                     | 0.49              |
| 1:A:130:ASN:ND2   | 1:Z:102:THR:HG23  | 2.28                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:65:LEU:CG     | 2:g:65:MET:HG3    | 2.39                     | 0.49              |
| 1:H:102:THR:HG23  | 1:I:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:O:65:LEU:CG     | 2:n:65:MET:HG3    | 2.39                     | 0.49              |
| 1:O:102:THR:HG23  | 1:P:130:ASN:ND2   | 2.28                     | 0.49              |
| 1:R:88:ALA:HB1    | 1:T:171:ILE:CD1   | 2.43                     | 0.49              |
| 1:W:88:ALA:HB1    | 1:Y:171:ILE:CD1   | 2.43                     | 0.49              |
| 2:e:52:THR:HB     | 2:e:59:THR:HG23   | 1.95                     | 0.49              |
| 2:h:52:THR:HB     | 2:h:59:THR:HG23   | 1.95                     | 0.49              |
| 2:k:21:ARG:HB2    | 2:k:243:GLU:HA    | 1.93                     | 0.49              |
| 2:m:52:THR:HB     | 2:m:59:THR:HG23   | 1.95                     | 0.49              |
| 2:n:52:THR:HB     | 2:n:59:THR:HG23   | 1.95                     | 0.49              |
| 3:3:180:ASN:C     | 3:3:182:THR:N     | 2.70                     | 0.49              |
| 3:4:56:SER:HA     | 5:AC:138:ALA:HB1  | 1.95                     | 0.49              |
| 3:6:231:VAL:CG1   | 3:ZC:9:LYS:HG2    | 2.30                     | 0.49              |
| 3:ZA:1:MET:CE     | 3:AN:226:VAL:HG21 | 2.43                     | 0.49              |
| 3:ZA:1:MET:HE3    | 3:AN:226:VAL:HG21 | 1.95                     | 0.49              |
| 3:ZD:184:LEU:HB3  | 3:ZD:192:TYR:HB3  | 1.95                     | 0.49              |
| 4:ZG:146:ALA:HB2  | 4:ZG:286:PRO:HD3  | 1.93                     | 0.49              |
| 4:ZH:78:SER:OG    | 4:ZH:355:LYS:N    | 2.35                     | 0.49              |
| 4:ZL:29:THR:CG2   | 4:ZQ:39:PHE:HB2   | 2.41                     | 0.49              |
| 4:ZR:126:PRO:HG2  | 4:ZR:310:GLN:HE21 | 1.78                     | 0.49              |
| 4:ZT:243:THR:HG22 | 4:ZT:262:SER:HB2  | 1.94                     | 0.49              |
| 4:ZU:293:GLN:HE21 | 4:ZU:303:ASN:HD21 | 1.61                     | 0.49              |
| 4:Zb:144:MET:SD   | 4:Zb:306:ASN:ND2  | 2.85                     | 0.49              |
| 5:AB:188:GLU:HG3  | 5:AB:189:ARG:HG2  | 1.94                     | 0.49              |
| 5:AC:71:LEU:HB2   | 3:AN:70:THR:HG21  | 1.90                     | 0.49              |
| 6:AX:294:ARG:HD2  | 6:AX:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:Af:365:ASN:CG   | 11:A8:72:HIS:ND1  | 2.70                     | 0.49              |
| 6:Aj:294:ARG:HD2  | 6:Aj:367:GLU:OE1  | 2.12                     | 0.49              |
| 6:Ao:294:ARG:HD2  | 6:Ao:367:GLU:OE1  | 2.13                     | 0.49              |
| 9:Au:92:LEU:HD13  | 9:Au:232:TRP:HZ2  | 1.77                     | 0.49              |
| 9:Au:130:GLY:O    | 9:Au:133:PRO:HD2  | 2.13                     | 0.49              |
| 9:Ay:143:ARG:NH2  | 9:Ay:180:LYS:HB3  | 2.28                     | 0.49              |
| 10:A2:48:ARG:HH11 | 11:A8:5:LEU:HD23  | 1.77                     | 0.49              |
| 12:BD:3:LEU:H     | 12:BD:3:LEU:HD12  | 1.77                     | 0.49              |
| 6:BV:266:VAL:HG22 | 6:BV:387:VAL:HG22 | 1.95                     | 0.49              |
| 1:C:102:THR:HG23  | 1:D:130:ASN:ND2   | 2.28                     | 0.48              |
| 1:D:65:LEU:CG     | 2:c:65:MET:HG3    | 2.39                     | 0.48              |
| 1:E:88:ALA:HB1    | 1:G:171:ILE:CD1   | 2.43                     | 0.48              |
| 1:G:62:TYR:CE1    | 2:e:129:VAL:HG13  | 2.48                     | 0.48              |
| 1:H:104:PHE:O     | 1:H:123:ASP:HA    | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:88:ALA:HB1    | 1:K:171:ILE:CD1   | 2.43                     | 0.48              |
| 1:L:102:THR:HG23  | 1:M:130:ASN:ND2   | 2.28                     | 0.48              |
| 2:f:21:ARG:HB2    | 2:f:243:GLU:HA    | 1.93                     | 0.48              |
| 2:l:52:THR:HB     | 2:l:59:THR:HG23   | 1.95                     | 0.48              |
| 2:m:219:ARG:NH1   | 2:n:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:q:219:ARG:NH1   | 2:r:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:r:253:VAL:HG13  | 2:r:264:MET:HG2   | 1.95                     | 0.48              |
| 2:t:253:VAL:HG13  | 2:t:264:MET:HG2   | 1.95                     | 0.48              |
| 2:v:219:ARG:NH1   | 2:w:94:PRO:HB2    | 2.28                     | 0.48              |
| 3:1:6:TRP:CB      | 5:AE:70:GLN:HB3   | 2.40                     | 0.48              |
| 3:4:226:VAL:HG11  | 3:9:242:ILE:CD1   | 2.43                     | 0.48              |
| 3:9:184:LEU:HB3   | 3:9:192:TYR:HB3   | 1.95                     | 0.48              |
| 3:ZA:85:ASN:HA    | 4:ZL:50:LEU:HD13  | 1.95                     | 0.48              |
| 3:ZB:172:GLN:HE22 | 3:ZB:205:THR:HG23 | 1.78                     | 0.48              |
| 3:ZB:227:ALA:HA   | 4:ZM:399:LEU:CD2  | 2.43                     | 0.48              |
| 4:ZI:198:VAL:HG22 | 4:ZI:212:THR:HG22 | 1.94                     | 0.48              |
| 4:ZP:181:LYS:HD3  | 4:Za:129:GLN:HE22 | 1.78                     | 0.48              |
| 4:ZP:391:THR:O    | 4:ZP:395:ILE:HG23 | 2.12                     | 0.48              |
| 4:ZT:95:SER:OG    | 4:ZT:332:ASN:O    | 2.23                     | 0.48              |
| 4:ZU:141:ASN:HA   | 4:ZU:289:LEU:HD13 | 1.94                     | 0.48              |
| 4:ZV:369:SER:HB3  | 4:Zb:382:TYR:OH   | 2.13                     | 0.48              |
| 4:ZV:372:LEU:CD1  | 4:Zg:399:LEU:HB3  | 2.43                     | 0.48              |
| 4:ZX:83:PHE:HB2   | 4:ZX:95:SER:O     | 2.13                     | 0.48              |
| 5:AA:228:GLU:OE1  | 3:AF:256:LYS:CG   | 2.49                     | 0.48              |
| 5:AD:35:ARG:HA    | 5:AD:210:ASN:HD21 | 1.78                     | 0.48              |
| 5:AE:173:ARG:HD2  | 3:AJ:46:TYR:CD1   | 2.48                     | 0.48              |
| 8:At:252:ALA:HB3  | 6:WK:163:SER:O    | 2.13                     | 0.48              |
| 9:Ay:143:ARG:HH22 | 9:Ay:180:LYS:HB3  | 1.78                     | 0.48              |
| 11:A9:11:PHE:CD1  | 11:A9:53:MET:HE2  | 2.48                     | 0.48              |
| 6:Ul:80:ALA:CB    | 6:Ul:83:SER:HB3   | 2.43                     | 0.48              |
| 6:UK:129:GLN:O    | 6:UK:133:GLN:N    | 2.29                     | 0.48              |
| 6:WF:145:GLU:HG2  | 6:WF:152:SER:HA   | 1.95                     | 0.48              |
| 6:WF:202:VAL:HB   | 6:WF:205:LEU:HB2  | 1.94                     | 0.48              |
| 6:WG:219:LEU:HD21 | 6:WG:222:GLN:O    | 2.13                     | 0.48              |
| 6:WN:145:GLU:O    | 6:WN:147:LEU:N    | 2.46                     | 0.48              |
| 6:WS:202:VAL:HB   | 6:WS:205:LEU:HB2  | 1.94                     | 0.48              |
| 6:WV:202:VAL:HB   | 6:WV:205:LEU:HB2  | 1.95                     | 0.48              |
| 6:BW:266:VAL:HG22 | 6:BW:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:B:104:PHE:O     | 1:B:123:ASP:HA    | 2.13                     | 0.48              |
| 1:E:104:PHE:O     | 1:E:123:ASP:HA    | 2.13                     | 0.48              |
| 1:K:104:PHE:O     | 1:K:123:ASP:HA    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:X:102:THR:HG23  | 1:Y:130:ASN:ND2   | 2.27                     | 0.48              |
| 1:Y:104:PHE:O     | 1:Y:123:ASP:HA    | 2.13                     | 0.48              |
| 1:Z:62:TYR:CE1    | 2:x:129:VAL:HG13  | 2.48                     | 0.48              |
| 2:k:346:MET:HE3   | 2:m:142:LEU:CD1   | 2.42                     | 0.48              |
| 2:v:253:VAL:HG13  | 2:v:264:MET:HG2   | 1.95                     | 0.48              |
| 3:0:251:ASP:OD1   | 3:AI:238:ARG:CZ   | 2.60                     | 0.48              |
| 3:5:28:ASN:OD1    | 3:ZA:72:VAL:HG23  | 2.14                     | 0.48              |
| 3:5:34:PHE:HB3    | 3:5:222:SER:HB3   | 1.95                     | 0.48              |
| 3:5:129:VAL:HG12  | 3:5:135:GLN:HA    | 1.96                     | 0.48              |
| 3:7:55:GLN:HG3    | 3:AF:169:GLN:HE21 | 1.77                     | 0.48              |
| 3:ZA:76:ALA:HA    | 4:ZF:47:LYS:CE    | 2.43                     | 0.48              |
| 3:ZA:189:GLU:HA   | 4:ZF:40:ALA:HB1   | 1.95                     | 0.48              |
| 3:ZB:29:VAL:O     | 3:ZB:222:SER:OG   | 2.31                     | 0.48              |
| 3:ZB:50:ARG:HB2   | 3:ZB:66:LEU:H     | 1.76                     | 0.48              |
| 3:ZC:240:TYR:CE2  | 4:ZH:395:ILE:HG22 | 2.48                     | 0.48              |
| 3:ZD:189:GLU:OE1  | 4:ZI:53:LYS:CE    | 2.61                     | 0.48              |
| 4:ZH:298:GLY:HA2  | 4:ZH:356:LEU:HD12 | 1.95                     | 0.48              |
| 4:ZJ:195:ASP:OD2  | 4:ZJ:195:ASP:N    | 2.36                     | 0.48              |
| 4:ZO:141:ASN:O    | 4:ZO:142:THR:C    | 2.56                     | 0.48              |
| 4:ZV:41:ASP:OD2   | 4:ZV:41:ASP:N     | 2.46                     | 0.48              |
| 4:ZV:182:GLY:HA2  | 4:Zg:131:GLY:HA3  | 1.95                     | 0.48              |
| 4:ZV:367:ASP:HB3  | 4:ZV:370:LYS:HD2  | 1.95                     | 0.48              |
| 4:ZY:102:LEU:HD11 | 4:ZY:139:ILE:HD12 | 1.95                     | 0.48              |
| 4:Zb:68:ASN:OD1   | 4:Zb:68:ASN:N     | 2.47                     | 0.48              |
| 4:Ze:352:ASN:OD1  | 4:Ze:352:ASN:N    | 2.43                     | 0.48              |
| 4:Zg:3:PHE:O      | 4:Zg:7:VAL:HG22   | 2.13                     | 0.48              |
| 4:Zg:196:MET:HE3  | 4:Zg:248:THR:HG22 | 1.95                     | 0.48              |
| 5:AB:225:ARG:HG2  | 5:AB:225:ARG:HH11 | 1.78                     | 0.48              |
| 3:AF:238:ARG:HG3  | 3:AL:254:LEU:HD13 | 1.94                     | 0.48              |
| 6:AV:294:ARG:HD2  | 6:AV:367:GLU:OE1  | 2.12                     | 0.48              |
| 6:AX:266:VAL:HG22 | 6:AX:387:VAL:HG22 | 1.95                     | 0.48              |
| 6:Af:266:VAL:HG22 | 6:Af:387:VAL:HG22 | 1.95                     | 0.48              |
| 6:Af:294:ARG:HD2  | 6:Af:367:GLU:OE1  | 2.13                     | 0.48              |
| 6:Ag:294:ARG:HD2  | 6:Ag:367:GLU:OE1  | 2.12                     | 0.48              |
| 6:Al:294:ARG:HH11 | 11:A7:68:THR:HG21 | 1.78                     | 0.48              |
| 9:Ay:73:LEU:HD13  | 9:Ay:186:GLY:HA3  | 1.94                     | 0.48              |
| 11:A9:49:LEU:O    | 11:A9:53:MET:HG2  | 2.13                     | 0.48              |
| 6:UO:80:ALA:CB    | 6:UO:83:SER:HB3   | 2.43                     | 0.48              |
| 6:WB:197:LEU:HA   | 6:WC:175:SER:OG   | 2.13                     | 0.48              |
| 6:WF:193:ALA:HB1  | 6:WG:213:VAL:HG11 | 1.94                     | 0.48              |
| 6:WJ:200:SER:OG   | 6:WK:175:SER:HB2  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WM:206:PRO:O    | 6:WM:207:PRO:C    | 2.56                     | 0.48              |
| 6:WR:202:VAL:HB   | 6:WR:205:LEU:HB2  | 1.95                     | 0.48              |
| 6:WW:202:VAL:HB   | 6:WW:205:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:104:PHE:O     | 1:A:123:ASP:HA    | 2.14                     | 0.48              |
| 1:V:88:ALA:HB1    | 1:X:171:ILE:CD1   | 2.43                     | 0.48              |
| 1:V:102:THR:HG23  | 1:W:130:ASN:ND2   | 2.27                     | 0.48              |
| 1:X:65:LEU:CG     | 2:w:65:MET:HG3    | 2.39                     | 0.48              |
| 1:X:104:PHE:O     | 1:X:123:ASP:HA    | 2.13                     | 0.48              |
| 2:l:219:ARG:NH1   | 2:m:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:n:219:ARG:NH1   | 2:o:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:o:52:THR:HB     | 2:o:59:THR:HG23   | 1.95                     | 0.48              |
| 2:x:253:VAL:HG13  | 2:x:264:MET:HG2   | 1.95                     | 0.48              |
| 3:0:1:MET:SD      | 3:0:1:MET:N       | 2.85                     | 0.48              |
| 3:3:50:ARG:HH21   | 3:AM:73:ARG:HH22  | 1.59                     | 0.48              |
| 3:5:238:ARG:NH1   | 3:5:241:GLU:OE2   | 2.45                     | 0.48              |
| 3:ZB:98:LYS:HE3   | 4:ZM:44:ALA:HB2   | 1.95                     | 0.48              |
| 3:ZB:248:SER:HB3  | 4:ZG:402:LEU:CD2  | 2.34                     | 0.48              |
| 4:ZH:33:LYS:HA    | 4:ZH:365:ASN:HD21 | 1.78                     | 0.48              |
| 4:ZK:394:GLN:O    | 4:ZK:397:ASN:HB3  | 2.13                     | 0.48              |
| 4:ZM:270:ASN:ND2  | 4:ZS:192:ASN:HA   | 2.25                     | 0.48              |
| 4:ZV:380:ARG:NH2  | 4:Zb:393:ASP:OD2  | 2.46                     | 0.48              |
| 4:ZZ:93:PHE:HB3   | 4:ZZ:333:VAL:HG13 | 1.94                     | 0.48              |
| 4:Zd:154:MET:HB2  | 4:Zd:279:THR:HG22 | 1.95                     | 0.48              |
| 4:Ze:178:TYR:HA   | 4:Ze:201:VAL:HG22 | 1.94                     | 0.48              |
| 5:AD:11:ALA:HB3   | 5:AD:230:GLN:HG2  | 1.95                     | 0.48              |
| 5:AD:28:ASN:ND2   | 3:AI:72:VAL:HB    | 2.27                     | 0.48              |
| 5:AE:48:GLY:HA3   | 11:A0:93:PRO:HB3  | 1.95                     | 0.48              |
| 5:AE:65:ASP:O     | 5:AE:210:ASN:ND2  | 2.45                     | 0.48              |
| 3:AK:100:GLN:H    | 3:AK:100:GLN:HG2  | 1.41                     | 0.48              |
| 6:AT:294:ARG:HD2  | 6:AT:367:GLU:OE1  | 2.13                     | 0.48              |
| 6:AW:294:ARG:HD2  | 6:AW:367:GLU:OE1  | 2.12                     | 0.48              |
| 6:AY:266:VAL:HG22 | 6:AY:387:VAL:HG22 | 1.95                     | 0.48              |
| 6:AO:266:VAL:HG22 | 6:AO:387:VAL:HG22 | 1.95                     | 0.48              |
| 7:As:55:ILE:HD11  | 9:Ax:205:MET:HE2  | 1.84                     | 0.48              |
| 8:At:106:MET:HE1  | 8:At:226:ILE:HG13 | 1.93                     | 0.48              |
| 11:A9:102:MET:HE3 | 11:A9:106:ARG:HE  | 1.78                     | 0.48              |
| 6:UK:98:LEU:HD12  | 6:UK:146:THR:HG1  | 1.78                     | 0.48              |
| 6:UL:127:SER:O    | 6:UL:131:ASN:HB2  | 2.13                     | 0.48              |
| 6:WA:202:VAL:HB   | 6:WA:205:LEU:HB2  | 1.94                     | 0.48              |
| 6:WC:197:LEU:HD11 | 6:WD:156:HIS:HD2  | 1.78                     | 0.48              |
| 6:WM:202:VAL:HB   | 6:WM:205:LEU:HB2  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WT:145:GLU:C    | 6:WT:147:LEU:N     | 2.72                     | 0.48              |
| 6:WT:202:VAL:HB   | 6:WT:205:LEU:HB2   | 1.95                     | 0.48              |
| 6:WV:192:SER:O    | 6:WV:195:VAL:N     | 2.47                     | 0.48              |
| 6:WW:115:LEU:HA   | 6:WW:118:GLN:OE1   | 2.13                     | 0.48              |
| 12:BC:27:ASN:OD1  | 12:BC:42:TYR:OH    | 2.27                     | 0.48              |
| 6:BT:266:VAL:HG22 | 6:BT:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:F:88:ALA:HB1    | 1:H:171:ILE:CD1    | 2.43                     | 0.48              |
| 1:H:88:ALA:HB1    | 1:J:171:ILE:CD1    | 2.42                     | 0.48              |
| 1:Q:102:THR:HG23  | 1:R:130:ASN:ND2    | 2.28                     | 0.48              |
| 1:R:102:THR:HG23  | 1:S:130:ASN:ND2    | 2.27                     | 0.48              |
| 1:U:102:THR:HG23  | 1:V:130:ASN:ND2    | 2.28                     | 0.48              |
| 2:a:346:MET:HE3   | 2:c:142:LEU:CD1    | 2.42                     | 0.48              |
| 2:f:219:ARG:NH1   | 2:g:94:PRO:HB2     | 2.28                     | 0.48              |
| 3:1:197:SER:CA    | 3:AK:124:GLN:HB3   | 2.43                     | 0.48              |
| 3:3:37:GLN:HE22   | 3:8:46:TYR:HE2     | 1.60                     | 0.48              |
| 3:4:73:ARG:HH22   | 3:9:50:ARG:NH1     | 2.10                     | 0.48              |
| 3:6:241:GLU:HG2   | 3:ZB:256:LYS:HG3   | 1.96                     | 0.48              |
| 3:7:235:GLN:HG2   | 3:ZD:5:LEU:CD2     | 2.40                     | 0.48              |
| 3:ZA:91:ASN:C     | 3:ZA:93:LYS:N      | 2.70                     | 0.48              |
| 4:ZK:58:THR:OG1   | 4:ZK:324:GLU:OE2   | 2.30                     | 0.48              |
| 4:ZL:165:PRO:HG2  | 4:ZL:201:VAL:HG13  | 1.94                     | 0.48              |
| 4:ZQ:380:ARG:HG3  | 4:ZW:396:LEU:HD12  | 1.94                     | 0.48              |
| 4:ZW:144:MET:SD   | 4:ZW:310:GLN:NE2   | 2.86                     | 0.48              |
| 4:Zb:33:LYS:O     | 4:Zb:59:GLN:NE2    | 2.46                     | 0.48              |
| 4:Zb:299:THR:HG22 | 4:Zb:314:GLN:HG3   | 1.95                     | 0.48              |
| 4:Zc:107:ASN:ND2  | 4:Zc:138:THR:OG1   | 2.46                     | 0.48              |
| 7:Ab:51:PHE:CE2   | 9:Au:202:SER:HA    | 2.47                     | 0.48              |
| 6:Ac:266:VAL:HG22 | 6:Ac:387:VAL:HG22  | 1.95                     | 0.48              |
| 6:AQ:266:VAL:HG22 | 6:AQ:387:VAL:HG22  | 1.95                     | 0.48              |
| 9:Ax:161:GLY:C    | 9:Ax:163:GLU:N     | 2.69                     | 0.48              |
| 11:A7:51:LYS:CG   | 11:A7:55:ARG:NH1   | 2.75                     | 0.48              |
| 11:A8:128:LYS:NZ  | 12:BC:134:GLN:HE21 | 2.11                     | 0.48              |
| 12:BA:27:ASN:ND2  | 12:BA:45:LYS:O     | 2.33                     | 0.48              |
| 6:WA:196:HIS:CD2  | 6:WB:219:LEU:HD22  | 2.49                     | 0.48              |
| 6:WB:145:GLU:C    | 6:WB:147:LEU:H     | 2.22                     | 0.48              |
| 6:WJ:202:VAL:HB   | 6:WJ:205:LEU:HB2   | 1.95                     | 0.48              |
| 1:O:62:TYR:CE1    | 2:m:129:VAL:HG13   | 2.48                     | 0.48              |
| 1:R:104:PHE:O     | 1:R:123:ASP:HA     | 2.14                     | 0.48              |
| 1:V:104:PHE:O     | 1:V:123:ASP:HA     | 2.13                     | 0.48              |
| 2:c:219:ARG:NH1   | 2:d:94:PRO:HB2     | 2.28                     | 0.48              |
| 2:g:219:ARG:NH1   | 2:h:94:PRO:HB2     | 2.28                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:52:THR:HB     | 2:i:59:THR:HG23   | 1.95                     | 0.48              |
| 2:v:52:THR:HB     | 2:v:59:THR:HG23   | 1.95                     | 0.48              |
| 2:x:52:THR:HB     | 2:x:59:THR:HG23   | 1.95                     | 0.48              |
| 2:y:52:THR:HB     | 2:y:59:THR:HG23   | 1.95                     | 0.48              |
| 3:1:45:LEU:CD1    | 5:AE:83:GLN:HA    | 2.37                     | 0.48              |
| 3:2:56:SER:HA     | 5:AA:138:ALA:HB1  | 1.85                     | 0.48              |
| 3:5:124:GLN:HB2   | 3:ZA:199:GLY:CA   | 2.42                     | 0.48              |
| 3:ZC:123:ASP:OD1  | 3:ZC:123:ASP:N    | 2.38                     | 0.48              |
| 4:ZI:93:PHE:HB3   | 4:ZI:333:VAL:HG13 | 1.95                     | 0.48              |
| 4:ZS:201:VAL:HG22 | 4:ZS:209:ALA:HB3  | 1.96                     | 0.48              |
| 4:ZV:5:GLN:HB2    | 4:ZV:50:LEU:O     | 2.13                     | 0.48              |
| 4:ZW:186:VAL:HG23 | 4:ZW:194:HIS:HB2  | 1.95                     | 0.48              |
| 4:ZY:21:GLY:HA2   | 4:ZY:24:ILE:HG22  | 1.94                     | 0.48              |
| 4:Zc:188:ASP:HA   | 4:Zc:257:ALA:HB2  | 1.95                     | 0.48              |
| 5:AB:59:ALA:O     | 3:AG:66:LEU:HD22  | 2.14                     | 0.48              |
| 6:AT:294:ARG:CG   | 11:A0:72:HIS:CE1  | 2.96                     | 0.48              |
| 6:AU:294:ARG:HD2  | 6:AU:367:GLU:OE1  | 2.13                     | 0.48              |
| 6:AV:266:VAL:HG22 | 6:AV:387:VAL:HG22 | 1.95                     | 0.48              |
| 11:A8:96:ASP:HB3  | 6:BL:318:ASN:OD1  | 2.13                     | 0.48              |
| 6:UN:80:ALA:CB    | 6:UN:83:SER:HB3   | 2.43                     | 0.48              |
| 6:WW:206:PRO:O    | 6:WW:207:PRO:C    | 2.56                     | 0.48              |
| 12:BC:94:PRO:HB2  | 12:BC:96:VAL:HG23 | 1.94                     | 0.48              |
| 12:BD:54:ALA:HB1  | 12:BD:55:PRO:CD   | 2.44                     | 0.48              |
| 1:D:104:PHE:O     | 1:D:123:ASP:HA    | 2.14                     | 0.48              |
| 1:G:104:PHE:O     | 1:G:123:ASP:HA    | 2.13                     | 0.48              |
| 1:N:104:PHE:O     | 1:N:123:ASP:HA    | 2.14                     | 0.48              |
| 1:U:88:ALA:HB1    | 1:W:171:ILE:CD1   | 2.43                     | 0.48              |
| 1:Y:62:TYR:CE1    | 2:w:129:VAL:HG13  | 2.48                     | 0.48              |
| 2:a:142:LEU:CD1   | 2:y:346:MET:HE3   | 2.42                     | 0.48              |
| 2:k:52:THR:HB     | 2:k:59:THR:HG23   | 1.95                     | 0.48              |
| 2:o:219:ARG:NH1   | 2:p:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:p:219:ARG:NH1   | 2:q:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:p:253:VAL:HG13  | 2:p:264:MET:HG2   | 1.95                     | 0.48              |
| 2:w:52:THR:HB     | 2:w:59:THR:HG23   | 1.95                     | 0.48              |
| 2:z:266:ARG:HG3   | 2:z:267:GLU:HG2   | 1.96                     | 0.48              |
| 3:6:86:LEU:HB2    | 4:ZH:42:MET:CE    | 2.27                     | 0.48              |
| 3:7:85:ASN:HA     | 4:ZI:50:LEU:HD22  | 1.96                     | 0.48              |
| 3:ZA:73:ARG:HB2   | 3:AN:218:TYR:OH   | 2.13                     | 0.48              |
| 3:ZA:240:TYR:CD2  | 4:ZF:395:ILE:CG2  | 2.90                     | 0.48              |
| 4:ZG:108:LEU:HD23 | 4:ZG:108:LEU:HA   | 1.71                     | 0.48              |
| 4:ZH:233:ASN:OD1  | 4:ZH:234:GLU:N    | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZJ:17:LEU:CD1   | 4:ZO:395:ILE:HD11 | 2.44                     | 0.48              |
| 4:ZN:267:MET:HE2  | 4:ZN:267:MET:HB3  | 1.78                     | 0.48              |
| 4:ZQ:228:THR:HG21 | 4:ZQ:244:VAL:HG11 | 1.96                     | 0.48              |
| 4:ZT:228:THR:HB   | 4:ZT:244:VAL:HG11 | 1.94                     | 0.48              |
| 4:Zb:85:LEU:HD13  | 4:Zb:114:MET:HB3  | 1.95                     | 0.48              |
| 4:Zc:139:ILE:HA   | 4:Zc:312:LEU:HD22 | 1.93                     | 0.48              |
| 5:AB:18:GLN:NE2   | 5:AB:223:ASN:OD1  | 2.46                     | 0.48              |
| 5:AB:34:PHE:HB3   | 5:AB:209:SER:HB3  | 1.96                     | 0.48              |
| 5:AB:220:MET:SD   | 3:AG:246:ALA:CA   | 3.00                     | 0.48              |
| 5:AC:217:MET:HE2  | 3:AN:258:THR:HA   | 1.84                     | 0.48              |
| 3:Al:62:LEU:HD21  | 12:BE:82:ASN:OD1  | 2.13                     | 0.48              |
| 3:AM:82:SER:HB2   | 3:AM:223:ASN:HD21 | 1.78                     | 0.48              |
| 6:AW:266:VAL:HG22 | 6:AW:387:VAL:HG22 | 1.95                     | 0.48              |
| 6:AZ:266:VAL:HG22 | 6:AZ:387:VAL:HG22 | 1.95                     | 0.48              |
| 7:Ar:17:ALA:HB2   | 9:Ax:195:ILE:HG23 | 1.95                     | 0.48              |
| 7:As:74:LEU:HD13  | 9:Ay:228:LEU:HB3  | 1.95                     | 0.48              |
| 9:Aw:148:ALA:HA   | 6:WA:164:LEU:HD13 | 1.95                     | 0.48              |
| 10:A2:86:ILE:HD11 | 11:A7:133:VAL:CG2 | 2.44                     | 0.48              |
| 6:UJ:98:LEU:HD22  | 6:UJ:147:LEU:CD2  | 2.39                     | 0.48              |
| 6:UJ:98:LEU:HD12  | 6:UJ:146:THR:HG1  | 1.77                     | 0.48              |
| 6:UM:80:ALA:CB    | 6:UM:83:SER:HB3   | 2.43                     | 0.48              |
| 6:WC:206:PRO:O    | 6:WC:207:PRO:C    | 2.56                     | 0.48              |
| 6:WF:206:PRO:O    | 6:WF:207:PRO:C    | 2.56                     | 0.48              |
| 6:WK:193:ALA:CB   | 6:WL:213:VAL:HG11 | 2.44                     | 0.48              |
| 6:WS:197:LEU:HD11 | 6:WT:156:HIS:HD2  | 1.78                     | 0.48              |
| 6:WS:200:SER:O    | 6:WT:158:ALA:HB3  | 2.05                     | 0.48              |
| 12:BC:97:ASP:O    | 12:BC:101:GLU:HG2 | 2.13                     | 0.48              |
| 1:E:102:THR:HG23  | 1:F:130:ASN:ND2   | 2.27                     | 0.48              |
| 1:P:65:LEU:CG     | 2:o:65:MET:HG3    | 2.39                     | 0.48              |
| 1:S:104:PHE:O     | 1:S:123:ASP:HA    | 2.14                     | 0.48              |
| 1:Z:50:SER:CB     | 2:w:32:ARG:NH1    | 2.77                     | 0.48              |
| 2:c:130:ASP:OD1   | 2:c:130:ASP:N     | 2.47                     | 0.48              |
| 2:d:130:ASP:OD1   | 2:d:130:ASP:N     | 2.47                     | 0.48              |
| 2:h:219:ARG:NH1   | 2:i:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:k:219:ARG:NH1   | 2:l:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:p:346:MET:HE3   | 2:r:142:LEU:CD1   | 2.42                     | 0.48              |
| 2:u:52:THR:HB     | 2:u:59:THR:HG23   | 1.95                     | 0.48              |
| 3:3:22:ILE:HD11   | 3:3:232:ASN:HB3   | 1.94                     | 0.48              |
| 3:4:22:ILE:HD11   | 3:4:232:ASN:HB3   | 1.94                     | 0.48              |
| 3:6:86:LEU:CD1    | 4:ZH:42:MET:HE1   | 2.37                     | 0.48              |
| 3:7:7:ILE:HG23    | 3:7:71:GLY:HA2    | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:45:LEU:HD13   | 3:AL:83:GLN:CG    | 2.44                     | 0.48              |
| 3:9:238:ARG:CZ    | 4:ZF:397:ASN:HB2  | 2.44                     | 0.48              |
| 3:ZA:45:LEU:CD1   | 3:AN:83:GLN:HG2   | 2.41                     | 0.48              |
| 4:ZF:10:LEU:HD21  | 4:ZK:399:LEU:HD21 | 1.96                     | 0.48              |
| 4:ZG:99:GLN:HG3   | 4:ZG:361:LEU:HD11 | 1.95                     | 0.48              |
| 4:ZJ:42:MET:SD    | 4:ZJ:53:LYS:HB2   | 2.54                     | 0.48              |
| 4:ZK:34:SER:HB3   | 4:ZK:366:VAL:HG12 | 1.94                     | 0.48              |
| 4:ZP:26:ASN:OD1   | 4:ZU:52:VAL:HB    | 2.13                     | 0.48              |
| 4:ZP:122:THR:OG1  | 4:ZP:129:GLN:NE2  | 2.46                     | 0.48              |
| 4:ZP:156:ILE:HD12 | 4:ZP:276:ILE:HG12 | 1.96                     | 0.48              |
| 4:ZR:101:LYS:HB2  | 4:ZW:324:GLU:OE1  | 2.13                     | 0.48              |
| 4:ZT:69:THR:HG21  | 4:ZT:361:LEU:HD12 | 1.95                     | 0.48              |
| 4:ZU:269:GLN:NE2  | 4:Za:190:GLN:HA   | 2.29                     | 0.48              |
| 4:ZZ:10:LEU:HG    | 4:ZZ:382:TYR:CZ   | 2.49                     | 0.48              |
| 4:Za:269:GLN:HG2  | 4:Zg:286:PRO:CG   | 2.44                     | 0.48              |
| 4:Zc:6:ALA:HB1    | 4:Zc:389:ILE:HG13 | 1.96                     | 0.48              |
| 4:Zf:294:ILE:HG12 | 4:Zf:300:VAL:HG22 | 1.96                     | 0.48              |
| 5:AA:70:GLN:HB2   | 3:AL:6:TRP:HD1    | 1.78                     | 0.48              |
| 5:AE:55:THR:H     | 12:BF:26:SER:HB2  | 1.78                     | 0.48              |
| 3:AL:19:MET:HB2   | 3:AL:236:VAL:HG11 | 1.96                     | 0.48              |
| 6:AY:294:ARG:CD   | 11:A9:68:THR:CG2  | 2.91                     | 0.48              |
| 6:Af:365:ASN:HD21 | 11:A8:65:LEU:HD11 | 1.78                     | 0.48              |
| 9:Ay:71:PHE:CZ    | 9:Ay:236:MET:HE1  | 2.49                     | 0.48              |
| 10:Az:69:ASN:ND2  | 11:A6:20:ALA:HB2  | 2.29                     | 0.48              |
| 6:UK:127:SER:O    | 6:UK:131:ASN:HB2  | 2.14                     | 0.48              |
| 6:UP:127:SER:O    | 6:UP:131:ASN:HB2  | 2.13                     | 0.48              |
| 12:BB:44:ALA:HB2  | 12:BB:96:VAL:HG22 | 1.96                     | 0.48              |
| 6:WB:128:GLU:HG2  | 6:WC:126:PHE:HD2  | 1.79                     | 0.48              |
| 6:WF:147:LEU:HA   | 6:WG:215:GLN:O    | 2.14                     | 0.48              |
| 6:WP:144:ILE:O    | 6:WP:147:LEU:HB2  | 2.13                     | 0.48              |
| 6:WT:196:HIS:HB3  | 6:WU:211:THR:CG2  | 2.30                     | 0.48              |
| 1:C:104:PHE:O     | 1:C:123:ASP:HA    | 2.13                     | 0.48              |
| 1:E:50:SER:CB     | 2:b:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:F:62:TYR:CE1    | 2:d:129:VAL:HG13  | 2.48                     | 0.48              |
| 1:G:88:ALA:HB1    | 1:I:171:ILE:CD1   | 2.43                     | 0.48              |
| 1:M:104:PHE:O     | 1:M:123:ASP:HA    | 2.13                     | 0.48              |
| 1:W:50:SER:CB     | 2:t:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:Y:50:SER:CB     | 2:v:32:ARG:NH1    | 2.77                     | 0.48              |
| 2:a:266:ARG:HG3   | 2:a:267:GLU:HG2   | 1.96                     | 0.48              |
| 2:d:52:THR:HB     | 2:d:59:THR:HG23   | 1.95                     | 0.48              |
| 2:h:266:ARG:HG3   | 2:h:267:GLU:HG2   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:m:273:CYS:CB    | 2:n:264:MET:O     | 2.42                     | 0.48              |
| 2:n:253:VAL:HG13  | 2:n:264:MET:HG2   | 1.95                     | 0.48              |
| 2:s:130:ASP:OD1   | 2:s:130:ASP:N     | 2.47                     | 0.48              |
| 2:w:346:MET:HE3   | 2:y:142:LEU:CD1   | 2.42                     | 0.48              |
| 2:y:266:ARG:HG3   | 2:y:267:GLU:HG2   | 1.96                     | 0.48              |
| 2:z:52:THR:HB     | 2:z:59:THR:HG23   | 1.95                     | 0.48              |
| 3:1:165:ALA:HB1   | 3:ZC:194:GLU:HG2  | 1.95                     | 0.48              |
| 3:5:241:GLU:CD    | 3:ZA:256:LYS:NZ   | 2.67                     | 0.48              |
| 3:ZA:95:VAL:HG11  | 3:ZA:214:LEU:HD23 | 1.95                     | 0.48              |
| 3:ZE:36:ARG:HB3   | 3:ZE:224:VAL:HG22 | 1.95                     | 0.48              |
| 4:ZK:102:LEU:O    | 4:ZP:322:ASN:HB2  | 2.13                     | 0.48              |
| 4:ZL:26:ASN:CG    | 4:ZQ:52:VAL:HG22  | 2.39                     | 0.48              |
| 4:ZM:93:PHE:HB3   | 4:ZM:333:VAL:HG13 | 1.95                     | 0.48              |
| 4:ZQ:317:LEU:HD11 | 4:ZQ:356:LEU:HD21 | 1.96                     | 0.48              |
| 4:ZQ:380:ARG:HB3  | 4:ZW:396:LEU:CD1  | 2.44                     | 0.48              |
| 4:ZT:210:VAL:HB   | 4:ZT:228:THR:HG22 | 1.94                     | 0.48              |
| 4:ZW:183:THR:HG21 | 4:Zh:132:ALA:HA   | 1.96                     | 0.48              |
| 5:AA:16:LEU:HD22  | 3:AF:253:MET:CE   | 2.44                     | 0.48              |
| 5:AA:109:PRO:HG3  | 3:AF:197:SER:HA   | 1.95                     | 0.48              |
| 5:AC:122:GLY:O    | 5:AC:123:GLU:C    | 2.56                     | 0.48              |
| 3:AN:2:ILE:HG21   | 3:AN:254:LEU:HD11 | 1.96                     | 0.48              |
| 7:Ab:8:MET:HE2    | 6:WS:124:SER:N    | 2.29                     | 0.48              |
| 6:Ah:294:ARG:HD2  | 6:Ah:367:GLU:OE1  | 2.12                     | 0.48              |
| 6:Ai:294:ARG:HD2  | 6:Ai:367:GLU:OE1  | 2.12                     | 0.48              |
| 6:Ai:296:ARG:HG2  | 6:Ai:296:ARG:HH11 | 1.79                     | 0.48              |
| 6:Ai:303:GLN:NE2  | 6:BK:319:GLN:CB   | 2.43                     | 0.48              |
| 7:As:60:ILE:HA    | 7:As:63:ILE:HG12  | 1.96                     | 0.48              |
| 8:At:182:ASN:HB3  | 8:At:239:PHE:HZ   | 1.79                     | 0.48              |
| 9:Aw:106:ASP:OD1  | 10:A2:31:THR:HA   | 2.14                     | 0.48              |
| 9:Ax:161:GLY:C    | 9:Ax:163:GLU:H    | 2.20                     | 0.48              |
| 6:UP:80:ALA:CB    | 6:UP:83:SER:HB3   | 2.43                     | 0.48              |
| 6:WA:196:HIS:HB3  | 6:WB:211:THR:CG2  | 2.36                     | 0.48              |
| 6:WC:187:ASP:O    | 6:WC:190:GLN:HB3  | 2.14                     | 0.48              |
| 6:WF:143:THR:OG1  | 6:WG:154:ARG:HG2  | 2.14                     | 0.48              |
| 6:WN:200:SER:CB   | 6:WO:173:SER:HB2  | 2.44                     | 0.48              |
| 1:A:50:SER:CB     | 2:x:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:B:50:SER:CB     | 2:y:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:C:50:SER:CB     | 2:z:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:D:50:SER:CB     | 2:a:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:F:50:SER:CB     | 2:c:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:G:50:SER:CB     | 2:d:32:ARG:NH1    | 2.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:50:SER:CB     | 2:e:32:ARG:NH1    | 2.77                     | 0.48              |
| 1:I:104:PHE:O     | 1:I:123:ASP:HA    | 2.14                     | 0.48              |
| 1:J:102:THR:HG23  | 1:K:130:ASN:ND2   | 2.28                     | 0.48              |
| 1:P:104:PHE:O     | 1:P:123:ASP:HA    | 2.14                     | 0.48              |
| 1:Q:104:PHE:O     | 1:Q:123:ASP:HA    | 2.14                     | 0.48              |
| 1:T:104:PHE:O     | 1:T:123:ASP:HA    | 2.13                     | 0.48              |
| 1:U:104:PHE:O     | 1:U:123:ASP:HA    | 2.13                     | 0.48              |
| 1:X:50:SER:CB     | 2:u:32:ARG:NH1    | 2.77                     | 0.48              |
| 2:b:266:ARG:HG3   | 2:b:267:GLU:HG2   | 1.96                     | 0.48              |
| 2:e:219:ARG:NH1   | 2:f:94:PRO:HB2    | 2.28                     | 0.48              |
| 2:g:266:ARG:HG3   | 2:g:267:GLU:HG2   | 1.96                     | 0.48              |
| 2:r:130:ASP:N     | 2:r:130:ASP:OD1   | 2.47                     | 0.48              |
| 2:s:266:ARG:HG3   | 2:s:267:GLU:HG2   | 1.96                     | 0.48              |
| 2:t:266:ARG:HG3   | 2:t:267:GLU:HG2   | 1.96                     | 0.48              |
| 2:z:130:ASP:N     | 2:z:130:ASP:OD1   | 2.47                     | 0.48              |
| 2:z:253:VAL:HG13  | 2:z:264:MET:HG2   | 1.95                     | 0.48              |
| 3:1:122:VAL:O     | 3:6:180:ASN:ND2   | 2.33                     | 0.48              |
| 3:1:137:GLN:HG3   | 3:1:137:GLN:O     | 2.12                     | 0.48              |
| 3:2:114:TYR:CD2   | 3:2:178:PHE:HZ    | 2.32                     | 0.48              |
| 3:4:136:VAL:O     | 3:4:137:GLN:C     | 2.57                     | 0.48              |
| 3:7:151:ILE:HG12  | 3:7:157:VAL:HG22  | 1.95                     | 0.48              |
| 3:8:227:ALA:CB    | 4:ZJ:399:LEU:HD22 | 2.44                     | 0.48              |
| 3:9:123:ASP:OD2   | 3:9:125:ASN:ND2   | 2.47                     | 0.48              |
| 3:9:130:THR:HG22  | 3:9:132:GLY:H     | 1.79                     | 0.48              |
| 3:ZA:57:SER:HA    | 3:AI:154:ASP:HB2  | 1.94                     | 0.48              |
| 4:ZI:147:LYS:HE2  | 4:ZI:282:ASN:HD22 | 1.79                     | 0.48              |
| 4:ZL:316:VAL:HG22 | 4:ZL:345:LEU:HD12 | 1.96                     | 0.48              |
| 4:ZU:269:GLN:HE22 | 4:Za:190:GLN:HA   | 1.78                     | 0.48              |
| 4:ZV:269:GLN:CG   | 4:Zb:286:PRO:HG2  | 2.43                     | 0.48              |
| 4:ZW:181:LYS:HZ2  | 4:Zh:129:GLN:NE2  | 2.12                     | 0.48              |
| 4:ZZ:367:ASP:HB2  | 4:ZZ:370:LYS:HG3  | 1.94                     | 0.48              |
| 4:Zb:96:ARG:HG3   | 4:Zb:96:ARG:O     | 2.14                     | 0.48              |
| 4:Zd:116:LEU:HD12 | 4:Zd:117:THR:N    | 2.29                     | 0.48              |
| 5:AD:26:LEU:HB3   | 3:AI:243:ASN:OD1  | 2.14                     | 0.48              |
| 5:AE:181:LEU:HD21 | 5:AE:193:LEU:HD11 | 1.96                     | 0.48              |
| 6:AI:266:VAL:HG22 | 6:AI:387:VAL:HG22 | 1.95                     | 0.48              |
| 6:Ap:266:VAL:HG22 | 6:Ap:387:VAL:HG22 | 1.95                     | 0.48              |
| 8:At:86:PHE:CZ    | 9:Au:88:VAL:HA    | 2.48                     | 0.48              |
| 6:UJ:80:ALA:CB    | 6:UJ:83:SER:HB3   | 2.43                     | 0.48              |
| 6:UL:180:LEU:HB2  | 6:UL:215:GLN:HE22 | 1.79                     | 0.48              |
| 6:WD:206:PRO:O    | 6:WD:207:PRO:C    | 2.56                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:WG:200:SER:OG   | 6:WH:175:SER:CB    | 2.45                     | 0.48              |
| 6:WH:187:ASP:OD2  | 6:WH:190:GLN:HB2   | 2.14                     | 0.48              |
| 12:BD:28:LEU:HD21 | 12:BD:102:MET:HE2  | 1.96                     | 0.48              |
| 6:BS:266:VAL:HG22 | 6:BS:387:VAL:HG22  | 1.95                     | 0.48              |
| 6:BX:266:VAL:HG22 | 6:BX:387:VAL:HG22  | 1.95                     | 0.48              |
| 1:E:65:LEU:CG     | 2:d:65:MET:HG3     | 2.39                     | 0.48              |
| 1:J:104:PHE:O     | 1:J:123:ASP:HA     | 2.14                     | 0.48              |
| 1:X:62:TYR:CE1    | 2:v:129:VAL:HG13   | 2.48                     | 0.48              |
| 2:c:346:MET:HE3   | 2:e:142:LEU:CD1    | 2.42                     | 0.48              |
| 2:d:219:ARG:NH1   | 2:e:94:PRO:HB2     | 2.28                     | 0.48              |
| 2:h:346:MET:HE3   | 2:j:142:LEU:CD1    | 2.42                     | 0.48              |
| 2:i:219:ARG:NH1   | 2:j:94:PRO:HB2     | 2.28                     | 0.48              |
| 2:i:266:ARG:HG3   | 2:i:267:GLU:HG2    | 1.96                     | 0.48              |
| 2:r:52:THR:HB     | 2:r:59:THR:HG23    | 1.95                     | 0.48              |
| 2:r:346:MET:HE2   | 2:t:142:LEU:HD11   | 1.95                     | 0.48              |
| 2:s:52:THR:HB     | 2:s:59:THR:HG23    | 1.95                     | 0.48              |
| 2:t:52:THR:HB     | 2:t:59:THR:HG23    | 1.95                     | 0.48              |
| 3:0:33:GLY:N      | 3:0:220:GLU:O      | 2.47                     | 0.48              |
| 3:1:73:ARG:CZ     | 5:AE:202:MET:SD    | 3.02                     | 0.48              |
| 3:3:64:SER:O      | 3:AM:76:ALA:HB1    | 2.14                     | 0.48              |
| 3:4:35:LYS:HE3    | 3:4:81:HIS:HA      | 1.95                     | 0.48              |
| 3:6:1:MET:HE2     | 3:AJ:226:VAL:CG1   | 2.38                     | 0.48              |
| 3:ZC:189:GLU:HA   | 4:ZH:40:ALA:HB1    | 1.96                     | 0.48              |
| 3:ZD:37:GLN:OE1   | 4:ZI:43:PHE:CZ     | 2.67                     | 0.48              |
| 3:ZD:97:ILE:HD11  | 3:ZD:103:PHE:CE2   | 2.49                     | 0.48              |
| 3:ZD:238:ARG:O    | 3:ZD:242:ILE:HG12  | 2.14                     | 0.48              |
| 4:ZG:27:SER:O     | 4:ZG:364:SER:OG    | 2.30                     | 0.48              |
| 4:ZH:159:ASN:ND2  | 4:ZH:162:ASP:OD2   | 2.46                     | 0.48              |
| 4:ZJ:87:ASP:OD2   | 4:ZJ:88:SER:N      | 2.45                     | 0.48              |
| 4:ZO:140:PRO:HD2  | 4:ZO:312:LEU:HD23  | 1.95                     | 0.48              |
| 4:Za:331:ASP:OD1  | 4:Zf:53:LYS:HE2    | 2.13                     | 0.48              |
| 4:Za:382:TYR:CG   | 4:Zf:395:ILE:HD12  | 2.49                     | 0.48              |
| 4:Zb:170:PHE:HE2  | 4:Zb:223:PRO:HG2   | 1.79                     | 0.48              |
| 4:Zc:110:ASN:OD1  | 4:Zc:114:MET:N     | 2.40                     | 0.48              |
| 5:AB:53:THR:CB    | 11:A7:92:GLN:HE21  | 2.27                     | 0.48              |
| 5:AB:202:MET:CE   | 3:AM:73:ARG:HH11   | 2.05                     | 0.48              |
| 5:AC:42:ARG:HG2   | 5:AC:58:THR:O      | 2.13                     | 0.48              |
| 5:AC:71:LEU:HB2   | 3:AN:70:THR:HG23   | 1.95                     | 0.48              |
| 5:AC:234:ILE:HG22 | 12:BC:106:MET:HE1  | 1.96                     | 0.48              |
| 5:AC:244:ALA:HA   | 12:BD:116:ILE:HD13 | 1.94                     | 0.48              |
| 5:AE:237:VAL:HG22 | 12:BF:21:LEU:HD21  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AI:16:GLN:HE22  | 3:AN:2:ILE:HD11   | 1.77                     | 0.48              |
| 3:AI:18:ASN:HB2   | 3:AI:41:PHE:HZ    | 1.79                     | 0.48              |
| 6:AR:296:ARG:HG2  | 6:AR:296:ARG:HH11 | 1.79                     | 0.48              |
| 7:Ar:14:MET:HE3   | 7:As:63:ILE:HD11  | 1.88                     | 0.48              |
| 8:At:9:TRP:CD1    | 8:At:9:TRP:H      | 2.31                     | 0.48              |
| 9:Au:99:PHE:C     | 9:Au:99:PHE:CD2   | 2.91                     | 0.48              |
| 9:Ax:153:LEU:CD2  | 6:WG:165:PHE:CE2  | 2.96                     | 0.48              |
| 6:WJ:171:SER:HB3  | 6:WJ:206:PRO:HG3  | 1.96                     | 0.48              |
| 6:WP:202:VAL:HB   | 6:WP:205:LEU:HB2  | 1.95                     | 0.48              |
| 6:BR:266:VAL:HG22 | 6:BR:387:VAL:HG22 | 1.95                     | 0.48              |
| 1:F:104:PHE:O     | 1:F:123:ASP:HA    | 2.14                     | 0.47              |
| 1:N:62:TYR:CE1    | 2:l:129:VAL:HG13  | 2.47                     | 0.47              |
| 1:T:88:ALA:HB1    | 1:V:171:ILE:CD1   | 2.43                     | 0.47              |
| 2:e:253:VAL:HG13  | 2:e:264:MET:HG2   | 1.95                     | 0.47              |
| 2:g:253:VAL:HG13  | 2:g:264:MET:HG2   | 1.95                     | 0.47              |
| 2:g:273:CYS:CB    | 2:h:264:MET:O     | 2.42                     | 0.47              |
| 2:h:253:VAL:HG13  | 2:h:264:MET:HG2   | 1.95                     | 0.47              |
| 2:j:52:THR:HB     | 2:j:59:THR:HG23   | 1.95                     | 0.47              |
| 2:l:54:GLN:OE1    | 3:AJ:202:ASN:OD1  | 2.32                     | 0.47              |
| 2:q:51:GLN:HG3    | 3:AI:209:ASN:HD21 | 1.73                     | 0.47              |
| 2:v:130:ASP:OD1   | 2:v:130:ASP:N     | 2.47                     | 0.47              |
| 3:0:42:GLU:HB3    | 3:0:75:VAL:HG21   | 1.96                     | 0.47              |
| 3:0:195:THR:HG22  | 3:0:196:GLN:H     | 1.79                     | 0.47              |
| 3:4:140:ILE:HD11  | 3:4:173:LEU:HD13  | 1.96                     | 0.47              |
| 3:5:238:ARG:CZ    | 3:ZB:255:GLN:HB2  | 2.43                     | 0.47              |
| 3:ZC:190:ASN:OD1  | 4:ZH:41:ASP:OD2   | 2.32                     | 0.47              |
| 4:ZH:87:ASP:OD2   | 4:ZH:87:ASP:N     | 2.39                     | 0.47              |
| 4:ZJ:110:ASN:ND2  | 4:ZJ:112:GLN:OE1  | 2.47                     | 0.47              |
| 4:ZP:102:LEU:O    | 4:ZU:322:ASN:HB2  | 2.14                     | 0.47              |
| 4:ZQ:233:ASN:HD21 | 4:ZQ:239:GLU:HB3  | 1.79                     | 0.47              |
| 4:ZS:103:ASP:OD2  | 4:ZS:105:ASN:N    | 2.44                     | 0.47              |
| 4:ZV:107:ASN:HD22 | 4:ZV:138:THR:HG22 | 1.79                     | 0.47              |
| 4:ZV:157:ASN:ND2  | 4:Zb:143:LEU:HD13 | 2.29                     | 0.47              |
| 4:ZW:183:THR:HG21 | 4:Zh:133:ASN:H    | 1.78                     | 0.47              |
| 4:ZW:317:LEU:HD11 | 4:ZW:356:LEU:HD21 | 1.96                     | 0.47              |
| 4:ZX:6:ALA:HB1    | 4:ZX:389:ILE:HG12 | 1.95                     | 0.47              |
| 5:AA:225:ARG:O    | 5:AA:229:MET:HG3  | 2.14                     | 0.47              |
| 5:AC:232:LYS:HG2  | 12:BD:102:MET:SD  | 2.54                     | 0.47              |
| 5:AD:240:ASN:ND2  | 12:BE:109:SER:OG  | 2.46                     | 0.47              |
| 3:AL:142:ILE:HD13 | 3:AL:149:ILE:HD13 | 1.96                     | 0.47              |
| 6:AR:266:VAL:HG22 | 6:AR:387:VAL:HG22 | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AW:296:ARG:HG2  | 6:AW:296:ARG:HH11 | 1.79                     | 0.47              |
| 6:Ag:266:VAL:HG22 | 6:Ag:387:VAL:HG22 | 1.95                     | 0.47              |
| 6:Aj:266:VAL:HG22 | 6:Aj:387:VAL:HG22 | 1.95                     | 0.47              |
| 6:AO:296:ARG:HG2  | 6:AO:296:ARG:HH11 | 1.79                     | 0.47              |
| 7:Aq:70:LEU:O     | 7:Aq:74:LEU:HG    | 2.14                     | 0.47              |
| 9:Aw:41:SER:HB2   | 10:A3:82:MET:HE3  | 1.95                     | 0.47              |
| 9:Ax:159:LEU:O    | 9:Ax:160:GLN:HB2  | 2.14                     | 0.47              |
| 9:Ay:80:THR:HB    | 9:Ay:83:ALA:HB2   | 1.96                     | 0.47              |
| 9:Ay:150:PHE:CE1  | 9:Ay:172:PRO:HB2  | 2.48                     | 0.47              |
| 11:A6:22:ARG:NH2  | 11:A6:108:GLN:OE1 | 2.47                     | 0.47              |
| 6:WA:216:SER:O    | 6:WW:190:GLN:HG2  | 2.14                     | 0.47              |
| 6:WC:145:GLU:O    | 6:WC:146:THR:C    | 2.56                     | 0.47              |
| 6:WI:193:ALA:HB1  | 6:WJ:213:VAL:HG11 | 1.94                     | 0.47              |
| 6:WU:142:ARG:O    | 6:WU:146:THR:HG23 | 2.14                     | 0.47              |
| 6:WU:206:PRO:O    | 6:WU:207:PRO:C    | 2.55                     | 0.47              |
| 1:E:47:ALA:HB1    | 2:b:178:GLN:HG3   | 1.96                     | 0.47              |
| 1:I:50:SER:CB     | 2:f:32:ARG:NH1    | 2.77                     | 0.47              |
| 1:L:104:PHE:O     | 1:L:123:ASP:HA    | 2.13                     | 0.47              |
| 1:O:68:ASP:OD1    | 2:n:64:ASN:ND2    | 2.48                     | 0.47              |
| 2:b:142:LEU:CD1   | 2:z:346:MET:HE3   | 2.42                     | 0.47              |
| 2:c:346:MET:HE2   | 2:e:142:LEU:HD11  | 1.95                     | 0.47              |
| 2:e:346:MET:HE2   | 2:g:142:LEU:HD11  | 1.95                     | 0.47              |
| 2:f:266:ARG:HG3   | 2:f:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:i:253:VAL:HG13  | 2:i:264:MET:HG2   | 1.95                     | 0.47              |
| 2:j:253:VAL:HG13  | 2:j:264:MET:HG2   | 1.95                     | 0.47              |
| 2:p:52:THR:HB     | 2:p:59:THR:HG23   | 1.95                     | 0.47              |
| 2:u:266:ARG:HG3   | 2:u:267:GLU:HG2   | 1.96                     | 0.47              |
| 3:1:1:MET:HE2     | 5:AE:213:PRO:HG3  | 1.97                     | 0.47              |
| 3:2:184:LEU:HB3   | 3:2:192:TYR:HB3   | 1.96                     | 0.47              |
| 3:5:235:GLN:HG3   | 3:ZB:5:LEU:HD21   | 1.96                     | 0.47              |
| 3:5:239:ALA:HB2   | 3:ZB:1:MET:CE     | 2.44                     | 0.47              |
| 3:6:16:GLN:O      | 3:6:19:MET:N      | 2.47                     | 0.47              |
| 3:8:40:VAL:O      | 3:8:75:VAL:N      | 2.45                     | 0.47              |
| 3:8:238:ARG:NH1   | 3:8:241:GLU:OE1   | 2.47                     | 0.47              |
| 3:ZC:20:ASP:OD1   | 4:ZH:2:SER:HB2    | 2.13                     | 0.47              |
| 3:ZC:31:THR:HB    | 4:ZH:39:PHE:O     | 2.14                     | 0.47              |
| 3:ZE:31:THR:CG2   | 4:ZJ:39:PHE:HB3   | 2.42                     | 0.47              |
| 4:ZL:380:ARG:NH1  | 4:ZR:397:ASN:OD1  | 2.44                     | 0.47              |
| 4:ZO:5:GLN:HG2    | 4:ZO:50:LEU:O     | 2.14                     | 0.47              |
| 4:ZQ:270:ASN:N    | 4:ZW:190:GLN:O    | 2.47                     | 0.47              |
| 4:ZV:387:GLN:OE1  | 4:Zb:400:VAL:HG13 | 2.09                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZW:171:SER:HB3  | 4:ZW:174:ASP:HB2   | 1.96                     | 0.47              |
| 4:ZY:319:ASN:ND2  | 4:ZY:352:ASN:O     | 2.46                     | 0.47              |
| 4:Za:68:ASN:OD1   | 4:Za:68:ASN:N      | 2.44                     | 0.47              |
| 4:Ze:196:MET:SD   | 4:Ze:212:THR:HB    | 2.54                     | 0.47              |
| 5:AB:21:VAL:HG23  | 3:AG:68:ILE:HG23   | 1.95                     | 0.47              |
| 5:AC:24:SER:HA    | 3:AH:7:ILE:CG2     | 2.44                     | 0.47              |
| 5:AE:244:ALA:HA   | 12:BF:116:ILE:HD13 | 1.95                     | 0.47              |
| 3:AF:155:GLY:HA2  | 3:AF:214:LEU:HD12  | 1.97                     | 0.47              |
| 3:AN:52:PRO:HG3   | 12:BD:80:PRO:HB3   | 1.96                     | 0.47              |
| 7:Ab:74:LEU:HB3   | 7:Ab:78:ARG:NH1    | 2.29                     | 0.47              |
| 6:Ae:296:ARG:HG2  | 6:Ae:296:ARG:HH11  | 1.79                     | 0.47              |
| 6:Ah:266:VAL:HG22 | 6:Ah:387:VAL:HG22  | 1.95                     | 0.47              |
| 6:Ai:303:GLN:NE2  | 6:BK:319:GLN:CD    | 2.72                     | 0.47              |
| 7:Aq:73:LEU:CD2   | 9:Aw:225:LEU:HD13  | 2.44                     | 0.47              |
| 8:At:205:ASN:HD21 | 9:Au:211:MET:HB2   | 1.79                     | 0.47              |
| 9:Ay:67:ILE:HG23  | 9:Ay:93:ALA:HB1    | 1.97                     | 0.47              |
| 9:Ay:142:THR:HG21 | 9:Ay:170:LEU:CD1   | 2.44                     | 0.47              |
| 9:Ay:159:LEU:CB   | 6:WI:165:PHE:HD2   | 2.26                     | 0.47              |
| 6:UL:129:GLN:O    | 6:UL:133:GLN:N     | 2.29                     | 0.47              |
| 6:UN:127:SER:O    | 6:UN:131:ASN:HB2   | 2.14                     | 0.47              |
| 6:WA:142:ARG:O    | 6:WA:146:THR:HG23  | 2.13                     | 0.47              |
| 6:WG:202:VAL:HB   | 6:WG:205:LEU:HB2   | 1.94                     | 0.47              |
| 6:WI:201:ALA:C    | 6:WJ:158:ALA:HB2   | 2.39                     | 0.47              |
| 6:WU:190:GLN:NE2  | 6:WV:216:SER:O     | 2.47                     | 0.47              |
| 1:D:47:ALA:HB1    | 2:a:178:GLN:HG3    | 1.96                     | 0.47              |
| 1:E:166:GLU:HB2   | 1:F:35:THR:CG2     | 2.30                     | 0.47              |
| 1:J:50:SER:CB     | 2:g:32:ARG:NH1     | 2.77                     | 0.47              |
| 1:M:62:TYR:HD1    | 2:k:129:VAL:HG11   | 1.62                     | 0.47              |
| 2:c:266:ARG:HG3   | 2:c:267:GLU:HG2    | 1.96                     | 0.47              |
| 2:f:277:GLN:HE22  | 2:f:347:SER:HB2    | 1.80                     | 0.47              |
| 2:g:346:MET:HE2   | 2:i:142:LEU:HD11   | 1.95                     | 0.47              |
| 2:j:219:ARG:NH1   | 2:k:94:PRO:HB2     | 2.28                     | 0.47              |
| 2:m:346:MET:HE2   | 2:o:142:LEU:HD11   | 1.95                     | 0.47              |
| 2:s:277:GLN:HE22  | 2:s:347:SER:HB2    | 1.80                     | 0.47              |
| 2:u:346:MET:HE3   | 2:w:142:LEU:CD1    | 2.42                     | 0.47              |
| 2:v:277:GLN:HE22  | 2:v:347:SER:HB2    | 1.80                     | 0.47              |
| 2:x:266:ARG:HG3   | 2:x:267:GLU:HG2    | 1.96                     | 0.47              |
| 2:y:130:ASP:OD1   | 2:y:130:ASP:N      | 2.47                     | 0.47              |
| 3:0:73:ARG:HH11   | 3:0:73:ARG:HB2     | 1.78                     | 0.47              |
| 3:4:2:ILE:HG22    | 3:4:254:LEU:HD11   | 1.95                     | 0.47              |
| 3:4:97:ILE:HD11   | 3:4:103:PHE:CE2    | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:ZA:95:VAL:O     | 3:ZA:118:GLY:HA3  | 2.13                     | 0.47              |
| 3:ZE:34:PHE:HB3   | 3:ZE:222:SER:HB3  | 1.95                     | 0.47              |
| 4:ZI:83:PHE:HB2   | 4:ZI:95:SER:O     | 2.14                     | 0.47              |
| 4:ZN:87:ASP:OD2   | 4:ZN:88:SER:N     | 2.39                     | 0.47              |
| 4:ZN:373:VAL:CG1  | 4:ZT:7:VAL:HG22   | 2.45                     | 0.47              |
| 4:ZP:27:SER:O     | 4:ZP:364:SER:OG   | 2.32                     | 0.47              |
| 4:ZQ:382:TYR:CE1  | 4:ZV:399:LEU:HD21 | 2.49                     | 0.47              |
| 4:ZW:294:ILE:HG12 | 4:ZW:300:VAL:HG22 | 1.96                     | 0.47              |
| 4:ZX:71:ARG:HB3   | 4:ZX:74:ASP:CG    | 2.39                     | 0.47              |
| 4:ZZ:373:VAL:HG11 | 4:Zf:7:VAL:HG22   | 1.96                     | 0.47              |
| 4:Zb:154:MET:HE1  | 4:Zb:276:ILE:HG12 | 1.96                     | 0.47              |
| 4:Zb:309:GLU:OE1  | 4:Zb:309:GLU:N    | 2.41                     | 0.47              |
| 4:Zg:87:ASP:OD1   | 4:Zg:91:SER:N     | 2.47                     | 0.47              |
| 5:AA:109:PRO:CG   | 3:AF:197:SER:O    | 2.59                     | 0.47              |
| 5:AB:217:MET:CE   | 3:AM:258:THR:HA   | 2.40                     | 0.47              |
| 5:AD:215:GLU:HG3  | 3:AJ:9:LYS:NZ     | 2.29                     | 0.47              |
| 5:AE:173:ARG:NH1  | 3:AJ:46:TYR:CZ    | 2.77                     | 0.47              |
| 3:AF:62:LEU:HD22  | 12:BB:83:PRO:HG2  | 1.91                     | 0.47              |
| 3:AG:115:THR:HB   | 3:AG:191:LEU:HD23 | 1.96                     | 0.47              |
| 6:Aa:266:VAL:HG22 | 6:Aa:387:VAL:HG22 | 1.95                     | 0.47              |
| 6:Af:296:ARG:HG2  | 6:Af:296:ARG:HH11 | 1.80                     | 0.47              |
| 6:Al:296:ARG:HG2  | 6:Al:296:ARG:HH11 | 1.80                     | 0.47              |
| 6:An:296:ARG:HG2  | 6:An:296:ARG:HH11 | 1.79                     | 0.47              |
| 7:Ar:4:GLU:HB3    | 6:WD:125:GLN:HB2  | 1.95                     | 0.47              |
| 8:At:144:LEU:C    | 6:WJ:164:LEU:HD21 | 2.39                     | 0.47              |
| 11:A8:24:GLU:HA   | 12:BC:6:ILE:HG12  | 1.96                     | 0.47              |
| 6:UL:103:GLN:CG   | 6:WH:182:PRO:HB3  | 2.43                     | 0.47              |
| 6:WA:170:LYS:H    | 6:WA:170:LYS:HD2  | 1.80                     | 0.47              |
| 6:WA:193:ALA:HB1  | 6:WB:213:VAL:CG1  | 2.43                     | 0.47              |
| 6:WC:169:GLN:NE2  | 6:WC:170:LYS:O    | 2.44                     | 0.47              |
| 6:WS:206:PRO:O    | 6:WS:207:PRO:C    | 2.56                     | 0.47              |
| 6:WU:115:LEU:HD21 | 6:WU:134:ARG:HD3  | 1.95                     | 0.47              |
| 1:K:50:SER:CB     | 2:h:32:ARG:NH1    | 2.77                     | 0.47              |
| 1:N:68:ASP:OD1    | 2:m:64:ASN:ND2    | 2.48                     | 0.47              |
| 1:Z:104:PHE:O     | 1:Z:123:ASP:HA    | 2.14                     | 0.47              |
| 2:a:52:THR:HB     | 2:a:59:THR:HG23   | 1.95                     | 0.47              |
| 2:a:277:GLN:HE22  | 2:a:347:SER:HB2   | 1.80                     | 0.47              |
| 2:d:253:VAL:HG13  | 2:d:264:MET:HG2   | 1.95                     | 0.47              |
| 2:f:253:VAL:HG13  | 2:f:264:MET:HG2   | 1.95                     | 0.47              |
| 2:i:277:GLN:HE22  | 2:i:347:SER:HB2   | 1.80                     | 0.47              |
| 2:l:273:CYS:CB    | 2:m:264:MET:O     | 2.42                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:q:52:THR:HB     | 2:q:59:THR:HG23    | 1.95                     | 0.47              |
| 2:q:277:GLN:HE22  | 2:q:347:SER:HB2    | 1.80                     | 0.47              |
| 2:r:266:ARG:HG3   | 2:r:267:GLU:HG2    | 1.96                     | 0.47              |
| 2:x:346:MET:HE3   | 2:z:142:LEU:CD1    | 2.42                     | 0.47              |
| 3:1:37:GLN:HG2    | 3:1:79:ARG:HG2     | 1.96                     | 0.47              |
| 3:5:44:LEU:O      | 3:5:70:THR:HB      | 2.15                     | 0.47              |
| 3:ZA:138:PRO:HD2  | 3:ZA:140:ILE:HD11  | 1.97                     | 0.47              |
| 3:ZC:238:ARG:NH2  | 4:ZI:397:ASN:HB2   | 2.28                     | 0.47              |
| 4:ZL:65:THR:HG22  | 4:ZW:50:LEU:HD13   | 1.96                     | 0.47              |
| 4:ZT:184:VAL:HG13 | 4:ZT:196:MET:HB2   | 1.96                     | 0.47              |
| 4:ZT:380:ARG:HH21 | 4:ZZ:397:ASN:HD21  | 1.62                     | 0.47              |
| 4:ZU:181:LYS:HZ3  | 4:ZU:197:ASN:HB3   | 1.79                     | 0.47              |
| 4:ZW:16:ASN:HB2   | 4:ZW:39:PHE:HZ     | 1.79                     | 0.47              |
| 4:ZW:211:TYR:CD1  | 4:ZW:226:ALA:HA    | 2.49                     | 0.47              |
| 4:Zc:83:PHE:HB2   | 4:Zc:95:SER:O      | 2.13                     | 0.47              |
| 4:Zd:20:ILE:O     | 4:Zd:24:ILE:HG13   | 2.14                     | 0.47              |
| 4:Zf:59:GLN:HB3   | 4:Zf:61:PHE:CE1    | 2.50                     | 0.47              |
| 5:AA:146:LEU:HB2  | 5:AA:155:VAL:HG23  | 1.95                     | 0.47              |
| 5:AA:224:ALA:O    | 5:AA:228:GLU:HG2   | 2.13                     | 0.47              |
| 5:AB:232:LYS:HD3  | 3:AH:260:LEU:O     | 2.13                     | 0.47              |
| 3:AF:9:LYS:HB2    | 12:BF:103:VAL:HG21 | 1.96                     | 0.47              |
| 3:AF:137:GLN:HA   | 3:AF:138:PRO:C     | 2.40                     | 0.47              |
| 3:AG:82:SER:HB3   | 3:AG:223:ASN:ND2   | 2.27                     | 0.47              |
| 3:AJ:62:LEU:HG    | 12:BF:84:LEU:CG    | 2.44                     | 0.47              |
| 3:AJ:176:THR:CG2  | 3:AJ:201:PRO:HB2   | 2.44                     | 0.47              |
| 3:AL:7:ILE:HG12   | 3:AL:70:THR:O      | 2.13                     | 0.47              |
| 3:AM:35:LYS:NZ    | 3:AM:220:GLU:OE2   | 2.44                     | 0.47              |
| 6:AT:296:ARG:HG2  | 6:AT:296:ARG:HH11  | 1.80                     | 0.47              |
| 6:AY:296:ARG:HH11 | 6:AY:296:ARG:HG2   | 1.80                     | 0.47              |
| 6:Am:266:VAL:HG22 | 6:Am:387:VAL:HG22  | 1.95                     | 0.47              |
| 6:An:266:VAL:HG22 | 6:An:387:VAL:HG22  | 1.95                     | 0.47              |
| 8:At:178:LEU:HD13 | 8:At:181:LEU:HD23  | 1.95                     | 0.47              |
| 9:Ay:86:ASN:C     | 9:Ay:88:VAL:N      | 2.72                     | 0.47              |
| 10:Az:77:LYS:HG3  | 11:A6:5:LEU:CD2    | 2.43                     | 0.47              |
| 11:A8:91:ASP:OD1  | 6:BM:313:PRO:HB3   | 2.14                     | 0.47              |
| 6:UO:127:SER:O    | 6:UO:131:ASN:HB2   | 2.13                     | 0.47              |
| 6:WC:190:GLN:C    | 6:WC:192:SER:N     | 2.72                     | 0.47              |
| 6:WW:142:ARG:O    | 6:WW:146:THR:HG23  | 2.14                     | 0.47              |
| 12:BE:42:TYR:O    | 12:BE:94:PRO:HB3   | 2.14                     | 0.47              |
| 1:C:47:ALA:HB1    | 2:z:178:GLN:HG3    | 1.96                     | 0.47              |
| 1:I:65:LEU:CG     | 2:h:65:MET:HG3     | 2.39                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:88:ALA:HB1    | 1:U:171:ILE:CD1   | 2.43                     | 0.47              |
| 2:b:130:ASP:N     | 2:b:130:ASP:OD1   | 2.47                     | 0.47              |
| 2:b:253:VAL:HG13  | 2:b:264:MET:HG2   | 1.95                     | 0.47              |
| 2:b:346:MET:HE3   | 2:d:142:LEU:CD1   | 2.42                     | 0.47              |
| 2:n:266:ARG:HG3   | 2:n:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:r:235:PHE:O     | 2:r:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:y:277:GLN:HE22  | 2:y:347:SER:HB2   | 1.80                     | 0.47              |
| 3:5:22:ILE:HG21   | 3:5:233:MET:HG3   | 1.96                     | 0.47              |
| 3:7:244:SER:CB    | 3:ZC:260:LEU:HD21 | 2.45                     | 0.47              |
| 3:ZE:48:THR:HG22  | 3:ZE:67:GLN:HE22  | 1.79                     | 0.47              |
| 4:ZG:103:ASP:O    | 4:ZG:104:GLU:C    | 2.56                     | 0.47              |
| 4:ZI:77:ILE:HG13  | 4:ZI:83:PHE:CZ    | 2.49                     | 0.47              |
| 4:ZJ:370:LYS:CE   | 4:ZP:11:ASN:HD21  | 2.25                     | 0.47              |
| 4:ZO:380:ARG:NH2  | 4:ZU:393:ASP:OD2  | 2.48                     | 0.47              |
| 4:ZR:180:LYS:HB3  | 4:ZR:200:PHE:HD1  | 1.79                     | 0.47              |
| 4:ZZ:180:LYS:HB3  | 4:ZZ:200:PHE:HB2  | 1.96                     | 0.47              |
| 4:Zb:171:SER:HB3  | 4:Zb:174:ASP:HB2  | 1.97                     | 0.47              |
| 4:Zg:79:GLN:HB2   | 4:Zg:354:GLY:HA3  | 1.96                     | 0.47              |
| 4:Zg:194:HIS:CE1  | 4:Zg:251:ILE:HD12 | 2.50                     | 0.47              |
| 5:AD:228:GLU:HB3  | 3:AJ:258:THR:HB   | 1.96                     | 0.47              |
| 5:AE:229:MET:HE2  | 3:AK:257:LEU:CD2  | 2.43                     | 0.47              |
| 3:AG:123:ASP:OD1  | 3:AG:127:GLN:HB3  | 2.14                     | 0.47              |
| 3:AI:32:ASN:HD22  | 3:AI:219:VAL:HB   | 1.80                     | 0.47              |
| 3:AI:73:ARG:NH1   | 3:AN:51:GLN:OE1   | 2.48                     | 0.47              |
| 6:AU:266:VAL:HG22 | 6:AU:387:VAL:HG22 | 1.95                     | 0.47              |
| 6:Am:296:ARG:HG2  | 6:Am:296:ARG:HH11 | 1.79                     | 0.47              |
| 6:Ao:266:VAL:HG22 | 6:Ao:387:VAL:HG22 | 1.95                     | 0.47              |
| 9:Ax:75:ARG:HD2   | 9:Ax:84:PRO:HD2   | 1.95                     | 0.47              |
| 10:Az:76:GLN:O    | 10:Az:77:LYS:C    | 2.57                     | 0.47              |
| 11:A8:10:ARG:HE   | 11:A8:53:MET:HE1  | 1.79                     | 0.47              |
| 6:WK:145:GLU:O    | 6:WK:146:THR:C    | 2.58                     | 0.47              |
| 6:WP:145:GLU:C    | 6:WP:147:LEU:N    | 2.72                     | 0.47              |
| 12:BC:46:GLN:HB3  | 6:BL:312:VAL:HG13 | 1.95                     | 0.47              |
| 6:BW:296:ARG:HG2  | 6:BW:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:E:62:TYR:CE1    | 2:c:129:VAL:HG13  | 2.48                     | 0.47              |
| 1:T:68:ASP:OD1    | 2:s:64:ASN:ND2    | 2.48                     | 0.47              |
| 1:W:62:TYR:CE1    | 2:u:129:VAL:HG13  | 2.48                     | 0.47              |
| 1:Y:166:GLU:HB2   | 1:Z:35:THR:CG2    | 2.30                     | 0.47              |
| 2:a:346:MET:HE2   | 2:c:142:LEU:HD11  | 1.95                     | 0.47              |
| 2:d:277:GLN:HE22  | 2:d:347:SER:HB2   | 1.80                     | 0.47              |
| 2:h:273:CYS:CB    | 2:i:264:MET:O     | 2.42                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:235:PHE:O     | 2:i:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:j:266:ARG:HG3   | 2:j:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:l:277:GLN:HE22  | 2:l:347:SER:HB2   | 1.80                     | 0.47              |
| 2:m:266:ARG:HG3   | 2:m:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:n:277:GLN:HE22  | 2:n:347:SER:HB2   | 1.80                     | 0.47              |
| 2:o:235:PHE:O     | 2:o:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:p:277:GLN:HE22  | 2:p:347:SER:HB2   | 1.80                     | 0.47              |
| 2:u:130:ASP:OD1   | 2:u:130:ASP:N     | 2.47                     | 0.47              |
| 2:u:253:VAL:HG13  | 2:u:264:MET:HG2   | 1.95                     | 0.47              |
| 2:w:253:VAL:HG13  | 2:w:264:MET:HG2   | 1.95                     | 0.47              |
| 2:x:51:GLN:HE21   | 3:AH:125:ASN:ND2  | 2.13                     | 0.47              |
| 3:1:260:LEU:HD11  | 3:AK:247:VAL:HG12 | 1.96                     | 0.47              |
| 3:2:237:GLN:HB2   | 3:7:249:THR:HG23  | 1.95                     | 0.47              |
| 3:3:230:LEU:HA    | 3:3:233:MET:HE2   | 1.95                     | 0.47              |
| 3:8:95:VAL:O      | 3:8:118:GLY:HA3   | 2.14                     | 0.47              |
| 3:ZB:238:ARG:HD3  | 4:ZH:396:LEU:HD13 | 1.96                     | 0.47              |
| 3:ZC:230:LEU:O    | 3:ZC:234:ILE:HG12 | 2.14                     | 0.47              |
| 4:ZH:67:THR:N     | 4:ZH:361:LEU:O    | 2.45                     | 0.47              |
| 4:ZH:114:MET:HE1  | 4:ZH:333:VAL:HG11 | 1.96                     | 0.47              |
| 4:ZL:84:ARG:HG2   | 4:ZL:117:THR:OG1  | 2.14                     | 0.47              |
| 4:ZM:86:VAL:HG13  | 4:ZM:117:THR:HG21 | 1.97                     | 0.47              |
| 4:ZR:186:VAL:HG22 | 4:ZR:194:HIS:HB2  | 1.94                     | 0.47              |
| 4:ZW:233:ASN:HD21 | 4:ZW:237:ILE:HB   | 1.79                     | 0.47              |
| 4:Ze:33:LYS:HG3   | 4:Ze:61:PHE:CD2   | 2.49                     | 0.47              |
| 5:AB:214:VAL:CA   | 3:AM:257:LEU:HD21 | 2.45                     | 0.47              |
| 5:AE:225:ARG:HD2  | 3:AK:254:LEU:HB3  | 1.97                     | 0.47              |
| 6:AV:296:ARG:HG2  | 6:AV:296:ARG:HH11 | 1.79                     | 0.47              |
| 6:Af:295:SER:OG   | 11:A8:65:LEU:HD13 | 2.14                     | 0.47              |
| 6:Ah:296:ARG:HG2  | 6:Ah:296:ARG:HH11 | 1.79                     | 0.47              |
| 7:Aq:29:LEU:HD23  | 7:Aq:30:ILE:HD13  | 1.96                     | 0.47              |
| 7:As:2:THR:OG1    | 7:As:4:GLU:OE1    | 2.29                     | 0.47              |
| 9:Av:66:ARG:NH2   | 9:Av:178:GLU:OE1  | 2.45                     | 0.47              |
| 11:A7:51:LYS:CD   | 11:A7:55:ARG:HH12 | 2.27                     | 0.47              |
| 11:A9:11:PHE:HD1  | 11:A9:53:MET:HE2  | 1.80                     | 0.47              |
| 6:UK:207:PRO:HG2  | 6:WE:187:ASP:OD1  | 2.10                     | 0.47              |
| 6:UM:127:SER:O    | 6:UM:131:ASN:HB2  | 2.14                     | 0.47              |
| 6:UN:98:LEU:HD22  | 6:UN:147:LEU:CD2  | 2.39                     | 0.47              |
| 6:WJ:200:SER:O    | 6:WK:158:ALA:HB2  | 2.15                     | 0.47              |
| 6:BI:319:GLN:HG2  | 6:BI:320:PRO:HD2  | 1.95                     | 0.47              |
| 6:BR:296:ARG:HG2  | 6:BR:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:B:47:ALA:HB1    | 2:y:178:GLN:HG3   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:65:LEU:CG     | 2:e:65:MET:HG3    | 2.39                     | 0.47              |
| 1:L:50:SER:CB     | 2:i:32:ARG:NH1    | 2.77                     | 0.47              |
| 1:M:62:TYR:CE1    | 2:k:129:VAL:HG13  | 2.47                     | 0.47              |
| 1:Q:65:LEU:CG     | 2:p:65:MET:HG3    | 2.39                     | 0.47              |
| 1:Y:65:LEU:CG     | 2:x:65:MET:HG3    | 2.39                     | 0.47              |
| 2:b:52:THR:HB     | 2:b:59:THR:HG23   | 1.95                     | 0.47              |
| 2:b:277:GLN:HE22  | 2:b:347:SER:HB2   | 1.80                     | 0.47              |
| 2:c:253:VAL:HG13  | 2:c:264:MET:HG2   | 1.95                     | 0.47              |
| 2:d:346:MET:HE3   | 2:f:142:LEU:CD1   | 2.42                     | 0.47              |
| 2:i:273:CYS:CB    | 2:j:264:MET:O     | 2.42                     | 0.47              |
| 2:i:346:MET:HE2   | 2:k:142:LEU:HD11  | 1.95                     | 0.47              |
| 2:j:235:PHE:O     | 2:j:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:l:235:PHE:O     | 2:l:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:l:253:VAL:HG13  | 2:l:264:MET:HG2   | 1.95                     | 0.47              |
| 2:l:266:ARG:HG3   | 2:l:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:o:266:ARG:HG3   | 2:o:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:p:235:PHE:O     | 2:p:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:q:235:PHE:O     | 2:q:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:s:253:VAL:HG13  | 2:s:264:MET:HG2   | 1.95                     | 0.47              |
| 2:t:277:GLN:HE22  | 2:t:347:SER:HB2   | 1.80                     | 0.47              |
| 2:x:277:GLN:HE22  | 2:x:347:SER:HB2   | 1.80                     | 0.47              |
| 3:0:70:THR:CG2    | 5:AD:71:LEU:H     | 2.27                     | 0.47              |
| 3:0:193:ILE:CD1   | 5:AD:152:PRO:CG   | 2.93                     | 0.47              |
| 3:2:165:ALA:HB1   | 3:ZD:194:GLU:HG2  | 1.97                     | 0.47              |
| 3:3:123:ASP:O     | 3:8:179:MET:HG3   | 2.15                     | 0.47              |
| 3:6:47:GLN:N      | 3:6:68:ILE:O      | 2.45                     | 0.47              |
| 3:6:57:SER:OG     | 3:AK:108:PRO:CG   | 2.51                     | 0.47              |
| 3:7:138:PRO:HD2   | 3:7:140:ILE:HG13  | 1.97                     | 0.47              |
| 3:9:50:ARG:HD3    | 3:9:66:LEU:HD12   | 1.97                     | 0.47              |
| 3:ZE:147:LEU:HD21 | 4:ZJ:352:ASN:HA   | 1.97                     | 0.47              |
| 4:ZH:24:ILE:O     | 4:ZH:27:SER:OG    | 2.26                     | 0.47              |
| 4:ZH:270:ASN:O    | 4:ZN:285:LYS:HE3  | 2.14                     | 0.47              |
| 4:ZI:17:LEU:CD1   | 4:ZN:395:ILE:HD11 | 2.44                     | 0.47              |
| 4:ZI:374:ASN:O    | 4:ZI:376:ILE:N    | 2.48                     | 0.47              |
| 4:ZJ:350:SER:OG   | 4:ZJ:351:GLY:N    | 2.48                     | 0.47              |
| 4:ZL:29:THR:HG22  | 4:ZQ:39:PHE:CB    | 2.41                     | 0.47              |
| 4:ZL:383:GLN:O    | 4:ZL:387:GLN:HG2  | 2.15                     | 0.47              |
| 4:ZO:33:LYS:HD2   | 4:ZO:61:PHE:HA    | 1.95                     | 0.47              |
| 4:ZO:159:ASN:ND2  | 4:ZO:162:ASP:OD2  | 2.43                     | 0.47              |
| 4:ZO:373:VAL:HG11 | 4:ZU:7:VAL:HG22   | 1.96                     | 0.47              |
| 4:ZQ:33:LYS:O     | 4:ZQ:59:GLN:NE2   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZR:281:GLN:NE2  | 4:ZR:283:GLY:O     | 2.47                     | 0.47              |
| 4:ZR:390:LYS:O    | 4:ZR:394:GLN:HG2   | 2.14                     | 0.47              |
| 4:ZS:6:ALA:O      | 4:ZS:9:GLY:N       | 2.47                     | 0.47              |
| 4:ZS:379:GLN:HG3  | 4:ZX:391:THR:HG23  | 1.96                     | 0.47              |
| 4:ZT:144:MET:HG3  | 4:ZT:310:GLN:NE2   | 2.29                     | 0.47              |
| 4:Za:93:PHE:HB3   | 4:Za:333:VAL:HG13  | 1.96                     | 0.47              |
| 4:Za:149:THR:HG21 | 4:Za:186:VAL:HB    | 1.97                     | 0.47              |
| 4:Za:269:GLN:HG2  | 4:Zg:286:PRO:HG2   | 1.97                     | 0.47              |
| 4:Zc:80:ASN:OD1   | 4:Zc:81:GLY:N      | 2.46                     | 0.47              |
| 4:Zd:116:LEU:HD12 | 4:Zd:117:THR:H     | 1.80                     | 0.47              |
| 4:Zf:2:SER:OG     | 4:Zf:3:PHE:N       | 2.46                     | 0.47              |
| 5:AD:50:SER:HB2   | 11:A9:91:ASP:O     | 2.15                     | 0.47              |
| 5:AD:229:MET:HG3  | 3:AJ:258:THR:CG2   | 2.23                     | 0.47              |
| 3:AG:7:ILE:HG23   | 3:AG:71:GLY:HA2    | 1.97                     | 0.47              |
| 3:AG:159:VAL:O    | 3:AG:168:VAL:N     | 2.48                     | 0.47              |
| 3:AH:1:MET:HE1    | 12:BC:75:LYS:HD3   | 1.97                     | 0.47              |
| 3:AI:44:LEU:HD22  | 12:BD:90:TYR:CE1   | 2.50                     | 0.47              |
| 3:AL:2:ILE:HG12   | 3:AL:254:LEU:HD11  | 1.97                     | 0.47              |
| 3:AN:151:ILE:HG12 | 3:AN:157:VAL:HG22  | 1.97                     | 0.47              |
| 6:AS:266:VAL:HG22 | 6:AS:387:VAL:HG22  | 1.95                     | 0.47              |
| 6:AT:297:GLN:OE1  | 11:A0:76:GLN:OE1   | 2.33                     | 0.47              |
| 6:AY:372:ILE:HB   | 10:A3:4:ILE:HG12   | 1.96                     | 0.47              |
| 7:Ab:85:PRO:CD    | 9:Av:238:SER:OG    | 2.61                     | 0.47              |
| 6:Ac:296:ARG:HG2  | 6:Ac:296:ARG:HH11  | 1.79                     | 0.47              |
| 6:Ak:266:VAL:HG22 | 6:Ak:387:VAL:HG22  | 1.95                     | 0.47              |
| 6:Al:266:VAL:HG22 | 6:Al:387:VAL:HG22  | 1.95                     | 0.47              |
| 6:An:276:GLU:CD   | 10:Az:11:ILE:CD1   | 2.87                     | 0.47              |
| 6:Ao:296:ARG:HG2  | 6:Ao:296:ARG:HH11  | 1.79                     | 0.47              |
| 6:Ao:357:SER:OG   | 6:BI:319:GLN:OE1   | 2.30                     | 0.47              |
| 6:Ap:296:ARG:HG2  | 6:Ap:296:ARG:HH11  | 1.79                     | 0.47              |
| 6:AQ:296:ARG:HG2  | 6:AQ:296:ARG:HH11  | 1.80                     | 0.47              |
| 7:Ar:6:VAL:HG22   | 9:Ax:187:PHE:CZ    | 2.50                     | 0.47              |
| 8:At:94:ALA:HB2   | 8:At:179:ILE:HA    | 1.96                     | 0.47              |
| 9:Av:59:LEU:HD11  | 10:A1:102:MET:CE   | 2.43                     | 0.47              |
| 9:Av:205:MET:CE   | 9:Aw:209:MET:HA    | 2.45                     | 0.47              |
| 10:A1:99:VAL:HA   | 10:A1:102:MET:HE3  | 1.97                     | 0.47              |
| 6:UI:127:SER:O    | 6:UI:131:ASN:HB2   | 2.13                     | 0.47              |
| 6:UJ:73:MET:HE1   | 6:UJ:99:ARG:HD2    | 1.95                     | 0.47              |
| 6:UL:98:LEU:HD22  | 6:UL:147:LEU:CD2   | 2.39                     | 0.47              |
| 6:UN:94:HIS:HB2   | 6:UN:146:THR:HG21  | 1.97                     | 0.47              |
| 12:BB:14:LEU:HD21 | 12:BB:116:ILE:HG13 | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WA:190:GLN:O    | 6:WA:191:ILE:C    | 2.57                     | 0.47              |
| 6:WB:206:PRO:O    | 6:WB:207:PRO:C    | 2.56                     | 0.47              |
| 6:WC:202:VAL:HB   | 6:WC:205:LEU:HB2  | 1.95                     | 0.47              |
| 6:WE:134:ARG:HB3  | 6:WE:134:ARG:NH2  | 2.27                     | 0.47              |
| 6:WF:187:ASP:H    | 6:WF:190:GLN:CD   | 2.22                     | 0.47              |
| 6:WH:200:SER:HG   | 6:WI:175:SER:HB2  | 1.77                     | 0.47              |
| 6:WO:202:VAL:HB   | 6:WO:205:LEU:HB2  | 1.95                     | 0.47              |
| 6:WT:186:LEU:HA   | 6:WT:190:GLN:OE1  | 2.15                     | 0.47              |
| 12:BF:5:ASN:N     | 6:BG:317:SER:O    | 2.48                     | 0.47              |
| 6:BT:296:ARG:HG2  | 6:BT:296:ARG:HH11 | 1.80                     | 0.47              |
| 6:BX:296:ARG:HH11 | 6:BX:296:ARG:HG2  | 1.79                     | 0.47              |
| 1:C:68:ASP:OD1    | 2:b:64:ASN:ND2    | 2.48                     | 0.47              |
| 1:M:68:ASP:OD1    | 2:l:64:ASN:ND2    | 2.48                     | 0.47              |
| 1:O:104:PHE:O     | 1:O:123:ASP:HA    | 2.14                     | 0.47              |
| 1:Q:166:GLU:HB2   | 1:R:35:THR:CG2    | 2.30                     | 0.47              |
| 1:W:104:PHE:O     | 1:W:123:ASP:HA    | 2.14                     | 0.47              |
| 1:Z:52:PHE:CD2    | 2:x:172:GLU:HB3   | 2.50                     | 0.47              |
| 2:c:277:GLN:HE22  | 2:c:347:SER:HB2   | 1.80                     | 0.47              |
| 2:d:266:ARG:HG3   | 2:d:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:e:266:ARG:HG3   | 2:e:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:e:346:MET:HE3   | 2:g:142:LEU:CD1   | 2.42                     | 0.47              |
| 2:h:235:PHE:O     | 2:h:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:j:277:GLN:HE22  | 2:j:347:SER:HB2   | 1.80                     | 0.47              |
| 2:k:235:PHE:O     | 2:k:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:k:253:VAL:HG13  | 2:k:264:MET:HG2   | 1.95                     | 0.47              |
| 2:k:277:GLN:HE22  | 2:k:347:SER:HB2   | 1.80                     | 0.47              |
| 2:m:346:MET:HE3   | 2:o:142:LEU:CD1   | 2.42                     | 0.47              |
| 2:q:130:ASP:OD1   | 2:q:130:ASP:N     | 2.47                     | 0.47              |
| 2:q:253:VAL:HG13  | 2:q:264:MET:HG2   | 1.95                     | 0.47              |
| 2:v:266:ARG:HG3   | 2:v:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:v:346:MET:HE3   | 2:x:142:LEU:CD1   | 2.42                     | 0.47              |
| 2:w:266:ARG:HG3   | 2:w:267:GLU:HG2   | 1.96                     | 0.47              |
| 2:y:253:VAL:HG13  | 2:y:264:MET:HG2   | 1.95                     | 0.47              |
| 3:0:89:THR:HG21   | 3:0:94:ASP:HB2    | 1.97                     | 0.47              |
| 3:4:74:PRO:O      | 3:9:66:LEU:HD11   | 2.15                     | 0.47              |
| 4:ZG:318:ALA:HB2  | 4:ZG:345:LEU:HD23 | 1.96                     | 0.47              |
| 4:ZH:355:LYS:N    | 4:ZH:355:LYS:HD3  | 2.29                     | 0.47              |
| 4:ZI:77:ILE:HG12  | 4:ZI:356:LEU:CD2  | 2.45                     | 0.47              |
| 4:ZN:41:ASP:N     | 4:ZN:41:ASP:OD2   | 2.42                     | 0.47              |
| 4:ZO:74:ASP:OD1   | 4:ZO:74:ASP:N     | 2.48                     | 0.47              |
| 4:ZP:367:ASP:O    | 4:ZP:371:GLU:HG2  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZQ:102:LEU:O    | 4:ZV:322:ASN:HB2   | 2.15                     | 0.47              |
| 4:ZS:170:PHE:HE2  | 4:ZS:223:PRO:HG2   | 1.79                     | 0.47              |
| 5:AE:9:MET:CB     | 12:BE:103:VAL:HG21 | 2.43                     | 0.47              |
| 5:AE:147:ASN:O    | 5:AE:148:PRO:C     | 2.58                     | 0.47              |
| 5:AE:234:ILE:CG2  | 12:BE:106:MET:HE1  | 2.45                     | 0.47              |
| 3:AL:95:VAL:O     | 3:AL:118:GLY:HA3   | 2.15                     | 0.47              |
| 6:AX:372:ILE:HB   | 10:A3:11:ILE:CG2   | 2.45                     | 0.47              |
| 6:AZ:296:ARG:HG2  | 6:AZ:296:ARG:HH11  | 1.80                     | 0.47              |
| 7:Ab:17:ALA:HB2   | 9:Av:195:ILE:HG23  | 1.97                     | 0.47              |
| 9:Au:144:GLU:N    | 6:WO:164:LEU:O     | 2.43                     | 0.47              |
| 9:Au:153:LEU:HD23 | 6:WR:165:PHE:HE2   | 1.80                     | 0.47              |
| 9:Ax:148:ALA:HB1  | 6:WF:165:PHE:CD1   | 2.49                     | 0.47              |
| 6:UM:98:LEU:CD1   | 6:UM:146:THR:HG1   | 2.28                     | 0.47              |
| 6:WD:202:VAL:HB   | 6:WD:205:LEU:HB2   | 1.94                     | 0.47              |
| 6:WG:112:GLY:HA3  | 6:WG:139:GLU:OE1   | 2.15                     | 0.47              |
| 12:BC:10:ALA:HB3  | 12:BC:119:LEU:HG   | 1.97                     | 0.47              |
| 6:BU:296:ARG:HH11 | 6:BU:296:ARG:HG2   | 1.79                     | 0.47              |
| 1:A:52:PHE:CD2    | 2:y:172:GLU:HB3    | 2.50                     | 0.47              |
| 1:L:52:PHE:CD2    | 2:j:172:GLU:HB3    | 2.50                     | 0.47              |
| 1:S:68:ASP:OD1    | 2:r:64:ASN:ND2     | 2.48                     | 0.47              |
| 1:U:165:GLY:C     | 1:V:35:THR:HG21    | 2.40                     | 0.47              |
| 1:U:166:GLU:HB2   | 1:V:35:THR:CG2     | 2.30                     | 0.47              |
| 1:Y:52:PHE:CD2    | 2:w:172:GLU:HB3    | 2.50                     | 0.47              |
| 2:c:52:THR:HB     | 2:c:59:THR:HG23    | 1.95                     | 0.47              |
| 2:e:235:PHE:O     | 2:e:239:ILE:HG12   | 2.15                     | 0.47              |
| 2:e:277:GLN:HE22  | 2:e:347:SER:HB2    | 1.80                     | 0.47              |
| 2:k:346:MET:HE2   | 2:m:142:LEU:HD11   | 1.95                     | 0.47              |
| 2:m:188:GLN:HG2   | 2:n:98:ARG:HD3     | 1.97                     | 0.47              |
| 2:m:253:VAL:HG13  | 2:m:264:MET:HG2    | 1.95                     | 0.47              |
| 2:m:277:GLN:HE22  | 2:m:347:SER:HB2    | 1.80                     | 0.47              |
| 2:n:188:GLN:HG2   | 2:o:98:ARG:HD3     | 1.97                     | 0.47              |
| 2:s:235:PHE:O     | 2:s:239:ILE:HG12   | 2.15                     | 0.47              |
| 3:6:56:SER:O      | 3:6:57:SER:C       | 2.57                     | 0.47              |
| 3:8:41:PHE:HA     | 3:8:74:PRO:HA      | 1.96                     | 0.47              |
| 4:ZG:195:ASP:O    | 4:ZG:215:SER:OG    | 2.33                     | 0.47              |
| 4:ZH:17:LEU:HD13  | 4:ZM:395:ILE:CD1   | 2.45                     | 0.47              |
| 4:ZQ:97:ASN:HD22  | 4:ZQ:332:ASN:ND2   | 2.13                     | 0.47              |
| 4:ZR:181:LYS:HD3  | 4:Zc:129:GLN:NE2   | 2.30                     | 0.47              |
| 4:ZS:188:ASP:HA   | 4:ZS:257:ALA:HB2   | 1.96                     | 0.47              |
| 4:ZS:380:ARG:HD3  | 4:ZS:380:ARG:HA    | 1.65                     | 0.47              |
| 4:ZW:269:GLN:HG2  | 4:Zc:286:PRO:HG2   | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:ZX:317:LEU:HD11  | 4:ZX:356:LEU:HD21  | 1.97                     | 0.47              |
| 4:Za:383:GLN:HB3   | 4:Zg:400:VAL:HG11  | 1.97                     | 0.47              |
| 5:AB:228:GLU:HA    | 3:AG:256:LYS:HG2   | 1.97                     | 0.47              |
| 5:AC:18:GLN:HE21   | 5:AC:41:LEU:HG     | 1.79                     | 0.47              |
| 5:AC:28:ASN:HD21   | 3:AH:43:ASP:CB     | 2.25                     | 0.47              |
| 5:AD:83:GLN:HG2    | 5:AD:84:GLN:H      | 1.79                     | 0.47              |
| 5:AD:241:GLU:OE1   | 11:A9:106:ARG:NH2  | 2.48                     | 0.47              |
| 3:AG:80:LEU:C      | 3:AG:82:SER:N      | 2.71                     | 0.47              |
| 3:AL:3:SER:C       | 3:AL:5:LEU:N       | 2.72                     | 0.47              |
| 3:AL:153:ARG:HE    | 3:AL:213:LEU:HD13  | 1.79                     | 0.47              |
| 3:AM:120:PHE:CD1   | 3:AM:136:VAL:HG21  | 2.50                     | 0.47              |
| 6:Ad:296:ARG:HH11  | 6:Ad:296:ARG:HG2   | 1.79                     | 0.47              |
| 7:Aq:11:THR:HA     | 7:Aq:14:MET:HE3    | 1.96                     | 0.47              |
| 7:Ar:31:THR:O      | 7:Ar:35:ILE:HG12   | 2.14                     | 0.47              |
| 10:Az:69:ASN:ND2   | 11:A6:20:ALA:CB    | 2.78                     | 0.47              |
| 10:A3:87:GLN:NE2   | 11:A9:134:LEU:O    | 2.48                     | 0.47              |
| 11:A6:23:GLN:NE2   | 12:BA:125:MET:HE1  | 2.30                     | 0.47              |
| 11:A7:117:GLN:HE22 | 12:BC:127:LEU:HD21 | 1.80                     | 0.47              |
| 11:A9:73:ILE:HD12  | 11:A9:74:PRO:HD2   | 1.95                     | 0.47              |
| 11:A9:95:LEU:HD13  | 6:BO:326:ALA:HB3   | 1.97                     | 0.47              |
| 6:UJ:127:SER:O     | 6:UJ:131:ASN:HB2   | 2.14                     | 0.47              |
| 6:UL:73:MET:HE3    | 6:UL:99:ARG:CD     | 2.41                     | 0.47              |
| 6:WN:142:ARG:O     | 6:WN:146:THR:HG23  | 2.14                     | 0.47              |
| 6:WU:190:GLN:HG2   | 6:WV:216:SER:O     | 2.15                     | 0.47              |
| 6:WW:145:GLU:O     | 6:WW:147:LEU:N     | 2.48                     | 0.47              |
| 12:BE:47:VAL:HG12  | 12:BE:67:VAL:HG22  | 1.96                     | 0.47              |
| 1:B:68:ASP:OD1     | 2:a:64:ASN:ND2     | 2.48                     | 0.47              |
| 1:D:52:PHE:CD2     | 2:b:172:GLU:HB3    | 2.50                     | 0.47              |
| 1:D:68:ASP:OD1     | 2:c:64:ASN:ND2     | 2.48                     | 0.47              |
| 1:E:68:ASP:OD1     | 2:d:64:ASN:ND2     | 2.47                     | 0.47              |
| 1:K:52:PHE:CD2     | 2:i:172:GLU:HB3    | 2.50                     | 0.47              |
| 1:M:50:SER:CB      | 2:j:32:ARG:NH1     | 2.77                     | 0.47              |
| 1:T:112:TYR:HD2    | 1:T:113:LEU:HD13   | 1.80                     | 0.47              |
| 1:T:165:GLY:C      | 1:U:35:THR:HG21    | 2.40                     | 0.47              |
| 1:Z:112:TYR:HD2    | 1:Z:113:LEU:HD13   | 1.80                     | 0.47              |
| 2:a:253:VAL:HG13   | 2:a:264:MET:HG2    | 1.95                     | 0.47              |
| 2:f:54:GLN:CD      | 3:AF:168:VAL:CG1   | 2.88                     | 0.47              |
| 2:f:235:PHE:O      | 2:f:239:ILE:HG12   | 2.15                     | 0.47              |
| 2:l:188:GLN:HG2    | 2:m:98:ARG:HD3     | 1.97                     | 0.47              |
| 2:o:188:GLN:HG2    | 2:p:98:ARG:HD3     | 1.97                     | 0.47              |
| 2:q:188:GLN:HG2    | 2:r:98:ARG:HD3     | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:188:GLN:HG2   | 2:s:98:ARG:HD3    | 1.97                     | 0.47              |
| 2:s:346:MET:HE3   | 2:u:142:LEU:CD1   | 2.42                     | 0.47              |
| 2:u:235:PHE:O     | 2:u:239:ILE:HG12  | 2.15                     | 0.47              |
| 2:y:319:LEU:HD21  | 2:z:264:MET:HE1   | 1.97                     | 0.47              |
| 3:0:2:ILE:HG13    | 5:AD:70:GLN:OE1   | 2.15                     | 0.47              |
| 3:1:18:ASN:O      | 3:1:22:ILE:HG13   | 2.15                     | 0.47              |
| 3:2:86:LEU:HG     | 3:ZD:45:LEU:HD12  | 1.97                     | 0.47              |
| 3:4:58:GLU:OE1    | 5:AC:160:ARG:NH1  | 2.47                     | 0.47              |
| 3:4:238:ARG:O     | 3:4:242:ILE:HG12  | 2.15                     | 0.47              |
| 3:5:226:VAL:CG1   | 3:ZA:242:ILE:HG21 | 2.45                     | 0.47              |
| 3:7:115:THR:HB    | 3:7:191:LEU:HD23  | 1.97                     | 0.47              |
| 3:ZC:40:VAL:HG23  | 3:ZC:75:VAL:HB    | 1.97                     | 0.47              |
| 3:ZD:28:ASN:OD1   | 4:ZI:52:VAL:CG1   | 2.54                     | 0.47              |
| 3:ZD:50:ARG:HB2   | 3:ZD:66:LEU:H     | 1.80                     | 0.47              |
| 4:ZM:267:MET:HE2  | 4:ZM:269:GLN:NE2  | 2.29                     | 0.47              |
| 4:ZN:380:ARG:HD2  | 4:ZT:396:LEU:HB3  | 1.95                     | 0.47              |
| 4:ZP:14:ALA:HB2   | 4:ZP:382:TYR:HE2  | 1.79                     | 0.47              |
| 4:ZS:149:THR:HG21 | 4:ZS:186:VAL:HG12 | 1.97                     | 0.47              |
| 4:Zg:146:ALA:HB2  | 4:Zg:286:PRO:HD3  | 1.95                     | 0.47              |
| 6:Aj:296:ARG:HG2  | 6:Aj:296:ARG:HH11 | 1.79                     | 0.47              |
| 7:Aq:85:PRO:HB3   | 9:Aw:242:SER:HA   | 1.96                     | 0.47              |
| 9:Av:152:ARG:HG3  | 6:WU:164:LEU:HA   | 1.97                     | 0.47              |
| 9:Aw:101:MET:HE3  | 9:Aw:101:MET:HB3  | 1.77                     | 0.47              |
| 10:A3:15:GLN:HG3  | 10:A3:16:ALA:N    | 2.30                     | 0.47              |
| 6:WA:200:SER:HG   | 6:WB:175:SER:HB2  | 1.77                     | 0.47              |
| 6:WB:145:GLU:O    | 6:WB:147:LEU:N    | 2.48                     | 0.47              |
| 6:WI:196:HIS:HB3  | 6:WJ:211:THR:CG2  | 2.32                     | 0.47              |
| 6:WJ:197:LEU:HD13 | 6:WK:175:SER:OG   | 2.09                     | 0.47              |
| 6:WV:164:LEU:HD12 | 6:WV:164:LEU:HA   | 1.76                     | 0.47              |
| 6:BS:296:ARG:HG2  | 6:BS:296:ARG:HH11 | 1.79                     | 0.47              |
| 1:A:47:ALA:HB1    | 2:x:178:GLN:HG3   | 1.96                     | 0.46              |
| 1:A:112:TYR:HD2   | 1:A:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:B:52:PHE:CD2    | 2:z:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:M:52:PHE:CD2    | 2:k:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:V:165:GLY:C     | 1:W:35:THR:HG21   | 2.40                     | 0.46              |
| 1:W:136:GLY:CA    | 1:Y:213:ILE:HG23  | 2.41                     | 0.46              |
| 1:W:165:GLY:C     | 1:X:35:THR:HG21   | 2.40                     | 0.46              |
| 1:X:52:PHE:CD2    | 2:v:172:GLU:HB3   | 2.50                     | 0.46              |
| 2:a:319:LEU:HD21  | 2:b:264:MET:HE1   | 1.98                     | 0.46              |
| 2:g:235:PHE:O     | 2:g:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:g:277:GLN:HE22  | 2:g:347:SER:HB2   | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:h:277:GLN:HE22  | 2:h:347:SER:HB2   | 1.80                     | 0.46              |
| 2:k:319:LEU:HD21  | 2:l:264:MET:HE1   | 1.97                     | 0.46              |
| 2:l:129:VAL:HG21  | 2:m:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:m:33:GLU:O      | 2:n:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:m:129:VAL:HG21  | 2:n:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:n:235:PHE:O     | 2:n:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:p:188:GLN:HG2   | 2:q:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:r:80:GLN:OE1    | 3:AI:174:ASN:CG   | 2.58                     | 0.46              |
| 3:2:232:ASN:O     | 3:2:236:VAL:HG13  | 2.15                     | 0.46              |
| 3:6:158:SER:HB3   | 3:6:167:PRO:HB2   | 1.96                     | 0.46              |
| 3:ZB:95:VAL:O     | 3:ZB:118:GLY:HA3  | 2.14                     | 0.46              |
| 4:ZG:397:ASN:O    | 4:ZG:400:VAL:N    | 2.48                     | 0.46              |
| 4:ZI:183:THR:HG22 | 4:ZI:197:ASN:ND2  | 2.30                     | 0.46              |
| 4:ZI:204:LYS:O    | 4:ZI:205:ASP:C    | 2.58                     | 0.46              |
| 4:ZK:374:ASN:O    | 4:ZK:375:MET:C    | 2.58                     | 0.46              |
| 4:ZL:28:ALA:O     | 4:ZQ:39:PHE:HD2   | 1.97                     | 0.46              |
| 4:ZO:331:ASP:HA   | 4:ZT:40:ALA:HB1   | 1.97                     | 0.46              |
| 4:ZP:25:ALA:HB1   | 4:ZU:52:VAL:CG1   | 2.44                     | 0.46              |
| 4:ZQ:181:LYS:HZ2  | 4:Zb:129:GLN:NE2  | 2.09                     | 0.46              |
| 4:ZQ:194:HIS:CE1  | 4:ZQ:251:ILE:HD12 | 2.50                     | 0.46              |
| 4:ZS:271:THR:OG1  | 4:ZS:273:ALA:O    | 2.29                     | 0.46              |
| 4:ZT:143:LEU:HD21 | 4:ZT:286:PRO:HB3  | 1.97                     | 0.46              |
| 4:ZV:93:PHE:HB3   | 4:ZV:333:VAL:CG2  | 2.46                     | 0.46              |
| 4:ZX:56:GLY:HA2   | 4:Zc:47:LYS:NZ    | 2.29                     | 0.46              |
| 4:ZY:210:VAL:HB   | 4:ZY:228:THR:HG22 | 1.97                     | 0.46              |
| 4:ZZ:234:GLU:HB3  | 4:Zf:255:THR:OG1  | 2.15                     | 0.46              |
| 5:AC:83:GLN:HG2   | 5:AC:84:GLN:N     | 2.30                     | 0.46              |
| 5:AE:229:MET:N    | 3:AK:258:THR:HG23 | 2.30                     | 0.46              |
| 3:AH:126:GLY:CA   | 3:AM:179:MET:HE3  | 2.45                     | 0.46              |
| 3:AH:196:GLN:C    | 3:AH:198:SER:H    | 2.23                     | 0.46              |
| 3:AI:229:GLU:O    | 3:AI:233:MET:HG3  | 2.15                     | 0.46              |
| 3:AK:188:GLY:O    | 3:AK:190:ASN:N    | 2.47                     | 0.46              |
| 6:AT:266:VAL:HG22 | 6:AT:387:VAL:HG22 | 1.95                     | 0.46              |
| 6:Aa:296:ARG:HG2  | 6:Aa:296:ARG:HH11 | 1.80                     | 0.46              |
| 6:Ao:278:THR:HG21 | 10:Az:7:ILE:CD1   | 2.44                     | 0.46              |
| 7:Aq:6:VAL:HG21   | 9:Ax:228:LEU:HD21 | 1.96                     | 0.46              |
| 7:Aq:8:MET:O      | 7:Aq:9:MET:C      | 2.57                     | 0.46              |
| 7:As:81:PHE:CE2   | 9:Ay:189:ILE:HD13 | 2.50                     | 0.46              |
| 9:Au:75:ARG:HD3   | 9:Au:89:LEU:HD11  | 1.97                     | 0.46              |
| 6:UI:129:GLN:O    | 6:UI:133:GLN:N    | 2.29                     | 0.46              |
| 6:UP:98:LEU:CD1   | 6:UP:146:THR:HG1  | 2.27                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WD:200:SER:OG   | 6:WE:175:SER:CB   | 2.47                     | 0.46              |
| 6:WG:122:GLY:O    | 6:WG:123:ILE:C    | 2.58                     | 0.46              |
| 6:WT:197:LEU:HA   | 6:WU:175:SER:OG   | 2.15                     | 0.46              |
| 6:WU:113:PHE:CE2  | 6:WU:139:GLU:HG3  | 2.48                     | 0.46              |
| 1:A:68:ASP:OD1    | 2:z:64:ASN:ND2    | 2.48                     | 0.46              |
| 1:B:112:TYR:HD2   | 1:B:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:C:52:PHE:CD2    | 2:a:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:J:52:PHE:CD2    | 2:h:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:M:50:SER:HB3    | 2:j:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:S:112:TYR:HD2   | 1:S:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:U:50:SER:HB3    | 2:r:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:V:62:TYR:CE1    | 2:t:129:VAL:HG13  | 2.48                     | 0.46              |
| 1:X:165:GLY:C     | 1:Y:35:THR:HG21   | 2.40                     | 0.46              |
| 1:Y:165:GLY:C     | 1:Z:35:THR:HG21   | 2.40                     | 0.46              |
| 2:a:264:MET:HE1   | 2:z:319:LEU:HD21  | 1.98                     | 0.46              |
| 2:i:33:GLU:O      | 2:j:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:j:33:GLU:O      | 2:k:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:j:319:LEU:HD21  | 2:k:264:MET:HE1   | 1.97                     | 0.46              |
| 2:l:80:GLN:OE1    | 5:AE:147:ASN:ND2  | 2.48                     | 0.46              |
| 2:n:33:GLU:O      | 2:o:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:o:33:GLU:O      | 2:p:170:ILE:HD13  | 2.15                     | 0.46              |
| 2:p:33:GLU:O      | 2:q:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:q:266:ARG:HG3   | 2:q:267:GLU:HG2   | 1.96                     | 0.46              |
| 2:u:277:GLN:HE22  | 2:u:347:SER:HB2   | 1.80                     | 0.46              |
| 2:x:56:PRO:CD     | 2:y:79:MET:HG2    | 2.45                     | 0.46              |
| 2:x:130:ASP:OD1   | 2:x:130:ASP:N     | 2.47                     | 0.46              |
| 2:x:319:LEU:HD21  | 2:y:264:MET:HE1   | 1.97                     | 0.46              |
| 3:0:257:LEU:HD21  | 5:AD:214:VAL:CA   | 2.45                     | 0.46              |
| 3:4:44:LEU:HD23   | 3:4:44:LEU:HA     | 1.76                     | 0.46              |
| 3:4:153:ARG:NH1   | 3:ZA:132:GLY:O    | 2.48                     | 0.46              |
| 3:4:260:LEU:HD12  | 3:AM:245:LYS:HE2  | 1.96                     | 0.46              |
| 3:ZA:12:LEU:HD13  | 4:ZF:399:LEU:HD11 | 1.98                     | 0.46              |
| 3:ZA:76:ALA:HB1   | 4:ZF:47:LYS:HD3   | 1.97                     | 0.46              |
| 4:ZH:206:ASN:HD21 | 4:ZN:253:GLY:HA3  | 1.80                     | 0.46              |
| 4:ZL:373:VAL:O    | 4:ZL:375:MET:N    | 2.47                     | 0.46              |
| 4:ZM:109:VAL:HG12 | 4:ZM:115:GLN:HA   | 1.98                     | 0.46              |
| 4:ZU:182:GLY:HA2  | 4:Zf:131:GLY:CA   | 2.21                     | 0.46              |
| 4:ZU:380:ARG:NH1  | 4:Za:393:ASP:OD1  | 2.48                     | 0.46              |
| 4:Zf:297:ASP:OD1  | 4:Zf:297:ASP:N    | 2.36                     | 0.46              |
| 4:Zg:294:ILE:HG12 | 4:Zg:300:VAL:HG22 | 1.97                     | 0.46              |
| 5:AB:21:VAL:CG2   | 3:AG:68:ILE:HG23  | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AC:71:LEU:CD1   | 3:AN:70:THR:CG2   | 2.77                     | 0.46              |
| 5:AE:54:ARG:HH12  | 12:BF:22:ASN:HD21 | 1.63                     | 0.46              |
| 3:AG:62:LEU:HD11  | 12:BC:84:LEU:CD1  | 2.45                     | 0.46              |
| 6:AU:296:ARG:HG2  | 6:AU:296:ARG:HH11 | 1.80                     | 0.46              |
| 6:AX:296:ARG:HG2  | 6:AX:296:ARG:HH11 | 1.79                     | 0.46              |
| 7:Ab:84:LEU:HB3   | 9:Av:238:SER:OG   | 2.15                     | 0.46              |
| 6:Ag:296:ARG:HH11 | 6:Ag:296:ARG:HG2  | 1.80                     | 0.46              |
| 6:Ak:296:ARG:HG2  | 6:Ak:296:ARG:HH11 | 1.80                     | 0.46              |
| 7:Ar:84:LEU:HD11  | 9:Ax:185:ILE:HG23 | 1.97                     | 0.46              |
| 9:Au:149:LEU:HB2  | 6:WQ:164:LEU:HD23 | 1.96                     | 0.46              |
| 9:Aw:138:MET:HE2  | 9:Aw:170:LEU:HG   | 1.98                     | 0.46              |
| 9:Ay:139:LEU:O    | 9:Ay:141:GLN:N    | 2.49                     | 0.46              |
| 10:A5:7:ILE:HG21  | 6:BR:278:THR:HG22 | 1.89                     | 0.46              |
| 11:A9:96:ASP:OD2  | 11:A9:96:ASP:N    | 2.48                     | 0.46              |
| 6:UN:136:LEU:HD23 | 6:UN:157:LEU:CD1  | 2.46                     | 0.46              |
| 6:UO:98:LEU:HD22  | 6:UO:147:LEU:CD2  | 2.39                     | 0.46              |
| 6:UO:136:LEU:HD23 | 6:UO:157:LEU:CD1  | 2.45                     | 0.46              |
| 6:WA:187:ASP:OD1  | 6:WA:190:GLN:N    | 2.42                     | 0.46              |
| 6:WF:124:SER:O    | 6:WF:127:SER:N    | 2.46                     | 0.46              |
| 6:WG:142:ARG:O    | 6:WG:146:THR:HG23 | 2.14                     | 0.46              |
| 1:A:31:VAL:CG1    | 1:Z:181:SER:HB2   | 2.45                     | 0.46              |
| 1:E:52:PHE:CD2    | 2:c:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:F:68:ASP:OD1    | 2:e:64:ASN:ND2    | 2.48                     | 0.46              |
| 1:H:68:ASP:OD1    | 2:g:64:ASN:ND2    | 2.47                     | 0.46              |
| 1:J:166:GLU:HB2   | 1:K:35:THR:CG2    | 2.30                     | 0.46              |
| 1:K:50:SER:HB3    | 2:h:32:ARG:HH11   | 1.80                     | 0.46              |
| 1:L:50:SER:HB3    | 2:i:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:N:52:PHE:CD2    | 2:l:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:T:50:SER:HB3    | 2:q:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:U:112:TYR:HD2   | 1:U:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:Y:112:TYR:HD2   | 1:Y:113:LEU:HD13  | 1.80                     | 0.46              |
| 2:b:319:LEU:HD21  | 2:c:264:MET:HE1   | 1.98                     | 0.46              |
| 2:e:208:ARG:O     | 2:e:212:SER:OG    | 2.16                     | 0.46              |
| 2:f:33:GLU:O      | 2:g:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:i:188:GLN:HG2   | 2:j:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:j:346:MET:HE2   | 2:l:142:LEU:HD11  | 1.95                     | 0.46              |
| 2:l:319:LEU:HD21  | 2:m:264:MET:HE1   | 1.98                     | 0.46              |
| 2:n:129:VAL:HG21  | 2:o:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:o:277:GLN:HE22  | 2:o:347:SER:HB2   | 1.80                     | 0.46              |
| 2:o:346:MET:HE2   | 2:q:142:LEU:HD11  | 1.95                     | 0.46              |
| 2:s:188:GLN:HG2   | 2:t:98:ARG:HD3    | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:u:93:TYR:OH     | 2:u:173:ARG:O     | 2.25                     | 0.46              |
| 2:w:346:MET:HE2   | 2:y:142:LEU:HD11  | 1.95                     | 0.46              |
| 3:2:38:ARG:NH2    | 3:AL:32:ASN:HD21  | 2.13                     | 0.46              |
| 3:3:194:GLU:OE2   | 3:3:201:PRO:HD3   | 2.16                     | 0.46              |
| 3:4:45:LEU:HD22   | 3:AH:98:LYS:CG    | 2.45                     | 0.46              |
| 3:ZA:237:GLN:OE1  | 4:ZF:391:THR:HG23 | 2.16                     | 0.46              |
| 3:ZC:252:GLN:O    | 3:ZC:256:LYS:HG2  | 2.16                     | 0.46              |
| 4:ZF:33:LYS:O     | 4:ZF:59:GLN:NE2   | 2.48                     | 0.46              |
| 4:ZG:358:ASN:OD1  | 4:ZG:359:GLY:N    | 2.47                     | 0.46              |
| 4:ZH:83:PHE:HB2   | 4:ZH:95:SER:O     | 2.15                     | 0.46              |
| 4:ZI:109:VAL:HG12 | 4:ZI:115:GLN:HA   | 1.97                     | 0.46              |
| 4:ZL:208:TRP:HE1  | 4:ZL:268:GLN:CD   | 2.23                     | 0.46              |
| 4:ZP:314:GLN:NE2  | 4:ZP:347:THR:OG1  | 2.47                     | 0.46              |
| 4:ZQ:382:TYR:HE1  | 4:ZV:399:LEU:CD2  | 2.28                     | 0.46              |
| 4:ZR:212:THR:HG21 | 4:ZR:246:ILE:HG13 | 1.97                     | 0.46              |
| 4:ZS:392:GLN:HA   | 4:ZS:395:ILE:HD12 | 1.97                     | 0.46              |
| 4:ZU:69:THR:HG22  | 4:ZU:71:ARG:H     | 1.79                     | 0.46              |
| 4:ZU:269:GLN:HG3  | 4:Za:286:PRO:HG2  | 1.97                     | 0.46              |
| 4:ZV:147:LYS:NZ   | 4:ZV:148:SER:O    | 2.43                     | 0.46              |
| 4:ZV:390:LYS:HB2  | 4:Za:402:LEU:HD22 | 1.96                     | 0.46              |
| 4:ZX:307:GLU:OE1  | 4:ZX:307:GLU:O    | 2.33                     | 0.46              |
| 4:Zc:93:PHE:CD1   | 4:Zc:114:MET:HE1  | 2.50                     | 0.46              |
| 4:Ze:44:ALA:HB3   | 4:Ze:50:LEU:HD11  | 1.97                     | 0.46              |
| 5:AC:152:PRO:HG2  | 3:AN:193:ILE:CD1  | 2.45                     | 0.46              |
| 5:AD:84:GLN:C     | 5:AD:86:GLY:H     | 2.23                     | 0.46              |
| 5:AE:52:ALA:C     | 5:AE:54:ARG:H     | 2.23                     | 0.46              |
| 3:AF:29:VAL:HG12  | 3:AK:235:GLN:HE22 | 1.81                     | 0.46              |
| 3:AH:11:GLY:O     | 3:AH:15:GLN:HG2   | 2.15                     | 0.46              |
| 3:AJ:200:ALA:HB1  | 3:AJ:201:PRO:HD2  | 1.97                     | 0.46              |
| 3:AJ:208:LEU:O    | 3:AJ:209:ASN:HB3  | 2.15                     | 0.46              |
| 3:AK:184:LEU:HB3  | 3:AK:192:TYR:HB3  | 1.97                     | 0.46              |
| 3:AL:249:THR:O    | 3:AL:253:MET:HG3  | 2.16                     | 0.46              |
| 6:AP:296:ARG:HG2  | 6:AP:296:ARG:HH11 | 1.79                     | 0.46              |
| 7:Ar:24:LEU:HD11  | 7:Ar:62:ILE:HD11  | 1.96                     | 0.46              |
| 8:At:72:TRP:HE1   | 8:At:161:SER:HB2  | 1.80                     | 0.46              |
| 8:At:144:LEU:HD11 | 9:Ay:146:ASP:OD1  | 2.15                     | 0.46              |
| 9:Au:68:ILE:HA    | 9:Au:68:ILE:HD12  | 1.82                     | 0.46              |
| 9:Au:190:PHE:CG   | 9:Av:220:PRO:HG3  | 2.51                     | 0.46              |
| 9:Ay:139:LEU:C    | 9:Ay:141:GLN:N    | 2.74                     | 0.46              |
| 10:A2:7:ILE:O     | 10:A2:11:ILE:HG23 | 2.16                     | 0.46              |
| 6:UP:136:LEU:HD23 | 6:UP:157:LEU:CD1  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WF:196:HIS:CD2  | 6:WG:219:LEU:HD22 | 2.51                     | 0.46              |
| 6:WH:145:GLU:O    | 6:WH:146:THR:C    | 2.57                     | 0.46              |
| 6:WM:187:ASP:OD1  | 6:WM:190:GLN:N    | 2.44                     | 0.46              |
| 6:WW:147:LEU:O    | 6:WW:148:GLY:C    | 2.59                     | 0.46              |
| 12:BC:3:LEU:O     | 12:BC:4:LEU:C     | 2.58                     | 0.46              |
| 6:BV:296:ARG:HG2  | 6:BV:296:ARG:HH11 | 1.80                     | 0.46              |
| 1:A:65:LEU:CG     | 2:z:65:MET:HG3    | 2.39                     | 0.46              |
| 1:C:181:SER:HB2   | 1:D:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:D:62:TYR:CE1    | 2:b:129:VAL:HG13  | 2.48                     | 0.46              |
| 1:M:136:GLY:CA    | 1:O:213:ILE:HG23  | 2.42                     | 0.46              |
| 1:N:50:SER:CB     | 2:k:32:ARG:NH1    | 2.77                     | 0.46              |
| 1:Q:52:PHE:CD2    | 2:o:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:S:50:SER:HB3    | 2:p:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:S:52:PHE:CD2    | 2:q:172:GLU:HB3   | 2.50                     | 0.46              |
| 2:a:142:LEU:HD11  | 2:y:346:MET:HE2   | 1.95                     | 0.46              |
| 2:b:80:GLN:HE22   | 3:AG:169:GLN:C    | 2.22                     | 0.46              |
| 2:b:235:PHE:O     | 2:b:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:e:33:GLU:O      | 2:f:170:ILE:HD13  | 2.15                     | 0.46              |
| 2:f:346:MET:HE3   | 2:h:142:LEU:CD1   | 2.42                     | 0.46              |
| 2:g:33:GLU:O      | 2:h:170:ILE:HD13  | 2.15                     | 0.46              |
| 2:i:319:LEU:HD21  | 2:j:264:MET:HE1   | 1.98                     | 0.46              |
| 2:j:188:GLN:HG2   | 2:k:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:k:129:VAL:HG21  | 2:l:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:o:253:VAL:HG13  | 2:o:264:MET:HG2   | 1.95                     | 0.46              |
| 2:v:235:PHE:O     | 2:v:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:w:277:GLN:HE22  | 2:w:347:SER:HB2   | 1.80                     | 0.46              |
| 3:0:70:THR:HG21   | 5:AD:71:LEU:HB2   | 1.96                     | 0.46              |
| 3:2:1:MET:HB2     | 3:AF:226:VAL:CG2  | 2.45                     | 0.46              |
| 3:4:173:LEU:HD23  | 3:4:214:LEU:HD13  | 1.97                     | 0.46              |
| 3:8:257:LEU:HG    | 3:AL:230:LEU:HD12 | 1.96                     | 0.46              |
| 3:ZA:128:LEU:HD12 | 3:ZA:140:ILE:HB   | 1.97                     | 0.46              |
| 3:ZC:95:VAL:HG11  | 3:ZC:214:LEU:HD23 | 1.98                     | 0.46              |
| 3:ZD:163:GLY:O    | 3:ZD:164:GLN:C    | 2.59                     | 0.46              |
| 4:ZF:210:VAL:O    | 4:ZF:227:SER:N    | 2.48                     | 0.46              |
| 4:ZF:233:ASN:HD21 | 4:ZF:237:ILE:HB   | 1.80                     | 0.46              |
| 4:ZF:269:GLN:OE1  | 4:ZL:286:PRO:HG3  | 2.15                     | 0.46              |
| 4:ZH:380:ARG:NH1  | 4:ZN:393:ASP:OD1  | 2.48                     | 0.46              |
| 4:ZL:140:PRO:HD2  | 4:ZL:312:LEU:HD22 | 1.98                     | 0.46              |
| 4:ZN:380:ARG:HD3  | 4:ZN:380:ARG:HA   | 1.68                     | 0.46              |
| 4:ZR:269:GLN:HE22 | 4:ZX:145:ALA:HB1  | 1.81                     | 0.46              |
| 4:ZS:143:LEU:HD23 | 4:ZS:143:LEU:H    | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZT:17:LEU:HD13  | 4:ZY:395:ILE:HD13 | 1.94                     | 0.46              |
| 4:ZU:109:VAL:HG12 | 4:ZU:115:GLN:HA   | 1.98                     | 0.46              |
| 4:ZX:245:ASN:C    | 4:ZX:246:ILE:HD13 | 2.40                     | 0.46              |
| 4:Zf:47:LYS:HE3   | 4:Zf:47:LYS:HB2   | 1.80                     | 0.46              |
| 4:Zg:328:SER:HG   | 4:Zg:334:TRP:CD1  | 2.32                     | 0.46              |
| 5:AC:31:THR:HG23  | 3:AH:41:PHE:O     | 2.16                     | 0.46              |
| 3:AF:61:THR:OG1   | 3:AF:62:LEU:N     | 2.46                     | 0.46              |
| 3:AI:113:ALA:HB1  | 3:AI:191:LEU:HB3  | 1.96                     | 0.46              |
| 3:AK:142:ILE:HD13 | 3:AK:149:ILE:HD13 | 1.96                     | 0.46              |
| 3:AL:188:GLY:O    | 3:AL:190:ASN:N    | 2.48                     | 0.46              |
| 6:AS:296:ARG:HG2  | 6:AS:296:ARG:HH11 | 1.79                     | 0.46              |
| 6:AY:370:ARG:NH2  | 10:A3:7:ILE:HD11  | 2.30                     | 0.46              |
| 6:Ag:295:SER:CB   | 11:A8:72:HIS:CA   | 2.93                     | 0.46              |
| 7:Aq:9:MET:HA     | 7:Aq:12:GLU:OE1   | 2.15                     | 0.46              |
| 9:Aw:40:LEU:HD22  | 11:A8:8:ALA:HB2   | 1.96                     | 0.46              |
| 10:A4:15:GLN:HG3  | 10:A4:16:ALA:N    | 2.30                     | 0.46              |
| 11:A0:67:LEU:HD11 | 11:A0:74:PRO:HA   | 1.97                     | 0.46              |
| 6:UM:73:MET:HE3   | 6:UM:99:ARG:CD    | 2.41                     | 0.46              |
| 6:WD:190:GLN:NE2  | 6:WE:216:SER:O    | 2.49                     | 0.46              |
| 6:WH:197:LEU:HA   | 6:WI:175:SER:CB   | 2.46                     | 0.46              |
| 6:WI:193:ALA:HB1  | 6:WJ:213:VAL:CG2  | 2.45                     | 0.46              |
| 6:WW:115:LEU:O    | 6:WW:116:LEU:C    | 2.57                     | 0.46              |
| 12:BC:43:ARG:HD2  | 12:BC:69:GLU:OE2  | 2.14                     | 0.46              |
| 1:A:181:SER:HB2   | 1:B:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:C:112:TYR:HD2   | 1:C:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:I:52:PHE:CD2    | 2:g:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:J:112:TYR:HD2   | 1:J:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:N:181:SER:HB2   | 1:O:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:R:112:TYR:HD2   | 1:R:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:T:52:PHE:CD2    | 2:r:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:W:52:PHE:CD2    | 2:u:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:X:181:SER:HB2   | 1:Y:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:Z:68:ASP:OD1    | 2:y:64:ASN:ND2    | 2.48                     | 0.46              |
| 2:c:319:LEU:HD21  | 2:d:264:MET:HE1   | 1.97                     | 0.46              |
| 2:e:54:GLN:OE1    | 3:7:58:GLU:HG2    | 2.16                     | 0.46              |
| 2:k:188:GLN:HG2   | 2:l:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:l:33:GLU:O      | 2:m:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:p:266:ARG:HG3   | 2:p:267:GLU:HG2   | 1.96                     | 0.46              |
| 2:t:235:PHE:O     | 2:t:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:t:346:MET:HE2   | 2:v:142:LEU:HD11  | 1.95                     | 0.46              |
| 2:z:277:GLN:HE22  | 2:z:347:SER:HB2   | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:0:242:ILE:CD1   | 3:AJ:230:LEU:HD11 | 2.42                     | 0.46              |
| 3:5:70:THR:HG23   | 3:AI:85:ASN:OD1   | 2.15                     | 0.46              |
| 3:5:100:GLN:HG3   | 3:5:100:GLN:O     | 2.14                     | 0.46              |
| 3:6:95:VAL:O      | 3:6:118:GLY:HA3   | 2.15                     | 0.46              |
| 3:ZE:5:LEU:HB2    | 3:ZE:250:THR:HG21 | 1.98                     | 0.46              |
| 4:ZI:197:ASN:HD22 | 4:ZI:197:ASN:N    | 2.14                     | 0.46              |
| 4:ZI:234:GLU:HB3  | 4:ZO:255:THR:OG1  | 2.15                     | 0.46              |
| 4:ZJ:24:ILE:O     | 4:ZJ:27:SER:OG    | 2.32                     | 0.46              |
| 4:ZJ:159:ASN:HB3  | 4:ZJ:162:ASP:OD2  | 2.15                     | 0.46              |
| 4:ZL:318:ALA:HB1  | 4:ZL:343:ALA:HB1  | 1.98                     | 0.46              |
| 4:ZN:235:ASN:C    | 4:ZT:190:GLN:HE22 | 2.24                     | 0.46              |
| 4:ZO:268:GLN:HE22 | 4:ZU:190:GLN:NE2  | 2.12                     | 0.46              |
| 4:ZP:144:MET:SD   | 4:ZP:306:ASN:ND2  | 2.77                     | 0.46              |
| 4:ZQ:369:SER:HA   | 4:Zb:399:LEU:CD1  | 2.42                     | 0.46              |
| 4:ZS:394:GLN:O    | 4:ZS:398:THR:HG22 | 2.16                     | 0.46              |
| 4:ZZ:99:GLN:HB3   | 4:ZZ:111:MET:HE3  | 1.96                     | 0.46              |
| 4:Zc:382:TYR:CG   | 4:Zh:395:ILE:CD1  | 2.99                     | 0.46              |
| 4:Zd:60:ASP:O     | 4:Zd:365:ASN:ND2  | 2.48                     | 0.46              |
| 5:AC:46:VAL:HG12  | 11:A8:93:PRO:HB2  | 1.97                     | 0.46              |
| 3:AI:178:PHE:CE1  | 3:AI:184:LEU:HD21 | 2.50                     | 0.46              |
| 3:AL:123:ASP:O    | 3:AL:124:GLN:C    | 2.59                     | 0.46              |
| 6:Af:297:GLN:NE2  | 11:A8:76:GLN:H    | 2.12                     | 0.46              |
| 8:At:103:GLY:O    | 8:At:106:MET:HB2  | 2.16                     | 0.46              |
| 9:Au:189:ILE:O    | 9:Au:192:PRO:HD2  | 2.15                     | 0.46              |
| 9:Av:158:PRO:HD3  | 6:WU:167:ARG:NH1  | 2.26                     | 0.46              |
| 9:Aw:46:VAL:HG22  | 10:A3:42:LEU:CD1  | 2.45                     | 0.46              |
| 11:A7:92:GLN:HE22 | 12:BC:22:ASN:HB2  | 1.80                     | 0.46              |
| 11:A0:65:LEU:HG   | 11:A0:75:ALA:CA   | 2.46                     | 0.46              |
| 6:UN:103:GLN:CG   | 6:WS:182:PRO:HB3  | 2.44                     | 0.46              |
| 6:WK:201:ALA:HA   | 6:WL:158:ALA:HB2  | 1.98                     | 0.46              |
| 6:WN:200:SER:HB2  | 6:WO:173:SER:CB   | 2.45                     | 0.46              |
| 1:E:112:TYR:HD2   | 1:E:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:G:65:LEU:CG     | 2:f:65:MET:HG3    | 2.39                     | 0.46              |
| 1:I:112:TYR:HD2   | 1:I:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:L:181:SER:HB2   | 1:M:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:O:50:SER:CB     | 2:l:32:ARG:NH1    | 2.77                     | 0.46              |
| 1:P:181:SER:HB2   | 1:Q:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:R:52:PHE:CD2    | 2:p:172:GLU:HB3   | 2.50                     | 0.46              |
| 2:a:188:GLN:HG2   | 2:b:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:a:235:PHE:O     | 2:a:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:g:56:PRO:CD     | 2:h:79:MET:HG2    | 2.45                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:g:192:GLU:H     | 2:g:192:GLU:HG3    | 1.52                     | 0.46              |
| 2:o:129:VAL:HG21  | 2:p:136:LEU:HD13   | 1.97                     | 0.46              |
| 2:t:188:GLN:HG2   | 2:u:98:ARG:HD3     | 1.97                     | 0.46              |
| 2:u:188:GLN:HG2   | 2:v:98:ARG:HD3     | 1.97                     | 0.46              |
| 2:w:319:LEU:HD21  | 2:x:264:MET:HE1    | 1.97                     | 0.46              |
| 2:y:56:PRO:CD     | 2:z:79:MET:HG2     | 2.45                     | 0.46              |
| 2:y:235:PHE:O     | 2:y:239:ILE:HG12   | 2.15                     | 0.46              |
| 2:z:235:PHE:O     | 2:z:239:ILE:HG12   | 2.15                     | 0.46              |
| 3:4:86:LEU:HB2    | 4:ZF:42:MET:HE1    | 1.98                     | 0.46              |
| 3:4:126:GLY:HA3   | 3:9:179:MET:CE     | 2.46                     | 0.46              |
| 3:7:94:ASP:OD2    | 3:ZC:38:ARG:NH1    | 2.43                     | 0.46              |
| 3:ZA:44:LEU:HD23  | 3:ZA:44:LEU:HA     | 1.81                     | 0.46              |
| 3:ZD:59:GLN:N     | 3:ZD:59:GLN:OE1    | 2.49                     | 0.46              |
| 4:ZG:319:ASN:OD1  | 4:ZG:344:LEU:HB3   | 2.16                     | 0.46              |
| 4:ZJ:146:ALA:HB2  | 4:ZJ:286:PRO:HD3   | 1.98                     | 0.46              |
| 4:ZL:233:ASN:OD1  | 4:ZL:237:ILE:N     | 2.48                     | 0.46              |
| 4:ZL:368:LEU:HD12 | 4:ZL:368:LEU:HA    | 1.68                     | 0.46              |
| 4:ZM:217:ASP:HB3  | 4:ZM:220:ALA:HB2   | 1.98                     | 0.46              |
| 4:ZO:196:MET:HE3  | 4:ZO:248:THR:HG22  | 1.98                     | 0.46              |
| 4:ZP:28:ALA:O     | 4:ZU:39:PHE:CD2    | 2.69                     | 0.46              |
| 4:ZQ:382:TYR:HE1  | 4:ZV:399:LEU:HD21  | 1.81                     | 0.46              |
| 4:ZU:195:ASP:OD2  | 4:ZU:216:SER:OG    | 2.22                     | 0.46              |
| 4:ZU:270:ASN:CG   | 4:Za:191:GLY:O     | 2.59                     | 0.46              |
| 4:ZV:372:LEU:HD13 | 4:Zg:399:LEU:HB3   | 1.97                     | 0.46              |
| 4:ZY:210:VAL:O    | 4:ZY:227:SER:N     | 2.49                     | 0.46              |
| 4:Za:16:ASN:O     | 4:Za:20:ILE:HG12   | 2.15                     | 0.46              |
| 4:Zh:374:ASN:HA   | 4:Zh:377:VAL:HG12  | 1.98                     | 0.46              |
| 5:AA:49:LEU:HD12  | 5:AA:50:SER:HB2    | 1.98                     | 0.46              |
| 5:AB:82:LEU:HD11  | 5:AB:88:LEU:HG     | 1.97                     | 0.46              |
| 5:AE:240:ASN:HD21 | 12:BF:109:SER:HA   | 1.80                     | 0.46              |
| 3:AG:62:LEU:CG    | 12:BC:84:LEU:HD11  | 2.45                     | 0.46              |
| 3:AL:42:GLU:OE1   | 3:AL:75:VAL:HG21   | 2.15                     | 0.46              |
| 6:AS:235:LEU:HD13 | 6:AT:244:ARG:HH22  | 1.81                     | 0.46              |
| 6:Ah:235:LEU:HD13 | 6:Ai:244:ARG:HH22  | 1.81                     | 0.46              |
| 6:AP:235:LEU:HD13 | 6:AQ:244:ARG:HH22  | 1.81                     | 0.46              |
| 9:Au:150:PHE:CZ   | 9:Au:172:PRO:HB2   | 2.51                     | 0.46              |
| 9:Av:171:LEU:HB3  | 9:Av:172:PRO:HD3   | 1.97                     | 0.46              |
| 9:Ay:159:LEU:HD13 | 9:Ay:165:VAL:HG22  | 1.98                     | 0.46              |
| 11:A6:113:SER:O   | 11:A6:117:GLN:HG3  | 2.15                     | 0.46              |
| 11:A7:109:PHE:CZ  | 12:BB:118:VAL:HG13 | 2.51                     | 0.46              |
| 6:UJ:136:LEU:HD23 | 6:UJ:157:LEU:CD1   | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UM:136:LEU:HD23 | 6:UM:157:LEU:CD1  | 2.45                     | 0.46              |
| 12:BA:36:GLY:HA2  | 12:BF:51:VAL:HG12 | 1.97                     | 0.46              |
| 6:WF:128:GLU:CG   | 6:WG:126:PHE:CD2  | 2.98                     | 0.46              |
| 6:WF:135:ALA:O    | 6:WF:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WR:145:GLU:O    | 6:WR:146:THR:C    | 2.59                     | 0.46              |
| 6:WT:135:ALA:O    | 6:WT:139:GLU:HG2  | 2.16                     | 0.46              |
| 12:BD:4:LEU:HD21  | 12:BD:126:MET:HE1 | 1.96                     | 0.46              |
| 1:D:112:TYR:HD2   | 1:D:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:G:68:ASP:OD1    | 2:f:64:ASN:ND2    | 2.48                     | 0.46              |
| 1:H:52:PHE:CD2    | 2:f:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:R:68:ASP:OD1    | 2:q:64:ASN:ND2    | 2.48                     | 0.46              |
| 1:V:112:TYR:HD2   | 1:V:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:W:112:TYR:HD2   | 1:W:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:X:112:TYR:HD2   | 1:X:113:LEU:HD13  | 1.80                     | 0.46              |
| 2:c:188:GLN:HG2   | 2:d:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:f:129:VAL:HG21  | 2:g:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:h:33:GLU:O      | 2:i:170:ILE:HD13  | 2.15                     | 0.46              |
| 2:h:319:LEU:HD21  | 2:i:264:MET:HE1   | 1.97                     | 0.46              |
| 2:m:235:PHE:O     | 2:m:239:ILE:HG12  | 2.15                     | 0.46              |
| 2:p:21:ARG:HA     | 2:p:21:ARG:HD2    | 1.75                     | 0.46              |
| 2:r:346:MET:HE3   | 2:t:142:LEU:CD1   | 2.42                     | 0.46              |
| 2:s:33:GLU:O      | 2:t:170:ILE:HD13  | 2.15                     | 0.46              |
| 2:s:129:VAL:HG21  | 2:t:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:t:129:VAL:HG21  | 2:u:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:x:235:PHE:O     | 2:x:239:ILE:HG12  | 2.15                     | 0.46              |
| 3:0:179:MET:SD    | 3:AJ:124:GLN:O    | 2.73                     | 0.46              |
| 3:1:237:GLN:O     | 3:1:241:GLU:HG2   | 2.16                     | 0.46              |
| 3:2:4:SER:OG      | 3:AL:20:ASP:OD1   | 2.33                     | 0.46              |
| 3:6:64:SER:O      | 3:6:64:SER:OG     | 2.23                     | 0.46              |
| 3:6:260:LEU:CD1   | 3:AJ:234:ILE:HD11 | 2.45                     | 0.46              |
| 3:ZE:240:TYR:HE2  | 4:ZJ:399:LEU:CD1  | 2.29                     | 0.46              |
| 4:ZF:117:THR:HA   | 4:ZF:136:PRO:HA   | 1.97                     | 0.46              |
| 4:ZF:392:GLN:HE22 | 4:ZF:396:LEU:HG   | 1.80                     | 0.46              |
| 4:ZH:269:GLN:HE22 | 4:ZN:146:ALA:H    | 1.64                     | 0.46              |
| 4:ZU:195:ASP:OD2  | 4:ZU:195:ASP:N    | 2.40                     | 0.46              |
| 4:ZX:144:MET:HE3  | 4:ZX:284:TYR:CE1  | 2.51                     | 0.46              |
| 5:AA:70:GLN:CD    | 3:AL:3:SER:OG     | 2.59                     | 0.46              |
| 5:AB:60:SER:CB    | 3:AG:65:GLY:O     | 2.61                     | 0.46              |
| 3:AG:122:VAL:O    | 3:AL:180:ASN:ND2  | 2.49                     | 0.46              |
| 3:AG:185:GLU:HG3  | 3:AL:67:GLN:NE2   | 2.31                     | 0.46              |
| 3:AJ:158:SER:HB3  | 3:AJ:167:PRO:HB2  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AK:80:LEU:HG    | 3:AK:223:ASN:HD21 | 1.81                     | 0.46              |
| 6:AX:235:LEU:HD13 | 6:AY:244:ARG:HH22 | 1.81                     | 0.46              |
| 6:AZ:235:LEU:HD13 | 6:Aa:244:ARG:HH22 | 1.81                     | 0.46              |
| 6:Ai:235:LEU:HD13 | 6:Aj:244:ARG:HH22 | 1.81                     | 0.46              |
| 6:Al:235:LEU:HD13 | 6:Am:244:ARG:HH22 | 1.81                     | 0.46              |
| 9:Aw:132:GLN:O    | 9:Aw:135:ARG:HG2  | 2.15                     | 0.46              |
| 11:A7:29:ASN:HD21 | 11:A7:41:ARG:H    | 1.61                     | 0.46              |
| 11:A8:128:LYS:HE2 | 12:BC:134:GLN:CG  | 2.45                     | 0.46              |
| 6:UI:98:LEU:CD1   | 6:UI:146:THR:HG1  | 2.28                     | 0.46              |
| 6:UL:136:LEU:HD23 | 6:UL:157:LEU:CD1  | 2.45                     | 0.46              |
| 6:WD:187:ASP:OD1  | 6:WD:190:GLN:N    | 2.46                     | 0.46              |
| 6:WG:135:ALA:O    | 6:WG:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WG:149:PRO:HG2  | 6:WG:190:GLN:HE22 | 1.79                     | 0.46              |
| 6:WK:197:LEU:HD13 | 6:WL:175:SER:OG   | 2.16                     | 0.46              |
| 6:WN:135:ALA:O    | 6:WN:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WQ:135:ALA:O    | 6:WQ:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WV:120:LYS:NZ   | 6:WV:123:ILE:CD1  | 2.74                     | 0.46              |
| 1:E:181:SER:HB2   | 1:F:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:H:112:TYR:HD2   | 1:H:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:J:65:LEU:CG     | 2:i:65:MET:HG3    | 2.39                     | 0.46              |
| 1:K:112:TYR:HD2   | 1:K:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:L:62:TYR:CE1    | 2:j:129:VAL:HG13  | 2.48                     | 0.46              |
| 1:L:68:ASP:OD1    | 2:k:64:ASN:ND2    | 2.48                     | 0.46              |
| 1:L:112:TYR:HD2   | 1:L:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:R:65:LEU:CG     | 2:q:65:MET:HG3    | 2.39                     | 0.46              |
| 1:Y:68:ASP:OD1    | 2:x:64:ASN:ND2    | 2.48                     | 0.46              |
| 1:Z:47:ALA:HB1    | 2:w:178:GLN:HG3   | 1.97                     | 0.46              |
| 2:j:129:VAL:HG21  | 2:k:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:k:33:GLU:O      | 2:l:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:k:266:ARG:HG3   | 2:k:267:GLU:HG2   | 1.96                     | 0.46              |
| 2:m:56:PRO:CD     | 2:n:79:MET:HG2    | 2.45                     | 0.46              |
| 2:n:56:PRO:CD     | 2:o:79:MET:HG2    | 2.45                     | 0.46              |
| 3:0:215:TYR:HE1   | 3:ZB:73:ARG:NH2   | 2.14                     | 0.46              |
| 3:2:253:MET:HG2   | 3:AL:240:TYR:CD2  | 2.51                     | 0.46              |
| 3:3:1:MET:HB3     | 3:AG:29:VAL:HG21  | 1.98                     | 0.46              |
| 3:8:260:LEU:HD13  | 3:AL:234:ILE:HD11 | 1.98                     | 0.46              |
| 3:ZB:27:ALA:O     | 4:ZG:52:VAL:HG11  | 2.16                     | 0.46              |
| 3:ZB:56:SER:HA    | 3:AJ:152:GLY:HA2  | 1.96                     | 0.46              |
| 4:ZH:17:LEU:CD1   | 4:ZM:395:ILE:HD11 | 2.46                     | 0.46              |
| 4:ZH:75:VAL:HG13  | 4:ZH:356:LEU:HB3  | 1.98                     | 0.46              |
| 4:ZM:17:LEU:CD1   | 4:ZR:395:ILE:HD11 | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZM:271:THR:OG1  | 4:ZM:273:ALA:O    | 2.27                     | 0.46              |
| 4:ZS:317:LEU:HD11 | 4:ZS:356:LEU:HD21 | 1.98                     | 0.46              |
| 4:ZW:199:TYR:HB2  | 4:ZW:211:TYR:HB2  | 1.98                     | 0.46              |
| 4:ZW:314:GLN:NE2  | 4:ZW:347:THR:OG1  | 2.49                     | 0.46              |
| 4:ZY:101:LYS:NZ   | 4:Zd:322:ASN:HD21 | 2.13                     | 0.46              |
| 4:ZY:109:VAL:HG12 | 4:ZY:115:GLN:HA   | 1.98                     | 0.46              |
| 4:ZY:373:VAL:HG21 | 4:Ze:10:LEU:HD23  | 1.98                     | 0.46              |
| 4:ZZ:234:GLU:O    | 4:Zf:190:GLN:CD   | 2.59                     | 0.46              |
| 4:Za:81:GLY:HA3   | 4:Za:317:LEU:HD23 | 1.97                     | 0.46              |
| 4:Ze:110:ASN:OD1  | 4:Ze:114:MET:N    | 2.49                     | 0.46              |
| 5:AA:202:MET:CG   | 3:AL:45:LEU:CD1   | 2.81                     | 0.46              |
| 3:AG:22:ILE:HG21  | 3:AG:233:MET:HG3  | 1.98                     | 0.46              |
| 3:AI:76:ALA:HA    | 3:AN:66:LEU:HB3   | 1.97                     | 0.46              |
| 3:AI:115:THR:HB   | 3:AI:191:LEU:HD23 | 1.97                     | 0.46              |
| 3:AK:70:THR:HG21  | 12:BF:76:LEU:O    | 2.16                     | 0.46              |
| 6:Ac:235:LEU:HD13 | 6:Ad:244:ARG:HH22 | 1.81                     | 0.46              |
| 6:Ao:235:LEU:HD13 | 6:Ap:244:ARG:HH22 | 1.81                     | 0.46              |
| 9:Au:149:LEU:HD22 | 9:Av:233:GLN:HG3  | 1.96                     | 0.46              |
| 9:Aw:109:TYR:HA   | 9:Aw:113:TYR:HB3  | 1.98                     | 0.46              |
| 10:A2:82:MET:HE3  | 11:A7:133:VAL:CG2 | 2.46                     | 0.46              |
| 6:UL:73:MET:HE1   | 6:UL:99:ARG:HD2   | 1.94                     | 0.46              |
| 12:BB:4:LEU:HB3   | 12:BB:7:PHE:HB2   | 1.98                     | 0.46              |
| 6:WA:187:ASP:OD2  | 6:WA:190:GLN:HG3  | 2.16                     | 0.46              |
| 6:WD:135:ALA:O    | 6:WD:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WH:139:GLU:HB3  | 6:WI:154:ARG:HH21 | 1.80                     | 0.46              |
| 6:WM:135:ALA:O    | 6:WM:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WV:135:ALA:O    | 6:WV:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WW:187:ASP:N    | 6:WW:190:GLN:HB2  | 2.31                     | 0.46              |
| 6:BW:235:LEU:HD13 | 6:BX:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:B:181:SER:HB2   | 1:C:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:F:50:SER:HB3    | 2:c:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:J:181:SER:HB2   | 1:K:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:O:90:LYS:HA     | 1:P:142:ASN:HA    | 1.98                     | 0.46              |
| 1:P:50:SER:CB     | 2:m:32:ARG:NH1    | 2.77                     | 0.46              |
| 1:R:181:SER:HB2   | 1:S:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:Z:65:LEU:CG     | 2:y:65:MET:HG3    | 2.39                     | 0.46              |
| 2:a:130:ASP:OD1   | 2:a:130:ASP:N     | 2.47                     | 0.46              |
| 2:b:188:GLN:HG2   | 2:c:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:c:33:GLU:O      | 2:d:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:d:33:GLU:O      | 2:e:170:ILE:HD13  | 2.16                     | 0.46              |
| 2:d:235:PHE:O     | 2:d:239:ILE:HG12  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:129:VAL:HG21  | 2:h:136:LEU:HD13  | 1.98                     | 0.46              |
| 2:h:188:GLN:HG2   | 2:i:98:ARG:HD3    | 1.97                     | 0.46              |
| 2:o:192:GLU:H     | 2:o:192:GLU:HG3   | 1.52                     | 0.46              |
| 2:o:258:ARG:HH12  | 2:q:140:ASN:HD21  | 1.64                     | 0.46              |
| 2:o:273:CYS:HB2   | 2:p:265:ASN:HA    | 1.98                     | 0.46              |
| 2:q:346:MET:HE3   | 2:s:142:LEU:CD1   | 2.42                     | 0.46              |
| 2:r:277:GLN:HE22  | 2:r:347:SER:HB2   | 1.80                     | 0.46              |
| 2:v:188:GLN:HG2   | 2:w:98:ARG:HD3    | 1.97                     | 0.46              |
| 3:2:1:MET:HB2     | 3:AF:226:VAL:HG21 | 1.98                     | 0.46              |
| 3:2:79:ARG:HH11   | 3:2:79:ARG:HG3    | 1.81                     | 0.46              |
| 3:4:56:SER:CA     | 5:AC:138:ALA:CB   | 2.94                     | 0.46              |
| 3:5:19:MET:HB2    | 3:5:236:VAL:HG11  | 1.97                     | 0.46              |
| 4:ZH:380:ARG:HB3  | 4:ZN:396:LEU:HD13 | 1.97                     | 0.46              |
| 4:ZI:234:GLU:HG3  | 4:ZO:253:GLY:O    | 2.15                     | 0.46              |
| 4:ZM:374:ASN:O    | 4:ZM:375:MET:C    | 2.59                     | 0.46              |
| 4:ZS:180:LYS:HD2  | 4:ZS:181:LYS:N    | 2.30                     | 0.46              |
| 4:Ze:269:GLN:HG2  | 4:Ze:270:ASN:H    | 1.80                     | 0.46              |
| 4:Zh:344:LEU:HD12 | 4:Zh:344:LEU:HA   | 1.80                     | 0.46              |
| 5:AB:132:GLY:CA   | 3:AG:179:MET:SD   | 3.03                     | 0.46              |
| 5:AE:51:LEU:CD1   | 12:BF:19:LYS:HD3  | 2.44                     | 0.46              |
| 3:AL:147:LEU:HD11 | 3:AL:162:GLN:HB2  | 1.98                     | 0.46              |
| 6:Ak:235:LEU:HD13 | 6:Al:244:ARG:HH22 | 1.81                     | 0.46              |
| 6:AP:278:THR:CG2  | 10:A5:21:ALA:HB3  | 2.44                     | 0.46              |
| 7:Ar:88:ILE:HB    | 9:Ax:181:THR:HG23 | 1.98                     | 0.46              |
| 9:Ay:83:ALA:CB    | 9:Ay:84:PRO:CD    | 2.94                     | 0.46              |
| 10:Az:77:LYS:O    | 10:Az:78:ALA:C    | 2.58                     | 0.46              |
| 10:A1:15:GLN:HG3  | 10:A1:16:ALA:N    | 2.30                     | 0.46              |
| 11:A8:73:ILE:HG22 | 11:A8:75:ALA:H    | 1.80                     | 0.46              |
| 6:UI:94:HIS:HB2   | 6:UI:146:THR:HG21 | 1.97                     | 0.46              |
| 6:UI:136:LEU:HD23 | 6:UI:157:LEU:CD1  | 2.45                     | 0.46              |
| 6:WB:147:LEU:O    | 6:WB:148:GLY:C    | 2.58                     | 0.46              |
| 6:WP:190:GLN:C    | 6:WP:192:SER:N    | 2.73                     | 0.46              |
| 6:BV:235:LEU:HD13 | 6:BW:244:ARG:HH22 | 1.81                     | 0.46              |
| 1:F:181:SER:HB2   | 1:G:31:VAL:CG1    | 2.45                     | 0.46              |
| 1:G:52:PHE:CD2    | 2:e:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:G:112:TYR:HD2   | 1:G:113:LEU:HD13  | 1.80                     | 0.46              |
| 1:O:52:PHE:CD2    | 2:m:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:P:90:LYS:HA     | 1:Q:142:ASN:HA    | 1.98                     | 0.46              |
| 1:R:50:SER:HB3    | 2:o:32:ARG:HH11   | 1.81                     | 0.46              |
| 1:U:52:PHE:CD2    | 2:s:172:GLU:HB3   | 2.50                     | 0.46              |
| 1:U:62:TYR:CE1    | 2:s:129:VAL:HG13  | 2.48                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:W:181:SER:HB2   | 1:X:31:VAL:CG1     | 2.45                     | 0.46              |
| 2:a:98:ARG:HD3    | 2:z:188:GLN:HG2    | 1.97                     | 0.46              |
| 2:b:142:LEU:HD11  | 2:z:346:MET:HE2    | 1.95                     | 0.46              |
| 2:c:235:PHE:O     | 2:c:239:ILE:HG12   | 2.15                     | 0.46              |
| 2:d:188:GLN:HG2   | 2:e:98:ARG:HD3     | 1.97                     | 0.46              |
| 2:e:129:VAL:HG21  | 2:f:136:LEU:HD13   | 1.98                     | 0.46              |
| 2:g:346:MET:HE3   | 2:i:142:LEU:CD1    | 2.42                     | 0.46              |
| 2:l:56:PRO:CD     | 2:m:79:MET:HG2     | 2.45                     | 0.46              |
| 2:m:258:ARG:HH12  | 2:o:140:ASN:HD21   | 1.64                     | 0.46              |
| 2:m:273:CYS:HB2   | 2:n:265:ASN:HA     | 1.98                     | 0.46              |
| 2:n:273:CYS:HB2   | 2:o:265:ASN:HA     | 1.98                     | 0.46              |
| 2:o:80:GLN:HE22   | 3:AJ:125:ASN:ND2   | 2.14                     | 0.46              |
| 2:q:33:GLU:O      | 2:r:170:ILE:HD13   | 2.15                     | 0.46              |
| 2:r:129:VAL:HG21  | 2:s:136:LEU:HD13   | 1.98                     | 0.46              |
| 2:t:130:ASP:OD1   | 2:t:130:ASP:N      | 2.47                     | 0.46              |
| 2:x:273:CYS:HB2   | 2:y:265:ASN:HA     | 1.98                     | 0.46              |
| 2:y:188:GLN:HG2   | 2:z:98:ARG:HD3     | 1.97                     | 0.46              |
| 3:0:227:ALA:HA    | 3:ZB:257:LEU:HD21  | 1.97                     | 0.46              |
| 3:1:67:GLN:HE22   | 3:AK:185:GLU:HA    | 1.81                     | 0.46              |
| 3:3:128:LEU:O     | 3:3:136:VAL:HG12   | 2.16                     | 0.46              |
| 3:5:257:LEU:O     | 3:5:260:LEU:HB2    | 2.16                     | 0.46              |
| 3:7:49:ILE:CD1    | 3:AF:90:ASN:HD21   | 2.29                     | 0.46              |
| 4:ZG:264:LEU:HD12 | 4:ZG:265:ASN:N     | 2.30                     | 0.46              |
| 4:ZO:156:ILE:HA   | 4:ZO:277:VAL:HG23  | 1.98                     | 0.46              |
| 4:ZP:245:ASN:C    | 4:ZP:246:ILE:HD13  | 2.40                     | 0.46              |
| 4:ZQ:380:ARG:HD3  | 4:ZQ:380:ARG:HA    | 1.70                     | 0.46              |
| 4:ZS:314:GLN:NE2  | 4:ZS:347:THR:OG1   | 2.47                     | 0.46              |
| 4:ZU:107:ASN:ND2  | 4:ZU:138:THR:HG22  | 2.31                     | 0.46              |
| 4:ZY:83:PHE:HB2   | 4:ZY:95:SER:O      | 2.16                     | 0.46              |
| 4:ZY:111:MET:CE   | 4:Zd:58:THR:OG1    | 2.63                     | 0.46              |
| 4:ZY:184:VAL:HG13 | 4:ZY:196:MET:HB2   | 1.97                     | 0.46              |
| 4:ZZ:5:GLN:HG2    | 4:ZZ:50:LEU:O      | 2.16                     | 0.46              |
| 4:Za:376:ILE:HG23 | 4:Zg:393:ASP:OD2   | 2.16                     | 0.46              |
| 4:Zb:380:ARG:HD2  | 4:Zh:396:LEU:HB3   | 1.98                     | 0.46              |
| 4:Zd:3:PHE:O      | 4:Zd:7:VAL:HG13    | 2.16                     | 0.46              |
| 4:Zf:101:LYS:HD3  | 4:Zf:102:LEU:N     | 2.31                     | 0.46              |
| 4:Zh:269:GLN:HG2  | 4:Zh:270:ASN:H     | 1.80                     | 0.46              |
| 5:AA:110:THR:HG23 | 5:AA:112:GLN:HG2   | 1.97                     | 0.46              |
| 5:AD:9:MET:HB2    | 12:BD:103:VAL:HG21 | 1.98                     | 0.46              |
| 3:AF:205:THR:HB   | 3:AF:208:LEU:HD12  | 1.98                     | 0.46              |
| 3:AG:62:LEU:HD12  | 12:BC:35:THR:HG21  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AG:180:ASN:O    | 3:AG:198:SER:HB3  | 2.16                     | 0.46              |
| 3:AJ:62:LEU:CG    | 12:BF:84:LEU:HD11 | 2.46                     | 0.46              |
| 3:AM:115:THR:HB   | 3:AM:191:LEU:HD23 | 1.97                     | 0.46              |
| 7:Ar:29:LEU:HB2   | 7:As:52:ILE:HG13  | 1.97                     | 0.46              |
| 8:At:86:PHE:CZ    | 9:Au:91:GLY:HA3   | 2.51                     | 0.46              |
| 8:At:145:TRP:HA   | 6:WJ:164:LEU:CD1  | 2.46                     | 0.46              |
| 9:Au:100:ILE:HG23 | 9:Au:101:MET:HE2  | 1.98                     | 0.46              |
| 10:A4:14:LEU:CD2  | 6:BW:278:THR:HG21 | 2.46                     | 0.46              |
| 11:A8:31:ALA:CB   | 12:BC:13:ALA:HB2  | 2.42                     | 0.46              |
| 6:UK:136:LEU:HD23 | 6:UK:157:LEU:CD1  | 2.45                     | 0.46              |
| 6:UL:98:LEU:HD11  | 6:UL:143:THR:O    | 2.16                     | 0.46              |
| 6:UN:129:GLN:O    | 6:UN:133:GLN:N    | 2.29                     | 0.46              |
| 6:WA:112:GLY:HA2  | 6:WA:135:ALA:CA   | 2.27                     | 0.46              |
| 6:WC:135:ALA:O    | 6:WC:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WD:147:LEU:O    | 6:WD:148:GLY:C    | 2.59                     | 0.46              |
| 6:WK:135:ALA:O    | 6:WK:139:GLU:HG2  | 2.16                     | 0.46              |
| 6:WK:145:GLU:O    | 6:WK:147:LEU:N    | 2.49                     | 0.46              |
| 6:WQ:160:PRO:HG2  | 6:WQ:170:LYS:O    | 2.16                     | 0.46              |
| 6:WR:135:ALA:O    | 6:WR:139:GLU:HG2  | 2.16                     | 0.46              |
| 1:C:136:GLY:CA    | 1:E:213:ILE:HG23  | 2.42                     | 0.45              |
| 1:F:52:PHE:CD2    | 2:d:172:GLU:HB3   | 2.50                     | 0.45              |
| 1:M:112:TYR:HD2   | 1:M:113:LEU:HD13  | 1.80                     | 0.45              |
| 1:N:47:ALA:HB1    | 2:k:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:O:47:ALA:HB1    | 2:l:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:P:52:PHE:CD2    | 2:n:172:GLU:HB3   | 2.50                     | 0.45              |
| 1:Q:112:TYR:HD2   | 1:Q:113:LEU:HD13  | 1.80                     | 0.45              |
| 1:S:90:LYS:HA     | 1:T:142:ASN:HA    | 1.98                     | 0.45              |
| 1:T:181:SER:HB2   | 1:U:31:VAL:CG1    | 2.45                     | 0.45              |
| 1:U:181:SER:HB2   | 1:V:31:VAL:CG1    | 2.45                     | 0.45              |
| 2:e:188:GLN:HG2   | 2:f:98:ARG:HD3    | 1.97                     | 0.45              |
| 2:j:93:TYR:OH     | 2:j:173:ARG:O     | 2.25                     | 0.45              |
| 2:t:258:ARG:HH12  | 2:v:140:ASN:HD21  | 1.64                     | 0.45              |
| 2:t:346:MET:HE3   | 2:v:142:LEU:CD1   | 2.42                     | 0.45              |
| 2:u:129:VAL:HG21  | 2:v:136:LEU:HD13  | 1.98                     | 0.45              |
| 2:u:273:CYS:HB2   | 2:v:265:ASN:HA    | 1.98                     | 0.45              |
| 2:v:319:LEU:HD21  | 2:w:264:MET:HE1   | 1.98                     | 0.45              |
| 3:0:129:VAL:HG12  | 3:0:135:GLN:HA    | 1.97                     | 0.45              |
| 3:8:180:ASN:OD1   | 3:8:183:GLY:N     | 2.44                     | 0.45              |
| 3:ZC:80:LEU:HD23  | 3:ZC:80:LEU:HA    | 1.75                     | 0.45              |
| 4:ZK:262:SER:OG   | 4:ZK:264:LEU:HG   | 2.16                     | 0.45              |
| 4:ZM:18:ASP:C     | 4:ZR:5:GLN:HE22   | 2.24                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZM:213:HIS:HB2  | 4:ZM:223:PRO:HG3   | 1.99                     | 0.45              |
| 4:ZP:16:ASN:HB2   | 4:ZP:39:PHE:HZ     | 1.79                     | 0.45              |
| 4:ZP:380:ARG:HD3  | 4:ZP:380:ARG:HA    | 1.67                     | 0.45              |
| 4:ZQ:93:PHE:HB3   | 4:ZQ:333:VAL:HG13  | 1.97                     | 0.45              |
| 4:ZQ:155:GLN:HE21 | 4:ZQ:277:VAL:HB    | 1.79                     | 0.45              |
| 4:ZT:70:GLY:O     | 4:ZT:71:ARG:C      | 2.58                     | 0.45              |
| 4:ZW:380:ARG:HD3  | 4:ZW:380:ARG:HA    | 1.65                     | 0.45              |
| 4:ZX:96:ARG:NH2   | 4:ZX:362:GLU:OE2   | 2.40                     | 0.45              |
| 5:AB:72:ASP:HB3   | 3:AM:6:TRP:CE3     | 2.51                     | 0.45              |
| 5:AE:53:THR:HG22  | 12:BF:67:VAL:HG11  | 1.98                     | 0.45              |
| 6:AU:235:LEU:HD13 | 6:AV:244:ARG:HH22  | 1.81                     | 0.45              |
| 6:AV:235:LEU:HD13 | 6:AW:244:ARG:HH22  | 1.81                     | 0.45              |
| 7:Ab:54:LYS:HB3   | 9:Av:207:LEU:CD2   | 2.45                     | 0.45              |
| 7:Ab:84:LEU:HD11  | 9:Av:185:ILE:HG23  | 1.97                     | 0.45              |
| 6:Af:235:LEU:HD13 | 6:Ag:244:ARG:HH22  | 1.81                     | 0.45              |
| 6:Al:294:ARG:CG   | 11:A7:66:THR:OG1   | 2.64                     | 0.45              |
| 7:As:2:THR:O      | 7:As:5:SER:OG      | 2.24                     | 0.45              |
| 9:Av:49:THR:CG2   | 10:A2:89:ARG:HG3   | 2.45                     | 0.45              |
| 9:Aw:44:THR:HG23  | 11:A8:133:VAL:HG11 | 1.96                     | 0.45              |
| 10:A5:7:ILE:HD11  | 6:BS:370:ARG:HH21  | 1.82                     | 0.45              |
| 6:UJ:98:LEU:HD11  | 6:UJ:143:THR:O     | 2.16                     | 0.45              |
| 6:UK:98:LEU:HD11  | 6:UK:143:THR:O     | 2.16                     | 0.45              |
| 6:UP:73:MET:HE3   | 6:UP:99:ARG:CD     | 2.41                     | 0.45              |
| 12:BA:30:ASN:ND2  | 12:BF:62:VAL:HB    | 2.31                     | 0.45              |
| 6:WI:193:ALA:HB1  | 6:WJ:213:VAL:CG1   | 2.45                     | 0.45              |
| 6:WI:197:LEU:HA   | 6:WJ:175:SER:OG    | 2.15                     | 0.45              |
| 6:WP:135:ALA:O    | 6:WP:139:GLU:HG2   | 2.16                     | 0.45              |
| 6:WP:147:LEU:O    | 6:WP:148:GLY:C     | 2.58                     | 0.45              |
| 6:WP:197:LEU:CD1  | 6:WQ:175:SER:OG    | 2.58                     | 0.45              |
| 6:WR:142:ARG:O    | 6:WR:146:THR:HG23  | 2.16                     | 0.45              |
| 6:WS:137:GLU:HG3  | 6:WS:155:VAL:O     | 2.16                     | 0.45              |
| 6:WT:128:GLU:CG   | 6:WU:126:PHE:CD2   | 2.99                     | 0.45              |
| 6:WV:190:GLN:HG2  | 6:WW:217:GLY:HA3   | 1.97                     | 0.45              |
| 12:BF:88:ASN:HB2  | 12:BF:90:TYR:CD2   | 2.50                     | 0.45              |
| 6:BQ:319:GLN:NE2  | 6:BW:305:GLY:O     | 2.49                     | 0.45              |
| 1:F:112:TYR:HD2   | 1:F:113:LEU:HD13   | 1.80                     | 0.45              |
| 1:J:50:SER:HB3    | 2:g:32:ARG:HH11    | 1.81                     | 0.45              |
| 1:L:90:LYS:HA     | 1:M:142:ASN:HA     | 1.98                     | 0.45              |
| 1:M:142:ASN:ND2   | 1:N:207:TYR:OH     | 2.28                     | 0.45              |
| 1:P:47:ALA:HB1    | 2:m:178:GLN:HG3    | 1.96                     | 0.45              |
| 1:V:136:GLY:CA    | 1:X:213:ILE:HG23   | 2.42                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:X:68:ASP:OD1    | 2:w:64:ASN:ND2    | 2.48                     | 0.45              |
| 1:Z:50:SER:HB3    | 2:w:32:ARG:HH11   | 1.81                     | 0.45              |
| 2:g:188:GLN:HG2   | 2:h:98:ARG:HD3    | 1.97                     | 0.45              |
| 2:k:56:PRO:CD     | 2:l:79:MET:HG2    | 2.45                     | 0.45              |
| 2:l:273:CYS:HB2   | 2:m:265:ASN:HA    | 1.98                     | 0.45              |
| 2:o:56:PRO:CD     | 2:p:79:MET:HG2    | 2.45                     | 0.45              |
| 2:t:33:GLU:O      | 2:u:170:ILE:HD13  | 2.15                     | 0.45              |
| 2:t:273:CYS:HB2   | 2:u:265:ASN:HA    | 1.98                     | 0.45              |
| 2:v:273:CYS:HB2   | 2:w:265:ASN:HA    | 1.99                     | 0.45              |
| 2:w:235:PHE:O     | 2:w:239:ILE:HG12  | 2.15                     | 0.45              |
| 2:w:273:CYS:HB2   | 2:x:265:ASN:HA    | 1.99                     | 0.45              |
| 2:y:273:CYS:HB2   | 2:z:265:ASN:HA    | 1.98                     | 0.45              |
| 3:2:64:SER:O      | 3:AL:76:ALA:HB1   | 2.16                     | 0.45              |
| 3:3:1:MET:HE3     | 3:AG:29:VAL:HG21  | 1.97                     | 0.45              |
| 3:3:98:LYS:HB3    | 3:3:213:LEU:HB2   | 1.98                     | 0.45              |
| 3:5:29:VAL:O      | 3:5:222:SER:OG    | 2.33                     | 0.45              |
| 3:8:56:SER:O      | 3:AG:152:GLY:C    | 2.59                     | 0.45              |
| 3:ZA:70:THR:HG22  | 3:ZA:71:GLY:N     | 2.29                     | 0.45              |
| 3:ZB:56:SER:HA    | 3:AJ:152:GLY:HA3  | 1.98                     | 0.45              |
| 3:ZC:85:ASN:HD22  | 4:ZN:4:SER:HB2    | 1.81                     | 0.45              |
| 4:ZQ:379:GLN:NE2  | 4:ZV:394:GLN:NE2  | 2.64                     | 0.45              |
| 4:ZR:125:PRO:HA   | 4:ZR:126:PRO:HD3  | 1.92                     | 0.45              |
| 4:ZX:41:ASP:OD1   | 4:ZX:41:ASP:N     | 2.42                     | 0.45              |
| 4:ZX:331:ASP:OD1  | 4:Zc:53:LYS:NZ    | 2.48                     | 0.45              |
| 4:ZY:194:HIS:CE1  | 4:ZY:251:ILE:HD12 | 2.51                     | 0.45              |
| 4:Zb:234:GLU:HG3  | 4:Zh:253:GLY:O    | 2.17                     | 0.45              |
| 4:Zf:5:GLN:HG2    | 4:Zf:50:LEU:O     | 2.15                     | 0.45              |
| 5:AB:243:ARG:O    | 5:AB:246:GLN:HG2  | 2.16                     | 0.45              |
| 5:AB:248:LEU:HD22 | 11:A7:109:PHE:CD2 | 2.52                     | 0.45              |
| 5:AC:53:THR:OG1   | 11:A8:92:GLN:CG   | 2.61                     | 0.45              |
| 5:AE:64:ALA:HB2   | 5:AE:173:ARG:HH21 | 1.80                     | 0.45              |
| 5:AE:220:MET:CE   | 3:AJ:246:ALA:HB2  | 2.46                     | 0.45              |
| 5:AE:221:ILE:HG21 | 3:AK:251:ASP:HB2  | 1.97                     | 0.45              |
| 3:AF:43:ASP:N     | 3:AF:43:ASP:OD1   | 2.45                     | 0.45              |
| 3:AG:16:GLN:HE21  | 3:AG:16:GLN:HB2   | 1.48                     | 0.45              |
| 3:AG:157:VAL:O    | 3:AG:170:VAL:N    | 2.49                     | 0.45              |
| 3:AG:188:GLY:O    | 3:AG:190:ASN:N    | 2.49                     | 0.45              |
| 3:AH:147:LEU:HB2  | 3:AH:160:THR:HG23 | 1.98                     | 0.45              |
| 3:AH:228:GLU:HG3  | 3:AN:9:LYS:HE3    | 1.99                     | 0.45              |
| 3:AM:25:ASN:HD21  | 3:AM:37:GLN:H     | 1.64                     | 0.45              |
| 7:Ab:81:PHE:CD2   | 9:Av:234:LEU:HB3  | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:At:39:PRO:HB3   | 10:A4:102:MET:SD  | 2.56                     | 0.45              |
| 9:Au:230:ASP:O    | 9:Au:234:LEU:HG   | 2.15                     | 0.45              |
| 6:UI:73:MET:HE3   | 6:UI:99:ARG:CD    | 2.41                     | 0.45              |
| 6:WJ:181:GLU:O    | 6:WJ:182:PRO:C    | 2.60                     | 0.45              |
| 6:WN:145:GLU:C    | 6:WN:147:LEU:N    | 2.74                     | 0.45              |
| 6:WN:197:LEU:CD1  | 6:WO:175:SER:HB3  | 2.42                     | 0.45              |
| 6:WP:142:ARG:O    | 6:WP:146:THR:HG23 | 2.16                     | 0.45              |
| 6:WU:112:GLY:HA2  | 6:WU:139:GLU:OE1  | 2.17                     | 0.45              |
| 6:WV:187:ASP:N    | 6:WV:190:GLN:HB2  | 2.31                     | 0.45              |
| 6:BT:235:LEU:HD13 | 6:BU:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:L:136:GLY:CA    | 1:N:213:ILE:HG23  | 2.42                     | 0.45              |
| 1:Q:47:ALA:HB1    | 2:n:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:Q:50:SER:CB     | 2:n:32:ARG:NH1    | 2.77                     | 0.45              |
| 1:V:52:PHE:CD2    | 2:t:172:GLU:HB3   | 2.50                     | 0.45              |
| 1:X:166:GLU:HB2   | 1:Y:35:THR:CG2    | 2.30                     | 0.45              |
| 2:a:79:MET:HG2    | 2:z:56:PRO:CD     | 2.45                     | 0.45              |
| 2:f:188:GLN:HG2   | 2:g:98:ARG:HD3    | 1.97                     | 0.45              |
| 2:g:319:LEU:HD21  | 2:h:264:MET:HE1   | 1.98                     | 0.45              |
| 2:h:273:CYS:HB2   | 2:i:265:ASN:HA    | 1.98                     | 0.45              |
| 2:j:346:MET:HE3   | 2:l:142:LEU:CD1   | 2.42                     | 0.45              |
| 2:l:78:ASN:HD21   | 5:AE:154:THR:CG2  | 2.29                     | 0.45              |
| 2:p:273:CYS:HB2   | 2:q:265:ASN:HA    | 1.99                     | 0.45              |
| 2:q:273:CYS:HB2   | 2:r:265:ASN:HA    | 1.99                     | 0.45              |
| 2:u:192:GLU:H     | 2:u:192:GLU:HG3   | 1.52                     | 0.45              |
| 2:v:33:GLU:O      | 2:w:170:ILE:HD13  | 2.15                     | 0.45              |
| 2:w:188:GLN:HG2   | 2:x:98:ARG:HD3    | 1.97                     | 0.45              |
| 3:0:20:ASP:OD1    | 3:5:3:SER:OG      | 2.34                     | 0.45              |
| 3:1:9:LYS:HB2     | 3:AJ:231:VAL:HG11 | 1.97                     | 0.45              |
| 3:1:251:ASP:CG    | 3:AJ:238:ARG:HH21 | 2.23                     | 0.45              |
| 3:4:9:LYS:HB2     | 3:AM:231:VAL:HG11 | 1.98                     | 0.45              |
| 3:5:184:LEU:HB3   | 3:5:192:TYR:HB3   | 1.99                     | 0.45              |
| 3:6:44:LEU:HD23   | 3:6:44:LEU:HA     | 1.83                     | 0.45              |
| 4:ZL:104:GLU:H    | 4:ZL:104:GLU:CD   | 2.24                     | 0.45              |
| 4:ZN:230:LEU:HD12 | 4:ZN:230:LEU:HA   | 1.85                     | 0.45              |
| 4:ZQ:42:MET:HE2   | 4:ZQ:50:LEU:HD22  | 1.98                     | 0.45              |
| 4:ZU:372:LEU:CD1  | 4:Zf:396:LEU:CD2  | 2.92                     | 0.45              |
| 4:ZZ:63:ASP:OD2   | 4:ZZ:79:GLN:N     | 2.50                     | 0.45              |
| 4:ZZ:205:ASP:CG   | 4:Zf:252:ASN:HA   | 2.40                     | 0.45              |
| 4:Zf:378:ALA:O    | 4:Zf:379:GLN:C    | 2.59                     | 0.45              |
| 5:AE:50:SER:OG    | 5:AE:51:LEU:HG    | 2.16                     | 0.45              |
| 3:AF:122:VAL:HG11 | 3:AF:142:ILE:HD12 | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AG:36:ARG:HD3   | 3:AG:80:LEU:HD22  | 1.97                     | 0.45              |
| 3:AG:185:GLU:HB2  | 3:AG:195:THR:CG2  | 2.46                     | 0.45              |
| 3:AJ:98:LYS:N     | 3:AJ:213:LEU:O    | 2.40                     | 0.45              |
| 3:AJ:159:VAL:O    | 3:AJ:168:VAL:HG22 | 2.17                     | 0.45              |
| 3:AL:3:SER:O      | 3:AL:4:SER:C      | 2.59                     | 0.45              |
| 3:AL:87:SER:OG    | 3:AL:88:GLN:N     | 2.47                     | 0.45              |
| 3:AN:238:ARG:O    | 3:AN:242:ILE:HG12 | 2.17                     | 0.45              |
| 6:AY:372:ILE:HG21 | 10:A3:4:ILE:CG1   | 2.45                     | 0.45              |
| 7:Ab:88:ILE:HG21  | 9:Av:242:SER:HB2  | 1.97                     | 0.45              |
| 6:Ad:372:ILE:HG21 | 10:A2:11:ILE:HG23 | 1.89                     | 0.45              |
| 6:An:235:LEU:HD13 | 6:Ao:244:ARG:HH22 | 1.81                     | 0.45              |
| 7:As:45:ASN:HB2   | 8:At:210:GLN:OE1  | 2.17                     | 0.45              |
| 8:At:144:LEU:CB   | 6:WJ:164:LEU:HD21 | 2.46                     | 0.45              |
| 9:Au:59:LEU:HD12  | 9:Av:88:VAL:CG2   | 2.46                     | 0.45              |
| 9:Aw:90:LEU:HD13  | 10:A2:100:MET:HA  | 1.98                     | 0.45              |
| 10:A4:72:MET:HE3  | 12:BE:130:LEU:CD2 | 2.47                     | 0.45              |
| 10:A5:62:GLY:HA2  | 6:BG:318:ASN:ND2  | 2.31                     | 0.45              |
| 6:UJ:103:GLN:OE1  | 6:WD:182:PRO:CG   | 2.65                     | 0.45              |
| 6:UJ:129:GLN:O    | 6:UJ:133:GLN:N    | 2.29                     | 0.45              |
| 6:UM:80:ALA:N     | 6:UM:85:ALA:O     | 2.49                     | 0.45              |
| 6:UN:80:ALA:N     | 6:UN:85:ALA:O     | 2.49                     | 0.45              |
| 6:WA:181:GLU:O    | 6:WA:182:PRO:C    | 2.60                     | 0.45              |
| 6:WT:190:GLN:HG2  | 6:WU:217:GLY:HA3  | 1.99                     | 0.45              |
| 6:WU:181:GLU:O    | 6:WU:182:PRO:C    | 2.60                     | 0.45              |
| 12:BC:37:PRO:O    | 6:BK:330:THR:OG1  | 2.33                     | 0.45              |
| 12:BE:68:ILE:HD11 | 6:BP:312:VAL:HG22 | 1.98                     | 0.45              |
| 6:BR:235:LEU:HD13 | 6:BS:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:E:50:SER:HB3    | 2:b:32:ARG:HH11   | 1.81                     | 0.45              |
| 1:K:90:LYS:HA     | 1:L:142:ASN:HA    | 1.98                     | 0.45              |
| 1:M:47:ALA:HB1    | 2:j:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:R:47:ALA:HB1    | 2:o:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:S:50:SER:CB     | 2:p:32:ARG:NH1    | 2.77                     | 0.45              |
| 1:V:181:SER:HB2   | 1:W:31:VAL:CG1    | 2.45                     | 0.45              |
| 2:h:56:PRO:CD     | 2:i:79:MET:HG2    | 2.45                     | 0.45              |
| 2:p:129:VAL:HG21  | 2:q:136:LEU:HD13  | 1.98                     | 0.45              |
| 2:r:33:GLU:O      | 2:s:170:ILE:HD13  | 2.16                     | 0.45              |
| 2:s:273:CYS:HB2   | 2:t:265:ASN:HA    | 1.98                     | 0.45              |
| 2:u:33:GLU:O      | 2:v:170:ILE:HD13  | 2.16                     | 0.45              |
| 2:w:33:GLU:O      | 2:x:170:ILE:HD13  | 2.15                     | 0.45              |
| 2:w:208:ARG:O     | 2:w:212:SER:OG    | 2.16                     | 0.45              |
| 3:3:1:MET:HB3     | 3:AG:29:VAL:CG2   | 2.46                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:4:44:LEU:HD22   | 3:AH:86:LEU:HD12   | 1.98                     | 0.45              |
| 3:8:255:GLN:O     | 3:8:259:GLN:HG2    | 2.16                     | 0.45              |
| 4:ZJ:24:ILE:HD13  | 4:ZO:384:SER:OG    | 2.16                     | 0.45              |
| 4:ZJ:183:THR:HG22 | 4:ZU:131:GLY:O     | 2.16                     | 0.45              |
| 4:ZJ:265:ASN:OD1  | 4:ZJ:265:ASN:O     | 2.35                     | 0.45              |
| 4:ZK:93:PHE:HB3   | 4:ZK:333:VAL:HG13  | 1.98                     | 0.45              |
| 4:ZP:17:LEU:CD1   | 4:ZU:395:ILE:HD11  | 2.45                     | 0.45              |
| 4:ZT:16:ASN:HB2   | 4:ZT:39:PHE:HZ     | 1.81                     | 0.45              |
| 4:ZW:122:THR:OG1  | 4:ZW:129:GLN:NE2   | 2.50                     | 0.45              |
| 4:ZX:230:LEU:HD22 | 4:ZX:238:LEU:HD11  | 1.98                     | 0.45              |
| 4:ZX:269:GLN:HG2  | 4:Zd:190:GLN:O     | 2.16                     | 0.45              |
| 4:ZY:33:LYS:NZ    | 4:ZY:362:GLU:OE2   | 2.49                     | 0.45              |
| 4:ZY:399:LEU:HD23 | 4:ZY:399:LEU:HA    | 1.84                     | 0.45              |
| 4:Ze:383:GLN:O    | 4:Ze:387:GLN:HG2   | 2.16                     | 0.45              |
| 4:Zf:38:SER:O     | 4:Zf:55:ALA:N      | 2.47                     | 0.45              |
| 4:Zg:29:THR:HB    | 4:Zg:32:PHE:HB2    | 1.98                     | 0.45              |
| 5:AB:131:GLU:HB2  | 3:AG:179:MET:HE3   | 1.99                     | 0.45              |
| 5:AB:240:ASN:HD22 | 12:BC:113:GLN:HE21 | 1.64                     | 0.45              |
| 5:AC:14:GLN:HG3   | 5:AC:58:THR:HA     | 1.97                     | 0.45              |
| 3:AF:79:ARG:NH1   | 3:AF:184:LEU:O     | 2.47                     | 0.45              |
| 3:AG:76:ALA:HA    | 3:AL:66:LEU:HB3    | 1.98                     | 0.45              |
| 3:AH:35:LYS:HG3   | 3:AH:81:HIS:ND1    | 2.32                     | 0.45              |
| 3:AK:44:LEU:HB2   | 3:AK:70:THR:HB     | 1.97                     | 0.45              |
| 3:AK:237:GLN:O    | 3:AK:241:GLU:HG3   | 2.17                     | 0.45              |
| 6:AR:244:ARG:HH22 | 6:Aa:235:LEU:HD13  | 1.81                     | 0.45              |
| 6:Ae:235:LEU:HD13 | 6:Af:244:ARG:HH22  | 1.81                     | 0.45              |
| 6:Aj:372:ILE:HD12 | 10:A1:11:ILE:CG2   | 2.28                     | 0.45              |
| 7:Aq:3:PRO:HB3    | 7:Ar:70:LEU:HD23   | 1.99                     | 0.45              |
| 9:Av:97:THR:O     | 9:Av:101:MET:HG2   | 2.16                     | 0.45              |
| 10:Az:15:GLN:HG3  | 10:Az:16:ALA:N     | 2.30                     | 0.45              |
| 11:A7:117:GLN:NE2 | 12:BC:127:LEU:HD21 | 2.31                     | 0.45              |
| 6:UO:164:LEU:HD22 | 6:UO:164:LEU:H     | 1.82                     | 0.45              |
| 6:WE:135:ALA:O    | 6:WE:139:GLU:HG2   | 2.16                     | 0.45              |
| 6:WF:166:VAL:HG22 | 6:WF:168:GLU:H     | 1.82                     | 0.45              |
| 6:WS:181:GLU:O    | 6:WS:182:PRO:C     | 2.60                     | 0.45              |
| 6:WU:135:ALA:O    | 6:WU:139:GLU:HG2   | 2.16                     | 0.45              |
| 12:BF:120:ASN:HA  | 12:BF:123:LYS:HE2  | 1.98                     | 0.45              |
| 1:A:50:SER:HB3    | 2:x:32:ARG:HH11    | 1.81                     | 0.45              |
| 1:B:90:LYS:HA     | 1:C:142:ASN:HA     | 1.98                     | 0.45              |
| 1:C:62:TYR:CE1    | 2:a:129:VAL:HG13   | 2.47                     | 0.45              |
| 1:D:181:SER:HB2   | 1:E:31:VAL:CG1     | 2.45                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:181:SER:HB2   | 1:I:31:VAL:CG1    | 2.45                     | 0.45              |
| 1:I:68:ASP:OD1    | 2:h:64:ASN:ND2    | 2.48                     | 0.45              |
| 1:Q:68:ASP:OD1    | 2:p:64:ASN:ND2    | 2.47                     | 0.45              |
| 1:R:50:SER:CB     | 2:o:32:ARG:NH1    | 2.77                     | 0.45              |
| 1:Y:50:SER:HB3    | 2:v:32:ARG:HH11   | 1.81                     | 0.45              |
| 1:Y:181:SER:HB2   | 1:Z:31:VAL:CG1    | 2.45                     | 0.45              |
| 2:a:265:ASN:HA    | 2:z:273:CYS:HB2   | 1.99                     | 0.45              |
| 2:d:129:VAL:HG21  | 2:e:136:LEU:HD13  | 1.98                     | 0.45              |
| 2:g:273:CYS:HB2   | 2:h:265:ASN:HA    | 1.98                     | 0.45              |
| 2:h:129:VAL:HG21  | 2:i:136:LEU:HD13  | 1.98                     | 0.45              |
| 2:p:130:ASP:OD1   | 2:p:130:ASP:N     | 2.47                     | 0.45              |
| 2:q:129:VAL:HG21  | 2:r:136:LEU:HD13  | 1.98                     | 0.45              |
| 2:u:319:LEU:HD21  | 2:v:264:MET:HE1   | 1.97                     | 0.45              |
| 2:x:188:GLN:HG2   | 2:y:98:ARG:HD3    | 1.97                     | 0.45              |
| 3:1:86:LEU:HD12   | 3:ZC:44:LEU:HD22  | 1.96                     | 0.45              |
| 3:4:238:ARG:HH21  | 3:ZA:251:ASP:CG   | 2.19                     | 0.45              |
| 3:5:100:GLN:HE21  | 3:5:177:THR:HG21  | 1.82                     | 0.45              |
| 3:7:106:MET:HE3   | 3:7:110:GLY:HA2   | 1.98                     | 0.45              |
| 3:8:45:LEU:HD23   | 3:8:45:LEU:HA     | 1.81                     | 0.45              |
| 4:ZI:18:ASP:HB3   | 4:ZN:5:GLN:HE22   | 1.81                     | 0.45              |
| 4:ZS:10:LEU:HD11  | 4:ZS:382:TYR:CE1  | 2.51                     | 0.45              |
| 4:ZT:380:ARG:HH21 | 4:ZZ:397:ASN:ND2  | 2.14                     | 0.45              |
| 4:ZV:119:TYR:HB2  | 4:ZV:314:GLN:HB3  | 1.99                     | 0.45              |
| 4:ZW:183:THR:CG2  | 4:Zh:132:ALA:HA   | 2.47                     | 0.45              |
| 5:AA:42:ARG:NH1   | 6:BI:328:ILE:HG22 | 2.31                     | 0.45              |
| 5:AA:58:THR:CG2   | 3:AF:50:ARG:NH2   | 2.79                     | 0.45              |
| 5:AC:24:SER:CA    | 3:AH:7:ILE:HG21   | 2.46                     | 0.45              |
| 5:AD:76:ARG:HG2   | 5:AD:78:LEU:H     | 1.82                     | 0.45              |
| 3:AG:147:LEU:HB2  | 3:AG:160:THR:HG23 | 1.98                     | 0.45              |
| 3:AL:44:LEU:HD21  | 3:AL:73:ARG:HD3   | 1.99                     | 0.45              |
| 6:AR:235:LEU:HD13 | 6:Ac:244:ARG:HH22 | 1.81                     | 0.45              |
| 6:AT:235:LEU:HD13 | 6:AU:244:ARG:HH22 | 1.81                     | 0.45              |
| 6:Af:363:THR:HG23 | 11:A8:73:ILE:HD12 | 1.98                     | 0.45              |
| 6:Am:278:THR:CG2  | 10:Az:21:ALA:HB3  | 2.39                     | 0.45              |
| 6:AO:235:LEU:HD13 | 6:AP:244:ARG:HH22 | 1.81                     | 0.45              |
| 9:Au:45:LEU:HD13  | 10:A1:86:ILE:HG12 | 1.98                     | 0.45              |
| 9:Au:160:GLN:HB2  | 6:WP:166:VAL:CG2  | 2.44                     | 0.45              |
| 9:Ay:83:ALA:O     | 9:Ay:85:PRO:N     | 2.50                     | 0.45              |
| 10:A1:84:MET:HE2  | 10:A1:84:MET:HB2  | 1.87                     | 0.45              |
| 10:A5:15:GLN:HG3  | 10:A5:16:ALA:N    | 2.30                     | 0.45              |
| 10:A5:75:MET:HE2  | 10:A5:75:MET:HB2  | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A6:104:ARG:O   | 11:A6:108:GLN:HG2 | 2.17                     | 0.45              |
| 11:A8:33:ALA:O    | 11:A8:98:ASN:ND2  | 2.50                     | 0.45              |
| 6:UJ:94:HIS:HB2   | 6:UJ:146:THR:HG21 | 1.97                     | 0.45              |
| 6:UM:164:LEU:HD22 | 6:UM:164:LEU:H    | 1.82                     | 0.45              |
| 6:UO:88:VAL:O     | 6:UO:89:PRO:C     | 2.60                     | 0.45              |
| 6:WB:113:PHE:CE2  | 6:WB:139:GLU:HG3  | 2.52                     | 0.45              |
| 6:WC:193:ALA:HB1  | 6:WD:213:VAL:HG21 | 1.98                     | 0.45              |
| 6:WJ:135:ALA:O    | 6:WJ:139:GLU:HG2  | 2.16                     | 0.45              |
| 6:WJ:159:MET:HE3  | 6:WJ:159:MET:HB3  | 1.78                     | 0.45              |
| 6:WK:193:ALA:HB1  | 6:WL:213:VAL:HG11 | 1.99                     | 0.45              |
| 6:WM:181:GLU:O    | 6:WM:182:PRO:C    | 2.60                     | 0.45              |
| 6:WW:135:ALA:O    | 6:WW:139:GLU:HG2  | 2.16                     | 0.45              |
| 1:K:62:TYR:CE1    | 2:i:129:VAL:HG13  | 2.47                     | 0.45              |
| 1:N:112:TYR:HD2   | 1:N:113:LEU:HD13  | 1.80                     | 0.45              |
| 1:P:150:VAL:HG12  | 1:P:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:R:90:LYS:HA     | 1:S:142:ASN:HA    | 1.98                     | 0.45              |
| 1:S:47:ALA:HB1    | 2:p:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:T:50:SER:CB     | 2:q:32:ARG:NH1    | 2.77                     | 0.45              |
| 1:T:90:LYS:HA     | 1:U:142:ASN:HA    | 1.98                     | 0.45              |
| 1:Y:47:ALA:HB1    | 2:v:178:GLN:HG3   | 1.97                     | 0.45              |
| 2:a:170:ILE:HD13  | 2:z:33:GLU:O      | 2.15                     | 0.45              |
| 2:a:273:CYS:HB2   | 2:b:265:ASN:HA    | 1.99                     | 0.45              |
| 2:b:273:CYS:HB2   | 2:c:265:ASN:HA    | 1.98                     | 0.45              |
| 2:d:273:CYS:HB2   | 2:e:265:ASN:HA    | 1.98                     | 0.45              |
| 2:i:129:VAL:HG21  | 2:j:136:LEU:HD13  | 1.98                     | 0.45              |
| 2:v:21:ARG:HA     | 2:v:21:ARG:HD2    | 1.74                     | 0.45              |
| 3:1:1:MET:CA      | 5:AE:211:VAL:O    | 2.64                     | 0.45              |
| 3:2:257:LEU:HG    | 3:AF:230:LEU:CD1  | 2.43                     | 0.45              |
| 3:4:95:VAL:O      | 3:4:118:GLY:HA3   | 2.16                     | 0.45              |
| 3:4:237:GLN:HB2   | 3:9:249:THR:HG23  | 1.98                     | 0.45              |
| 3:6:218:TYR:CZ    | 4:ZH:53:LYS:HG3   | 2.49                     | 0.45              |
| 3:9:85:ASN:HB3    | 4:ZK:4:SER:CB     | 2.46                     | 0.45              |
| 3:ZA:37:GLN:NE2   | 3:ZA:77:THR:OG1   | 2.50                     | 0.45              |
| 3:ZD:185:GLU:OE1  | 4:ZI:46:SER:HB2   | 2.16                     | 0.45              |
| 3:ZE:235:GLN:NE2  | 4:ZK:7:VAL:HG21   | 2.32                     | 0.45              |
| 4:ZG:65:THR:HG22  | 4:ZR:50:LEU:HD22  | 1.98                     | 0.45              |
| 4:ZI:8:SER:HB3    | 4:ZI:52:VAL:H     | 1.81                     | 0.45              |
| 4:ZJ:269:GLN:OE1  | 4:ZP:190:GLN:HA   | 2.17                     | 0.45              |
| 4:ZK:210:VAL:HB   | 4:ZK:228:THR:HG22 | 1.98                     | 0.45              |
| 4:ZM:139:ILE:HA   | 4:ZM:312:LEU:HD13 | 1.97                     | 0.45              |
| 4:ZM:380:ARG:NE   | 4:ZS:393:ASP:OD1  | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZS:156:ILE:HG13 | 4:ZS:276:ILE:HA   | 1.99                     | 0.45              |
| 4:ZV:18:ASP:HB3   | 4:Za:5:GLN:NE2    | 2.31                     | 0.45              |
| 4:Zd:5:GLN:HG2    | 4:Zd:50:LEU:O     | 2.17                     | 0.45              |
| 4:Zd:184:VAL:HG13 | 4:Zd:196:MET:HB2  | 1.98                     | 0.45              |
| 5:AA:83:GLN:HA    | 3:AL:45:LEU:HD22  | 1.97                     | 0.45              |
| 5:AB:151:PRO:HB2  | 5:AB:153:ASN:OD1  | 2.17                     | 0.45              |
| 5:AC:68:PRO:HG2   | 3:AN:47:GLN:HB2   | 1.98                     | 0.45              |
| 5:AD:57:VAL:HB    | 12:BE:30:ASN:ND2  | 2.32                     | 0.45              |
| 5:AE:48:GLY:HA3   | 6:BQ:324:ASN:ND2  | 2.29                     | 0.45              |
| 5:AE:77:PRO:O     | 5:AE:203:SER:OG   | 2.34                     | 0.45              |
| 5:AE:131:GLU:HG2  | 3:AJ:179:MET:CE   | 2.46                     | 0.45              |
| 3:AJ:62:LEU:HG    | 12:BF:84:LEU:CD1  | 2.45                     | 0.45              |
| 3:AK:102:PHE:HB3  | 3:AK:114:TYR:HB3  | 1.99                     | 0.45              |
| 3:AL:140:ILE:HG21 | 3:AL:157:VAL:HG11 | 1.98                     | 0.45              |
| 7:Aq:44:ILE:HA    | 7:Aq:44:ILE:HD13  | 1.74                     | 0.45              |
| 9:Au:135:ARG:O    | 9:Au:138:MET:N    | 2.50                     | 0.45              |
| 9:Aw:59:LEU:HD22  | 9:Ax:88:VAL:HG23  | 1.99                     | 0.45              |
| 9:Ax:148:ALA:HB1  | 6:WF:165:PHE:HD1  | 1.82                     | 0.45              |
| 10:A1:87:GLN:NE2  | 11:A7:134:LEU:O   | 2.49                     | 0.45              |
| 6:UN:164:LEU:H    | 6:UN:164:LEU:HD22 | 1.82                     | 0.45              |
| 6:UP:80:ALA:N     | 6:UP:85:ALA:O     | 2.49                     | 0.45              |
| 6:WC:131:ASN:O    | 6:WC:132:TYR:C    | 2.60                     | 0.45              |
| 6:WD:167:ARG:C    | 6:WD:167:ARG:HE   | 2.25                     | 0.45              |
| 6:WE:143:THR:HA   | 6:WE:146:THR:HG23 | 1.97                     | 0.45              |
| 6:WE:161:LYS:H    | 6:WE:161:LYS:HD3  | 1.82                     | 0.45              |
| 6:WI:147:LEU:O    | 6:WI:148:GLY:C    | 2.60                     | 0.45              |
| 6:WQ:181:GLU:O    | 6:WQ:182:PRO:C    | 2.60                     | 0.45              |
| 6:BS:235:LEU:HD13 | 6:BT:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:A:142:ASN:HA    | 1:Z:90:LYS:HA     | 1.98                     | 0.45              |
| 1:E:90:LYS:HA     | 1:F:142:ASN:HA    | 1.98                     | 0.45              |
| 1:G:150:VAL:HG12  | 1:G:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:L:47:ALA:HB1    | 2:i:178:GLN:HG3   | 1.97                     | 0.45              |
| 1:L:150:VAL:HG12  | 1:L:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:Q:150:VAL:HG12  | 1:Q:165:GLY:HA3   | 1.99                     | 0.45              |
| 2:c:273:CYS:HB2   | 2:d:265:ASN:HA    | 1.98                     | 0.45              |
| 2:f:54:GLN:CG     | 3:AF:168:VAL:HG13 | 2.32                     | 0.45              |
| 2:f:273:CYS:HB2   | 2:g:265:ASN:HA    | 1.99                     | 0.45              |
| 2:k:258:ARG:HH12  | 2:m:140:ASN:HD21  | 1.64                     | 0.45              |
| 2:k:273:CYS:HB2   | 2:l:265:ASN:HA    | 1.99                     | 0.45              |
| 2:n:21:ARG:HA     | 2:n:21:ARG:HD2    | 1.74                     | 0.45              |
| 2:o:80:GLN:NE2    | 3:AJ:125:ASN:ND2  | 2.65                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:273:CYS:HB2   | 2:s:265:ASN:HA    | 1.99                     | 0.45              |
| 2:x:33:GLU:O      | 2:y:170:ILE:HD13  | 2.16                     | 0.45              |
| 3:1:28:ASN:ND2    | 3:6:43:ASP:OD1    | 2.49                     | 0.45              |
| 3:ZC:145:ASN:HA   | 4:ZH:352:ASN:ND2  | 2.28                     | 0.45              |
| 4:ZH:233:ASN:HD21 | 4:ZH:237:ILE:HB   | 1.82                     | 0.45              |
| 4:ZJ:74:ASP:O     | 4:ZJ:359:GLY:N    | 2.36                     | 0.45              |
| 4:ZK:204:LYS:HZ2  | 4:ZK:207:GLU:HG3  | 1.82                     | 0.45              |
| 4:ZP:373:VAL:O    | 4:ZP:375:MET:N    | 2.50                     | 0.45              |
| 4:ZS:34:SER:HB3   | 4:ZS:366:VAL:HG22 | 1.98                     | 0.45              |
| 4:ZU:10:LEU:HD23  | 4:ZU:10:LEU:HA    | 1.84                     | 0.45              |
| 4:Za:352:ASN:O    | 4:Za:352:ASN:OD1  | 2.35                     | 0.45              |
| 4:Zc:210:VAL:HB   | 4:Zc:228:THR:HG22 | 1.99                     | 0.45              |
| 5:AA:26:LEU:HD22  | 3:AF:242:ILE:CG2  | 2.36                     | 0.45              |
| 3:AI:174:ASN:HA   | 3:AI:206:PRO:HD3  | 1.99                     | 0.45              |
| 3:AJ:130:THR:OG1  | 3:AJ:131:ALA:N    | 2.50                     | 0.45              |
| 6:AW:235:LEU:HD13 | 6:AX:244:ARG:HH22 | 1.81                     | 0.45              |
| 7:Ab:66:GLY:O     | 7:Ab:67:PRO:C     | 2.59                     | 0.45              |
| 8:At:66:PHE:O     | 11:A6:4:ARG:HG3   | 2.17                     | 0.45              |
| 6:UI:98:LEU:HD11  | 6:UI:143:THR:O    | 2.16                     | 0.45              |
| 6:UL:98:LEU:HD12  | 6:UL:146:THR:HG1  | 1.78                     | 0.45              |
| 6:UO:73:MET:HE1   | 6:UO:99:ARG:HD2   | 1.95                     | 0.45              |
| 6:UO:73:MET:HE3   | 6:UO:99:ARG:CD    | 2.41                     | 0.45              |
| 6:WA:217:GLY:HA3  | 6:WW:190:GLN:HG2  | 1.98                     | 0.45              |
| 6:WC:190:GLN:C    | 6:WC:192:SER:H    | 2.23                     | 0.45              |
| 6:WO:135:ALA:O    | 6:WO:139:GLU:HG2  | 2.16                     | 0.45              |
| 6:WO:219:LEU:HG   | 6:WO:221:THR:H    | 1.82                     | 0.45              |
| 6:WP:190:GLN:C    | 6:WP:192:SER:H    | 2.24                     | 0.45              |
| 6:BL:316:LEU:HD12 | 6:BL:316:LEU:HA   | 1.77                     | 0.45              |
| 6:BU:235:LEU:HD13 | 6:BV:244:ARG:HH22 | 1.81                     | 0.45              |
| 1:E:142:ASN:ND2   | 1:F:207:TYR:OH    | 2.28                     | 0.45              |
| 1:E:150:VAL:HG12  | 1:E:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:F:150:VAL:HG12  | 1:F:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:H:150:VAL:HG12  | 1:H:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:I:150:VAL:HG12  | 1:I:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:J:150:VAL:HG12  | 1:J:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:K:68:ASP:OD1    | 2:j:64:ASN:ND2    | 2.48                     | 0.45              |
| 1:N:150:VAL:HG12  | 1:N:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:O:112:TYR:HD2   | 1:O:113:LEU:HD13  | 1.80                     | 0.45              |
| 1:O:150:VAL:HG12  | 1:O:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:P:112:TYR:HD2   | 1:P:113:LEU:HD13  | 1.80                     | 0.45              |
| 1:P:166:GLU:HB2   | 1:Q:35:THR:CG2    | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:150:VAL:HG12  | 1:R:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:S:142:ASN:ND2   | 1:T:207:TYR:OH    | 2.28                     | 0.45              |
| 1:U:50:SER:CB     | 2:r:32:ARG:NH1    | 2.77                     | 0.45              |
| 2:a:136:LEU:HD13  | 2:z:129:VAL:HG21  | 1.98                     | 0.45              |
| 2:b:33:GLU:O      | 2:c:170:ILE:HD13  | 2.16                     | 0.45              |
| 2:c:21:ARG:HA     | 2:c:21:ARG:HD2    | 1.74                     | 0.45              |
| 2:f:319:LEU:HD21  | 2:g:264:MET:HE1   | 1.98                     | 0.45              |
| 2:h:47:GLY:H      | 2:h:83:ASN:HD22   | 1.64                     | 0.45              |
| 2:i:47:GLY:H      | 2:i:83:ASN:HD22   | 1.64                     | 0.45              |
| 2:i:273:CYS:HB2   | 2:j:265:ASN:HA    | 1.99                     | 0.45              |
| 2:j:47:GLY:H      | 2:j:83:ASN:HD22   | 1.64                     | 0.45              |
| 2:j:273:CYS:HB2   | 2:k:265:ASN:HA    | 1.99                     | 0.45              |
| 2:l:346:MET:HE2   | 2:n:142:LEU:HD11  | 1.95                     | 0.45              |
| 2:m:21:ARG:HA     | 2:m:21:ARG:HD2    | 1.74                     | 0.45              |
| 2:p:56:PRO:CD     | 2:q:79:MET:HG2    | 2.45                     | 0.45              |
| 2:v:129:VAL:HG21  | 2:w:136:LEU:HD13  | 1.97                     | 0.45              |
| 2:y:129:VAL:HG21  | 2:z:136:LEU:HD13  | 1.98                     | 0.45              |
| 3:0:21:VAL:HG21   | 3:0:39:ALA:HB2    | 1.99                     | 0.45              |
| 3:0:226:VAL:HB    | 3:ZB:2:ILE:CD1    | 2.39                     | 0.45              |
| 3:2:10:THR:OG1    | 3:2:71:GLY:HA3    | 2.17                     | 0.45              |
| 3:2:141:THR:C     | 3:2:142:ILE:HD13  | 2.41                     | 0.45              |
| 3:ZD:238:ARG:HD3  | 3:ZD:238:ARG:HA   | 1.46                     | 0.45              |
| 4:ZM:235:ASN:ND2  | 4:ZS:189:SER:OG   | 2.49                     | 0.45              |
| 4:ZN:99:GLN:HG2   | 4:ZN:361:LEU:HD11 | 1.98                     | 0.45              |
| 4:ZP:382:TYR:HE1  | 4:ZU:399:LEU:CD1  | 2.30                     | 0.45              |
| 4:ZR:178:TYR:HA   | 4:ZR:201:VAL:HG22 | 1.98                     | 0.45              |
| 4:ZR:204:LYS:HG2  | 4:ZR:205:ASP:N    | 2.32                     | 0.45              |
| 4:ZR:288:ASP:N    | 4:ZR:305:SER:OG   | 2.43                     | 0.45              |
| 4:ZS:86:VAL:HG23  | 4:ZS:117:THR:HG21 | 1.98                     | 0.45              |
| 4:ZV:102:LEU:HD21 | 4:ZV:106:ARG:HA   | 1.98                     | 0.45              |
| 4:ZV:382:TYR:CE1  | 4:Za:395:ILE:HG23 | 2.52                     | 0.45              |
| 4:ZW:10:LEU:HD21  | 4:Zb:399:LEU:HD21 | 1.97                     | 0.45              |
| 4:Zd:269:GLN:HG2  | 4:Zd:270:ASN:H    | 1.82                     | 0.45              |
| 4:Ze:107:ASN:HD22 | 4:Ze:138:THR:HG22 | 1.82                     | 0.45              |
| 4:Zh:154:MET:HG2  | 4:Zh:279:THR:HG22 | 1.98                     | 0.45              |
| 5:AB:40:ALA:HB1   | 12:BC:34:VAL:HG21 | 1.99                     | 0.45              |
| 5:AB:107:VAL:HG22 | 5:AB:113:LEU:CD2  | 2.46                     | 0.45              |
| 5:AC:70:GLN:HB3   | 3:AN:6:TRP:CE3    | 2.43                     | 0.45              |
| 5:AD:10:GLY:O     | 5:AD:14:GLN:HG2   | 2.16                     | 0.45              |
| 6:AS:244:ARG:HH22 | 6:BX:235:LEU:HD13 | 1.81                     | 0.45              |
| 6:Ap:235:LEU:HD13 | 6:AO:244:ARG:HH22 | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:At:158:PRO:HD2  | 8:At:162:ASN:ND2  | 2.32                     | 0.45              |
| 9:Aw:187:PHE:CE1  | 9:Ax:224:MET:HB2  | 2.52                     | 0.45              |
| 9:Ay:142:THR:HG21 | 9:Ay:170:LEU:HD11 | 1.97                     | 0.45              |
| 6:UN:73:MET:HE3   | 6:UN:99:ARG:CD    | 2.41                     | 0.45              |
| 6:WB:112:GLY:HA2  | 6:WB:139:GLU:OE1  | 2.17                     | 0.45              |
| 6:WB:181:GLU:O    | 6:WB:182:PRO:C    | 2.60                     | 0.45              |
| 6:WD:145:GLU:C    | 6:WD:147:LEU:N    | 2.74                     | 0.45              |
| 6:WG:190:GLN:HG3  | 6:WH:217:GLY:HA3  | 1.99                     | 0.45              |
| 6:WL:181:GLU:O    | 6:WL:182:PRO:C    | 2.60                     | 0.45              |
| 6:WQ:214:ASP:OD1  | 6:WQ:218:HIS:N    | 2.49                     | 0.45              |
| 6:WV:181:GLU:O    | 6:WV:182:PRO:C    | 2.60                     | 0.45              |
| 1:A:63:GLN:OE1    | 2:y:131:SER:CB    | 2.65                     | 0.45              |
| 1:C:63:GLN:OE1    | 2:a:131:SER:CB    | 2.65                     | 0.45              |
| 1:D:90:LYS:HA     | 1:E:142:ASN:HA    | 1.98                     | 0.45              |
| 1:E:63:GLN:OE1    | 2:c:131:SER:CB    | 2.65                     | 0.45              |
| 1:M:150:VAL:HG12  | 1:M:165:GLY:HA3   | 1.99                     | 0.45              |
| 1:Q:50:SER:HB3    | 2:n:32:ARG:HH11   | 1.81                     | 0.45              |
| 1:T:47:ALA:HB1    | 2:q:178:GLN:HG3   | 1.96                     | 0.45              |
| 1:W:68:ASP:OD1    | 2:v:64:ASN:ND2    | 2.47                     | 0.45              |
| 2:e:273:CYS:HB2   | 2:f:265:ASN:HA    | 1.99                     | 0.45              |
| 2:k:47:GLY:H      | 2:k:83:ASN:HD22   | 1.64                     | 0.45              |
| 2:l:346:MET:HE3   | 2:n:142:LEU:CD1   | 2.42                     | 0.45              |
| 2:o:346:MET:HE3   | 2:q:142:LEU:CD1   | 2.42                     | 0.45              |
| 2:r:192:GLU:H     | 2:r:192:GLU:HG3   | 1.52                     | 0.45              |
| 3:8:154:ASP:OD1   | 3:8:154:ASP:N     | 2.49                     | 0.45              |
| 3:ZC:7:ILE:HG23   | 3:ZC:71:GLY:HA2   | 1.97                     | 0.45              |
| 3:ZC:88:GLN:NE2   | 3:ZC:218:TYR:OH   | 2.50                     | 0.45              |
| 3:ZE:257:LEU:HA   | 3:ZE:257:LEU:HD23 | 1.83                     | 0.45              |
| 4:ZF:71:ARG:HB2   | 4:ZF:74:ASP:OD2   | 2.17                     | 0.45              |
| 4:ZP:73:LEU:HD21  | 4:ZP:292:TYR:CE1  | 2.52                     | 0.45              |
| 4:ZQ:373:VAL:O    | 4:ZQ:377:VAL:HG23 | 2.17                     | 0.45              |
| 4:ZR:111:MET:N    | 4:ZR:111:MET:SD   | 2.90                     | 0.45              |
| 4:ZS:105:ASN:HB2  | 4:ZS:107:ASN:ND2  | 2.30                     | 0.45              |
| 4:ZV:391:THR:O    | 4:ZV:395:ILE:HG12 | 2.16                     | 0.45              |
| 4:ZW:104:GLU:OE2  | 4:ZW:104:GLU:N    | 2.35                     | 0.45              |
| 4:ZY:337:THR:HG23 | 4:ZY:339:ALA:H    | 1.82                     | 0.45              |
| 4:ZZ:112:GLN:OE1  | 4:ZZ:112:GLN:N    | 2.50                     | 0.45              |
| 4:Zd:93:PHE:HB3   | 4:Zd:333:VAL:HG13 | 1.97                     | 0.45              |
| 4:Ze:80:ASN:OD1   | 4:Ze:81:GLY:N     | 2.50                     | 0.45              |
| 5:AC:10:GLY:O     | 5:AC:14:GLN:HG2   | 2.17                     | 0.45              |
| 5:AC:47:ASP:O     | 6:BM:324:ASN:ND2  | 2.49                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AC:49:LEU:HG    | 6:BM:322:PRO:HD2   | 1.99                     | 0.45              |
| 5:AD:35:ARG:O     | 5:AD:173:ARG:NH2   | 2.37                     | 0.45              |
| 3:AI:175:LEU:HD12 | 3:AI:206:PRO:HB3   | 1.97                     | 0.45              |
| 3:AJ:234:ILE:O    | 3:AJ:238:ARG:HG2   | 2.17                     | 0.45              |
| 3:AM:43:ASP:HA    | 3:AM:72:VAL:HA     | 1.99                     | 0.45              |
| 6:AV:278:THR:CG2  | 10:A3:21:ALA:HB3   | 2.31                     | 0.45              |
| 6:AQ:235:LEU:HD13 | 6:BR:244:ARG:HH22  | 1.81                     | 0.45              |
| 7:As:6:VAL:O      | 7:As:9:MET:HG3     | 2.16                     | 0.45              |
| 8:At:248:PHE:HB2  | 6:WK:164:LEU:HD12  | 1.93                     | 0.45              |
| 9:Ay:159:LEU:O    | 6:WI:165:PHE:HB2   | 2.17                     | 0.45              |
| 10:Az:79:SER:HB2  | 10:A5:91:LYS:CE    | 2.47                     | 0.45              |
| 10:A4:77:LYS:CE   | 11:A0:13:GLN:NE2   | 2.61                     | 0.45              |
| 6:UL:80:ALA:N     | 6:UL:85:ALA:O      | 2.49                     | 0.45              |
| 12:BA:37:PRO:HD3  | 12:BF:51:VAL:HG13  | 1.99                     | 0.45              |
| 6:WB:167:ARG:C    | 6:WB:169:GLN:H     | 2.25                     | 0.45              |
| 6:WS:219:LEU:HG   | 6:WS:221:THR:H     | 1.82                     | 0.45              |
| 12:BF:128:LYS:O   | 12:BF:131:THR:HG22 | 2.17                     | 0.45              |
| 1:A:130:ASN:HD22  | 1:Z:102:THR:HG23   | 1.82                     | 0.45              |
| 1:B:63:GLN:OE1    | 2:z:131:SER:CB     | 2.65                     | 0.45              |
| 1:B:102:THR:HG23  | 1:C:130:ASN:HD22   | 1.82                     | 0.45              |
| 1:C:90:LYS:HA     | 1:D:142:ASN:HA     | 1.98                     | 0.45              |
| 1:D:63:GLN:OE1    | 2:b:131:SER:CB     | 2.65                     | 0.45              |
| 1:D:150:VAL:HG12  | 1:D:165:GLY:HA3    | 1.99                     | 0.45              |
| 1:E:102:THR:HG23  | 1:F:130:ASN:HD22   | 1.82                     | 0.45              |
| 1:I:181:SER:HB2   | 1:J:31:VAL:CG1     | 2.45                     | 0.45              |
| 1:K:150:VAL:HG12  | 1:K:165:GLY:HA3    | 1.99                     | 0.45              |
| 1:R:62:TYR:HD1    | 2:p:129:VAL:HG11   | 1.62                     | 0.45              |
| 1:S:181:SER:HB2   | 1:T:31:VAL:CG1     | 2.45                     | 0.45              |
| 1:T:62:TYR:CE1    | 2:r:129:VAL:HG13   | 2.48                     | 0.45              |
| 1:W:150:VAL:HG12  | 1:W:165:GLY:HA3    | 1.99                     | 0.45              |
| 1:Y:150:VAL:HG12  | 1:Y:165:GLY:HA3    | 1.99                     | 0.45              |
| 1:Z:63:GLN:OE1    | 2:x:131:SER:CB     | 2.65                     | 0.45              |
| 2:i:188:GLN:HE21  | 2:i:188:GLN:HB2    | 1.63                     | 0.45              |
| 2:j:56:PRO:CD     | 2:k:79:MET:HG2     | 2.45                     | 0.45              |
| 2:l:47:GLY:H      | 2:l:83:ASN:HD22    | 1.64                     | 0.45              |
| 2:o:47:GLY:H      | 2:o:83:ASN:HD22    | 1.64                     | 0.45              |
| 2:q:346:MET:HE2   | 2:s:142:LEU:HD11   | 1.95                     | 0.45              |
| 2:r:258:ARG:HH12  | 2:t:140:ASN:HD21   | 1.64                     | 0.45              |
| 2:w:47:GLY:H      | 2:w:83:ASN:HD22    | 1.64                     | 0.45              |
| 3:0:49:ILE:HB     | 3:0:66:LEU:HG      | 1.98                     | 0.45              |
| 3:0:184:LEU:HB3   | 3:0:192:TYR:HB3    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:1:MET:HB3     | 3:AF:29:VAL:HG13  | 1.98                     | 0.45              |
| 3:2:55:GLN:CG     | 5:AA:142:THR:HG21 | 2.47                     | 0.45              |
| 3:6:16:GLN:O      | 3:6:17:THR:C      | 2.58                     | 0.45              |
| 3:6:138:PRO:O     | 3:6:139:ALA:HB2   | 2.16                     | 0.45              |
| 3:6:254:LEU:HD21  | 3:AJ:226:VAL:HG21 | 1.97                     | 0.45              |
| 3:7:1:MET:HB2     | 3:AK:226:VAL:HG21 | 1.98                     | 0.45              |
| 3:ZB:20:ASP:OD1   | 4:ZG:2:SER:HB2    | 2.17                     | 0.45              |
| 3:ZD:66:LEU:HD23  | 3:ZD:66:LEU:HA    | 1.83                     | 0.45              |
| 4:ZF:396:LEU:HD23 | 4:ZF:396:LEU:HA   | 1.84                     | 0.45              |
| 4:ZJ:233:ASN:ND2  | 4:ZJ:235:ASN:H    | 2.14                     | 0.45              |
| 4:ZL:95:SER:OG    | 4:ZL:332:ASN:O    | 2.25                     | 0.45              |
| 4:ZQ:233:ASN:ND2  | 4:ZQ:239:GLU:HB3  | 2.31                     | 0.45              |
| 4:Za:139:ILE:HA   | 4:Za:312:LEU:HD22 | 1.98                     | 0.45              |
| 5:AB:51:LEU:O     | 5:AB:53:THR:OG1   | 2.27                     | 0.45              |
| 5:AB:71:LEU:CB    | 3:AM:70:THR:HG22  | 2.47                     | 0.45              |
| 5:AB:220:MET:SD   | 3:AG:246:ALA:CB   | 3.05                     | 0.45              |
| 5:AE:55:THR:HG22  | 12:BF:30:ASN:HD21 | 1.82                     | 0.45              |
| 3:AG:35:LYS:HG3   | 3:AG:81:HIS:ND1   | 2.31                     | 0.45              |
| 3:AI:6:TRP:NE1    | 12:BD:77:VAL:CB   | 2.75                     | 0.45              |
| 7:Ab:10:GLY:O     | 7:Ab:14:MET:HG2   | 2.16                     | 0.45              |
| 6:Ae:372:ILE:HD12 | 10:A2:3:ALA:C     | 2.42                     | 0.45              |
| 6:Ag:295:SER:HB3  | 11:A8:72:HIS:CA   | 2.45                     | 0.45              |
| 6:Am:235:LEU:HD13 | 6:An:244:ARG:HH22 | 1.81                     | 0.45              |
| 7:Ar:37:ILE:HA    | 7:As:44:ILE:HD11  | 1.99                     | 0.45              |
| 8:At:123:PRO:HB2  | 8:At:126:ALA:HB3  | 1.99                     | 0.45              |
| 9:Ay:152:ARG:NH2  | 6:WJ:164:LEU:O    | 2.50                     | 0.45              |
| 10:Az:79:SER:HB2  | 10:A5:91:LYS:HE3  | 1.99                     | 0.45              |
| 10:A5:59:PHE:HZ   | 12:BF:4:LEU:HD21  | 1.81                     | 0.45              |
| 6:UL:164:LEU:HD22 | 6:UL:164:LEU:H    | 1.82                     | 0.45              |
| 6:UM:88:VAL:O     | 6:UM:89:PRO:C     | 2.60                     | 0.45              |
| 6:UO:94:HIS:HB2   | 6:UO:146:THR:HG21 | 1.97                     | 0.45              |
| 6:WF:124:SER:O    | 6:WF:125:GLN:C    | 2.58                     | 0.45              |
| 6:WH:135:ALA:O    | 6:WH:139:GLU:HG2  | 2.16                     | 0.45              |
| 6:WN:200:SER:C    | 6:WO:173:SER:OG   | 2.60                     | 0.45              |
| 6:WT:159:MET:HE3  | 6:WT:159:MET:HB2  | 1.83                     | 0.45              |
| 6:WW:181:GLU:O    | 6:WW:182:PRO:C    | 2.60                     | 0.45              |
| 6:WW:192:SER:O    | 6:WW:195:VAL:HB   | 2.17                     | 0.45              |
| 1:A:166:GLU:HB2   | 1:B:35:THR:CG2    | 2.30                     | 0.44              |
| 1:C:150:VAL:HG12  | 1:C:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:F:63:GLN:OE1    | 2:d:131:SER:CB    | 2.65                     | 0.44              |
| 1:G:63:GLN:OE1    | 2:e:131:SER:CB    | 2.65                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:102:THR:HG23  | 1:H:130:ASN:HD22  | 1.83                     | 0.44              |
| 1:I:102:THR:HG23  | 1:J:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:I:126:ALA:HB3   | 1:K:232:MET:HE1   | 1.99                     | 0.44              |
| 1:J:68:ASP:OD1    | 2:i:64:ASN:ND2    | 2.48                     | 0.44              |
| 1:K:47:ALA:HB1    | 2:h:178:GLN:HG3   | 1.97                     | 0.44              |
| 1:N:90:LYS:HA     | 1:O:142:ASN:HA    | 1.98                     | 0.44              |
| 1:O:142:ASN:ND2   | 1:P:207:TYR:OH    | 2.28                     | 0.44              |
| 1:S:65:LEU:CG     | 2:r:65:MET:HG3    | 2.39                     | 0.44              |
| 1:S:150:VAL:HG12  | 1:S:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:T:150:VAL:HG12  | 1:T:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:U:47:ALA:HB1    | 2:r:178:GLN:HG3   | 1.96                     | 0.44              |
| 1:V:150:VAL:HG12  | 1:V:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:X:102:THR:HG23  | 1:Y:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:X:150:VAL:HG12  | 1:X:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:Y:63:GLN:OE1    | 2:w:131:SER:CB    | 2.65                     | 0.44              |
| 2:a:56:PRO:CD     | 2:b:79:MET:HG2    | 2.45                     | 0.44              |
| 2:a:129:VAL:HG21  | 2:b:136:LEU:HD13  | 1.98                     | 0.44              |
| 2:f:47:GLY:H      | 2:f:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:m:47:GLY:H      | 2:m:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:n:47:GLY:H      | 2:n:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:r:56:PRO:CD     | 2:s:79:MET:HG2    | 2.45                     | 0.44              |
| 2:s:56:PRO:CD     | 2:t:79:MET:HG2    | 2.45                     | 0.44              |
| 2:w:130:ASP:OD1   | 2:w:130:ASP:N     | 2.47                     | 0.44              |
| 2:x:129:VAL:HG21  | 2:y:136:LEU:HD13  | 1.98                     | 0.44              |
| 2:y:33:GLU:O      | 2:z:170:ILE:HD13  | 2.16                     | 0.44              |
| 3:1:52:PRO:CB     | 12:BF:87:ALA:O    | 2.66                     | 0.44              |
| 3:7:1:MET:HE2     | 3:AK:29:VAL:HG11  | 1.98                     | 0.44              |
| 3:8:195:THR:O     | 3:8:196:GLN:C     | 2.60                     | 0.44              |
| 3:9:140:ILE:HG23  | 3:9:171:GLY:HA3   | 1.99                     | 0.44              |
| 3:ZB:8:ALA:HB1    | 3:ZB:247:VAL:HG23 | 1.99                     | 0.44              |
| 3:ZB:184:LEU:HB3  | 3:ZB:192:TYR:HB3  | 1.99                     | 0.44              |
| 3:ZD:49:ILE:HB    | 3:ZD:66:LEU:HB3   | 1.99                     | 0.44              |
| 3:ZD:91:ASN:HB2   | 3:ZD:94:ASP:OD2   | 2.17                     | 0.44              |
| 3:ZD:208:LEU:HD13 | 3:ZD:208:LEU:HA   | 1.80                     | 0.44              |
| 4:ZG:230:LEU:HB3  | 4:ZG:238:LEU:HD11 | 1.98                     | 0.44              |
| 4:ZI:2:SER:O      | 4:ZI:2:SER:OG     | 2.31                     | 0.44              |
| 4:ZI:352:ASN:OD1  | 4:ZI:352:ASN:N    | 2.49                     | 0.44              |
| 4:ZO:180:LYS:HB3  | 4:ZO:200:PHE:HB2  | 1.98                     | 0.44              |
| 4:ZQ:214:ASP:OD2  | 4:ZQ:214:ASP:N    | 2.42                     | 0.44              |
| 4:ZU:3:PHE:HE2    | 4:ZU:396:LEU:HD12 | 1.82                     | 0.44              |
| 4:ZZ:281:GLN:OE1  | 4:ZZ:281:GLN:N    | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zc:69:THR:HG21  | 4:Zc:361:LEU:HD12 | 1.99                     | 0.44              |
| 5:AD:249:SER:OG   | 12:BD:117:GLU:OE1 | 2.35                     | 0.44              |
| 3:AG:189:GLU:O    | 3:AG:191:LEU:HG   | 2.17                     | 0.44              |
| 3:AJ:200:ALA:HB1  | 3:AJ:201:PRO:CD   | 2.47                     | 0.44              |
| 3:AL:1:MET:HE3    | 3:AL:1:MET:HB2    | 1.73                     | 0.44              |
| 3:AL:107:LEU:HB2  | 3:AL:111:THR:O    | 2.17                     | 0.44              |
| 3:AN:47:GLN:HG2   | 3:AN:68:ILE:HB    | 1.99                     | 0.44              |
| 6:AZ:236:LYS:CE   | 6:UP:167:ARG:HH11 | 2.29                     | 0.44              |
| 7:Aq:84:LEU:HD22  | 9:Aw:185:ILE:HG23 | 2.00                     | 0.44              |
| 9:Av:57:ILE:O     | 9:Av:61:MET:HB2   | 2.17                     | 0.44              |
| 9:Aw:143:ARG:HA   | 6:WW:165:PHE:HA   | 1.99                     | 0.44              |
| 9:Ay:221:PHE:O    | 9:Ay:224:MET:HE2  | 2.17                     | 0.44              |
| 6:UI:164:LEU:HD22 | 6:UI:164:LEU:H    | 1.82                     | 0.44              |
| 6:UK:94:HIS:HB2   | 6:UK:146:THR:HG21 | 1.97                     | 0.44              |
| 6:UK:164:LEU:H    | 6:UK:164:LEU:HD22 | 1.82                     | 0.44              |
| 6:UM:73:MET:HE1   | 6:UM:99:ARG:HD2   | 1.95                     | 0.44              |
| 6:UM:98:LEU:HD11  | 6:UM:143:THR:O    | 2.17                     | 0.44              |
| 6:WP:181:GLU:O    | 6:WP:182:PRO:C    | 2.60                     | 0.44              |
| 6:WP:186:LEU:HA   | 6:WP:190:GLN:OE1  | 2.17                     | 0.44              |
| 6:WT:181:GLU:O    | 6:WT:182:PRO:C    | 2.60                     | 0.44              |
| 1:A:150:VAL:HG12  | 1:A:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:G:181:SER:HB2   | 1:H:31:VAL:CG1    | 2.45                     | 0.44              |
| 1:H:63:GLN:OE1    | 2:f:131:SER:CB    | 2.65                     | 0.44              |
| 1:I:63:GLN:OE1    | 2:g:131:SER:CB    | 2.65                     | 0.44              |
| 1:M:90:LYS:HA     | 1:N:142:ASN:HA    | 1.98                     | 0.44              |
| 1:S:102:THR:HG23  | 1:T:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:U:150:VAL:HG12  | 1:U:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:V:47:ALA:HB1    | 2:s:178:GLN:HG3   | 1.96                     | 0.44              |
| 1:W:90:LYS:HA     | 1:X:142:ASN:HA    | 1.98                     | 0.44              |
| 1:X:47:ALA:HB1    | 2:u:178:GLN:HG3   | 1.96                     | 0.44              |
| 1:X:63:GLN:OE1    | 2:v:131:SER:CB    | 2.65                     | 0.44              |
| 2:b:129:VAL:HG21  | 2:c:136:LEU:HD13  | 1.98                     | 0.44              |
| 2:e:80:GLN:HE22   | 3:AL:106:MET:HE2  | 1.81                     | 0.44              |
| 2:t:319:LEU:HD21  | 2:u:264:MET:HE1   | 1.98                     | 0.44              |
| 2:v:47:GLY:H      | 2:v:83:ASN:HD22   | 1.64                     | 0.44              |
| 3:1:231:VAL:HG11  | 3:7:9:LYS:HB2     | 1.99                     | 0.44              |
| 3:5:208:LEU:C     | 3:5:210:GLY:H     | 2.25                     | 0.44              |
| 3:7:167:PRO:HG3   | 4:ZI:338:GLN:OE1  | 2.15                     | 0.44              |
| 3:ZE:44:LEU:HD23  | 3:ZE:44:LEU:HA    | 1.82                     | 0.44              |
| 4:ZG:107:ASN:O    | 4:ZG:109:VAL:HG13 | 2.16                     | 0.44              |
| 4:ZG:147:LYS:HB2  | 4:ZG:147:LYS:HE2  | 1.66                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZH:93:PHE:HB3   | 4:ZH:333:VAL:HG13 | 2.00                     | 0.44              |
| 4:ZI:75:VAL:HG11  | 4:ZI:356:LEU:HD13 | 1.98                     | 0.44              |
| 4:ZL:380:ARG:NE   | 4:ZR:393:ASP:OD1  | 2.50                     | 0.44              |
| 4:ZN:159:ASN:ND2  | 4:ZN:162:ASP:OD2  | 2.49                     | 0.44              |
| 4:ZR:269:GLN:HG2  | 4:ZX:190:GLN:HA   | 2.00                     | 0.44              |
| 4:ZZ:99:GLN:HE21  | 4:ZZ:111:MET:HE3  | 1.81                     | 0.44              |
| 4:Ze:156:ILE:HD11 | 4:Ze:180:LYS:HE2  | 1.99                     | 0.44              |
| 5:AC:225:ARG:HA   | 5:AC:225:ARG:HD3  | 1.67                     | 0.44              |
| 3:AF:22:ILE:HG21  | 3:AF:233:MET:HG2  | 1.99                     | 0.44              |
| 3:AG:47:GLN:O     | 3:AG:67:GLN:HA    | 2.17                     | 0.44              |
| 3:AG:62:LEU:HD12  | 12:BC:35:THR:CG2  | 2.47                     | 0.44              |
| 7:Ab:83:ASN:O     | 7:Ab:84:LEU:C     | 2.60                     | 0.44              |
| 9:Av:52:THR:HG22  | 10:A1:91:LYS:CE   | 2.47                     | 0.44              |
| 9:Av:204:LEU:HD12 | 9:Av:214:PRO:HB3  | 1.99                     | 0.44              |
| 9:Aw:66:ARG:HB2   | 9:Aw:178:GLU:OE1  | 2.17                     | 0.44              |
| 9:Ay:86:ASN:ND2   | 10:A4:103:GLN:HA  | 2.32                     | 0.44              |
| 11:A6:49:LEU:O    | 11:A6:53:MET:HG2  | 2.17                     | 0.44              |
| 6:UI:55:PHE:O     | 6:UI:85:ALA:HA    | 2.18                     | 0.44              |
| 6:UI:73:MET:HE1   | 6:UI:99:ARG:HD2   | 1.95                     | 0.44              |
| 6:UM:75:ILE:HG21  | 6:UM:96:LEU:HD11  | 1.99                     | 0.44              |
| 6:UN:88:VAL:O     | 6:UN:89:PRO:C     | 2.60                     | 0.44              |
| 6:WF:114:GLU:HA   | 6:WF:117:ASP:HB2  | 1.99                     | 0.44              |
| 6:WF:200:SER:O    | 6:WG:158:ALA:HB2  | 2.16                     | 0.44              |
| 6:WI:145:GLU:C    | 6:WI:147:LEU:N    | 2.74                     | 0.44              |
| 6:WL:159:MET:HE3  | 6:WL:159:MET:HB2  | 1.69                     | 0.44              |
| 1:D:50:SER:HB3    | 2:a:32:ARG:HH11   | 1.81                     | 0.44              |
| 1:G:90:LYS:HA     | 1:H:142:ASN:HA    | 1.98                     | 0.44              |
| 1:J:47:ALA:HB1    | 2:g:178:GLN:HG3   | 1.96                     | 0.44              |
| 1:K:102:THR:HG23  | 1:L:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:K:136:GLY:CA    | 1:M:213:ILE:HG23  | 2.42                     | 0.44              |
| 1:Q:142:ASN:ND2   | 1:R:207:TYR:OH    | 2.28                     | 0.44              |
| 1:V:63:GLN:OE1    | 2:t:131:SER:CB    | 2.65                     | 0.44              |
| 1:W:63:GLN:OE1    | 2:u:131:SER:CB    | 2.65                     | 0.44              |
| 1:X:50:SER:HB3    | 2:u:32:ARG:HH11   | 1.81                     | 0.44              |
| 1:Y:90:LYS:HA     | 1:Z:142:ASN:HA    | 1.98                     | 0.44              |
| 1:Z:150:VAL:HG12  | 1:Z:165:GLY:HA3   | 1.99                     | 0.44              |
| 2:g:47:GLY:H      | 2:g:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:q:47:GLY:H      | 2:q:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:s:21:ARG:HA     | 2:s:21:ARG:HD2    | 1.74                     | 0.44              |
| 2:t:56:PRO:CD     | 2:u:79:MET:HG2    | 2.45                     | 0.44              |
| 3:4:9:LYS:HE3     | 3:AM:228:GLU:HG3  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:6:59:GLN:HE21   | 3:6:59:GLN:HB3    | 1.53                     | 0.44              |
| 3:8:85:ASN:HB3    | 4:ZJ:4:SER:HB2    | 1.98                     | 0.44              |
| 3:ZA:240:TYR:CD2  | 4:ZF:395:ILE:HG12 | 2.52                     | 0.44              |
| 3:ZD:76:ALA:HB1   | 4:ZI:47:LYS:NZ    | 2.33                     | 0.44              |
| 4:ZI:324:GLU:O    | 4:ZI:326:LEU:N    | 2.50                     | 0.44              |
| 4:ZK:126:PRO:HG2  | 4:ZK:310:GLN:HG3  | 2.00                     | 0.44              |
| 4:ZL:160:SER:HA   | 4:ZL:268:GLN:HE21 | 1.82                     | 0.44              |
| 4:ZL:367:ASP:HB3  | 4:ZL:370:LYS:CG   | 2.47                     | 0.44              |
| 4:ZR:182:GLY:O    | 4:ZR:197:ASN:HA   | 2.17                     | 0.44              |
| 4:ZT:29:THR:HG23  | 4:ZY:39:PHE:O     | 2.17                     | 0.44              |
| 4:ZV:16:ASN:HB2   | 4:ZV:39:PHE:HZ    | 1.83                     | 0.44              |
| 4:ZY:74:ASP:OD2   | 4:ZY:361:LEU:HD11 | 2.18                     | 0.44              |
| 4:ZZ:109:VAL:HG12 | 4:ZZ:115:GLN:HA   | 1.98                     | 0.44              |
| 4:Za:111:MET:HE2  | 4:Zf:56:GLY:HA3   | 1.99                     | 0.44              |
| 4:Zd:114:MET:HE3  | 4:Zd:114:MET:HB3  | 1.83                     | 0.44              |
| 5:AA:70:GLN:CB    | 3:AL:6:TRP:CB     | 2.87                     | 0.44              |
| 5:AB:87:TRP:HB2   | 5:AB:164:VAL:HG23 | 1.98                     | 0.44              |
| 5:AB:227:PHE:CB   | 3:AG:253:MET:HG2  | 2.46                     | 0.44              |
| 5:AD:14:GLN:HG3   | 5:AD:58:THR:HA    | 1.99                     | 0.44              |
| 3:AI:62:LEU:HG    | 12:BE:84:LEU:HD21 | 2.00                     | 0.44              |
| 3:AI:97:ILE:HD12  | 3:AI:116:ARG:HG2  | 1.98                     | 0.44              |
| 3:AM:154:ASP:O    | 3:AM:154:ASP:OD1  | 2.35                     | 0.44              |
| 6:AX:370:ARG:NH2  | 10:A3:14:LEU:HD11 | 2.32                     | 0.44              |
| 7:Aq:52:ILE:HD13  | 7:Aq:52:ILE:HA    | 1.83                     | 0.44              |
| 8:At:8:GLN:O      | 8:At:12:TRP:HD1   | 2.00                     | 0.44              |
| 8:At:75:MET:O     | 8:At:79:LEU:HG    | 2.17                     | 0.44              |
| 8:At:242:HIS:CG   | 6:WJ:125:GLN:HB2  | 2.52                     | 0.44              |
| 9:Au:51:LEU:HD21  | 10:Az:88:VAL:HG13 | 1.98                     | 0.44              |
| 9:Ax:147:LEU:HD21 | 9:Ax:165:VAL:HG11 | 1.99                     | 0.44              |
| 9:Ay:114:GLN:HB3  | 9:Ay:115:PRO:HD3  | 2.00                     | 0.44              |
| 6:UL:88:VAL:O     | 6:UL:89:PRO:C     | 2.60                     | 0.44              |
| 6:UO:55:PHE:O     | 6:UO:85:ALA:HA    | 2.18                     | 0.44              |
| 6:UO:98:LEU:HD11  | 6:UO:143:THR:O    | 2.17                     | 0.44              |
| 6:UP:164:LEU:H    | 6:UP:164:LEU:HD22 | 1.82                     | 0.44              |
| 6:WD:129:GLN:O    | 6:WD:130:VAL:C    | 2.60                     | 0.44              |
| 6:WE:181:GLU:O    | 6:WE:182:PRO:C    | 2.60                     | 0.44              |
| 6:WE:200:SER:O    | 6:WF:158:ALA:HB3  | 2.18                     | 0.44              |
| 6:WF:148:GLY:N    | 6:WG:215:GLN:O    | 2.39                     | 0.44              |
| 6:WN:181:GLU:O    | 6:WN:182:PRO:C    | 2.60                     | 0.44              |
| 6:WO:181:GLU:O    | 6:WO:182:PRO:C    | 2.60                     | 0.44              |
| 6:WR:181:GLU:O    | 6:WR:182:PRO:C    | 2.60                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WT:167:ARG:HG2  | 6:WT:168:GLU:N    | 2.31                     | 0.44              |
| 1:B:150:VAL:HG12  | 1:B:165:GLY:HA3   | 1.99                     | 0.44              |
| 1:D:126:ALA:HB3   | 1:F:232:MET:HE1   | 1.99                     | 0.44              |
| 1:D:166:GLU:HB2   | 1:E:35:THR:CG2    | 2.30                     | 0.44              |
| 1:E:126:ALA:HB3   | 1:G:232:MET:HE1   | 1.99                     | 0.44              |
| 1:J:63:GLN:OE1    | 2:h:131:SER:CB    | 2.65                     | 0.44              |
| 1:J:126:ALA:HB3   | 1:L:232:MET:HE1   | 2.00                     | 0.44              |
| 1:K:181:SER:HB2   | 1:L:31:VAL:CG1    | 2.45                     | 0.44              |
| 1:O:102:THR:HG23  | 1:P:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:Q:102:THR:HG23  | 1:R:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:U:63:GLN:OE1    | 2:s:131:SER:CB    | 2.65                     | 0.44              |
| 1:V:50:SER:CB     | 2:s:32:ARG:NH1    | 2.77                     | 0.44              |
| 1:V:102:THR:HG23  | 1:W:130:ASN:HD22  | 1.82                     | 0.44              |
| 2:e:319:LEU:HD21  | 2:f:264:MET:HE1   | 1.97                     | 0.44              |
| 2:i:56:PRO:CD     | 2:j:79:MET:HG2    | 2.45                     | 0.44              |
| 2:i:258:ARG:HH12  | 2:k:140:ASN:HD21  | 1.64                     | 0.44              |
| 2:i:346:MET:HE3   | 2:k:142:LEU:CD1   | 2.42                     | 0.44              |
| 2:u:56:PRO:CD     | 2:v:79:MET:HG2    | 2.45                     | 0.44              |
| 2:w:129:VAL:HG21  | 2:x:136:LEU:HD13  | 1.98                     | 0.44              |
| 2:x:47:GLY:H      | 2:x:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:z:47:GLY:H      | 2:z:83:ASN:HD22   | 1.64                     | 0.44              |
| 3:1:114:TYR:CD2   | 3:1:178:PHE:HZ    | 2.36                     | 0.44              |
| 3:1:254:LEU:O     | 3:1:258:THR:HG23  | 2.17                     | 0.44              |
| 3:3:10:THR:OG1    | 3:3:71:GLY:HA3    | 2.17                     | 0.44              |
| 3:4:1:MET:HE3     | 3:AH:226:VAL:HG21 | 1.99                     | 0.44              |
| 3:4:33:GLY:N      | 3:4:220:GLU:O     | 2.49                     | 0.44              |
| 3:7:51:GLN:HB3    | 3:7:54:ALA:HB2    | 1.99                     | 0.44              |
| 3:9:36:ARG:HH21   | 3:9:80:LEU:HD22   | 1.82                     | 0.44              |
| 3:ZE:208:LEU:HB3  | 3:ZE:209:ASN:H    | 1.61                     | 0.44              |
| 4:ZG:102:LEU:HD23 | 4:ZG:102:LEU:HA   | 1.84                     | 0.44              |
| 4:ZN:202:LYS:HZ3  | 4:ZN:203:THR:C    | 2.25                     | 0.44              |
| 4:ZN:202:LYS:HB2  | 4:ZN:208:TRP:CZ3  | 2.52                     | 0.44              |
| 4:ZO:139:ILE:HA   | 4:ZO:312:LEU:HD22 | 1.98                     | 0.44              |
| 4:ZP:83:PHE:O     | 4:ZP:94:TYR:HA    | 2.16                     | 0.44              |
| 4:ZP:195:ASP:OD2  | 4:ZP:216:SER:OG   | 2.25                     | 0.44              |
| 4:ZQ:288:ASP:O    | 4:ZQ:305:SER:N    | 2.50                     | 0.44              |
| 4:ZR:185:THR:OG1  | 4:Zc:133:ASN:ND2  | 2.50                     | 0.44              |
| 4:ZS:27:SER:O     | 4:ZS:364:SER:OG   | 2.34                     | 0.44              |
| 4:ZY:392:GLN:HA   | 4:ZY:395:ILE:HD12 | 1.99                     | 0.44              |
| 4:Zc:375:MET:SD   | 4:Zh:388:THR:HA   | 2.57                     | 0.44              |
| 4:Ze:10:LEU:HD11  | 4:Ze:382:TYR:CE1  | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:80:VAL:O     | 5:AB:103:GLY:HA3  | 2.17                     | 0.44              |
| 5:AB:206:LEU:HD22 | 3:AG:38:ARG:HH22  | 1.81                     | 0.44              |
| 5:AC:57:VAL:HB    | 12:BD:30:ASN:ND2  | 2.33                     | 0.44              |
| 5:AC:167:GLU:OE1  | 5:AC:167:GLU:N    | 2.50                     | 0.44              |
| 7:Ab:85:PRO:HB3   | 9:Av:241:GLN:HG3  | 2.00                     | 0.44              |
| 7:Aq:20:LEU:HD11  | 7:Aq:73:LEU:HD13  | 2.00                     | 0.44              |
| 9:Ax:140:ARG:HD3  | 6:WC:167:ARG:HE   | 1.82                     | 0.44              |
| 9:Ax:194:LEU:HD11 | 9:Ay:220:PRO:CG   | 2.42                     | 0.44              |
| 9:Ax:214:PRO:HG2  | 9:Ay:212:VAL:HG23 | 1.98                     | 0.44              |
| 10:A4:86:ILE:HD11 | 11:A9:133:VAL:HA  | 1.99                     | 0.44              |
| 10:A5:76:GLN:HE21 | 12:BA:123:LYS:HB2 | 1.82                     | 0.44              |
| 11:A7:51:LYS:O    | 11:A7:55:ARG:HG2  | 2.18                     | 0.44              |
| 6:Ul:103:GLN:NE2  | 6:WB:182:PRO:HB3  | 2.32                     | 0.44              |
| 6:UL:94:HIS:HB2   | 6:UL:146:THR:HG21 | 1.97                     | 0.44              |
| 6:WC:130:VAL:HG12 | 6:WC:134:ARG:HD2  | 1.99                     | 0.44              |
| 6:WI:181:GLU:O    | 6:WI:182:PRO:C    | 2.60                     | 0.44              |
| 6:WN:219:LEU:HG   | 6:WN:221:THR:H    | 1.82                     | 0.44              |
| 6:WP:196:HIS:CD2  | 6:WQ:219:LEU:HD13 | 2.52                     | 0.44              |
| 6:WW:134:ARG:HH21 | 6:WW:134:ARG:CB   | 2.30                     | 0.44              |
| 1:B:136:GLY:CA    | 1:D:213:ILE:HG23  | 2.42                     | 0.44              |
| 1:J:62:TYR:CE1    | 2:h:129:VAL:HG13  | 2.48                     | 0.44              |
| 1:J:142:ASN:ND2   | 1:K:207:TYR:OH    | 2.28                     | 0.44              |
| 1:M:102:THR:HG23  | 1:N:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:P:232:MET:HE3   | 1:P:232:MET:HB2   | 1.90                     | 0.44              |
| 1:Q:90:LYS:HA     | 1:R:142:ASN:HA    | 1.98                     | 0.44              |
| 1:Q:232:MET:HE3   | 1:Q:232:MET:HB2   | 1.90                     | 0.44              |
| 1:U:102:THR:HG23  | 1:V:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:U:136:GLY:CA    | 1:W:213:ILE:HG23  | 2.42                     | 0.44              |
| 1:V:68:ASP:OD1    | 2:u:64:ASN:ND2    | 2.47                     | 0.44              |
| 1:X:90:LYS:HA     | 1:Y:142:ASN:HA    | 1.98                     | 0.44              |
| 2:a:33:GLU:O      | 2:b:170:ILE:HD13  | 2.16                     | 0.44              |
| 2:a:47:GLY:H      | 2:a:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:d:47:GLY:H      | 2:d:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:e:78:ASN:OD1    | 2:e:78:ASN:N      | 2.51                     | 0.44              |
| 2:i:78:ASN:OD1    | 2:i:78:ASN:N      | 2.51                     | 0.44              |
| 2:q:56:PRO:CD     | 2:r:79:MET:HG2    | 2.45                     | 0.44              |
| 2:x:21:ARG:HA     | 2:x:21:ARG:HD2    | 1.74                     | 0.44              |
| 2:y:47:GLY:H      | 2:y:83:ASN:HD22   | 1.64                     | 0.44              |
| 3:6:26:LEU:HD11   | 3:6:233:MET:HE2   | 1.98                     | 0.44              |
| 3:6:184:LEU:HB3   | 3:6:192:TYR:HB3   | 1.99                     | 0.44              |
| 3:ZA:31:THR:HG22  | 4:ZF:39:PHE:CB    | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:ZC:46:TYR:HA     | 3:ZC:69:GLY:HA2    | 2.00                     | 0.44              |
| 4:ZG:181:LYS:HE2   | 4:ZR:129:GLN:HG2   | 2.00                     | 0.44              |
| 4:ZI:297:ASP:OD2   | 4:ZI:297:ASP:N     | 2.44                     | 0.44              |
| 4:ZN:271:THR:HG22  | 4:ZT:286:PRO:HB2   | 1.99                     | 0.44              |
| 4:ZP:22:ASN:HB2    | 4:ZU:5:GLN:HE21    | 1.82                     | 0.44              |
| 4:ZR:184:VAL:HG13  | 4:ZR:196:MET:HB2   | 1.98                     | 0.44              |
| 4:ZS:183:THR:HB    | 4:Zd:132:ALA:HA    | 2.00                     | 0.44              |
| 4:ZV:156:ILE:HG22  | 4:ZV:276:ILE:HG12  | 2.00                     | 0.44              |
| 4:ZX:188:ASP:HA    | 4:ZX:257:ALA:HB2   | 1.99                     | 0.44              |
| 4:ZZ:74:ASP:O      | 4:ZZ:359:GLY:N     | 2.50                     | 0.44              |
| 4:Zd:93:PHE:HB2    | 4:Zd:114:MET:HE1   | 1.98                     | 0.44              |
| 4:Zg:71:ARG:NH1    | 4:Zg:74:ASP:OD1    | 2.51                     | 0.44              |
| 5:AB:18:GLN:HG2    | 5:AB:223:ASN:HD21  | 1.82                     | 0.44              |
| 3:AJ:127:GLN:HE22  | 3:AJ:139:ALA:CB    | 2.28                     | 0.44              |
| 6:AY:294:ARG:HD2   | 11:A9:68:THR:CG2   | 2.48                     | 0.44              |
| 6:Ad:265:GLN:NE2   | 6:UN:218:HIS:NE2   | 2.66                     | 0.44              |
| 6:Ag:235:LEU:HD13  | 6:Ah:244:ARG:HH22  | 1.81                     | 0.44              |
| 9:Av:211:MET:HE1   | 9:Aw:210:MET:CE    | 2.48                     | 0.44              |
| 9:Ax:160:GLN:CA    | 6:WE:167:ARG:HG3   | 2.46                     | 0.44              |
| 10:A4:84:MET:SD    | 11:A0:134:LEU:HD21 | 2.58                     | 0.44              |
| 10:A5:59:PHE:CZ    | 12:BF:4:LEU:HD21   | 2.52                     | 0.44              |
| 11:A8:88:ARG:HH12  | 11:A8:108:GLN:HG3  | 1.82                     | 0.44              |
| 6:UK:80:ALA:N      | 6:UK:85:ALA:O      | 2.49                     | 0.44              |
| 6:UN:55:PHE:O      | 6:UN:85:ALA:HA     | 2.18                     | 0.44              |
| 6:UP:75:ILE:HG21   | 6:UP:96:LEU:HD11   | 2.00                     | 0.44              |
| 6:WB:142:ARG:O     | 6:WB:146:THR:HG23  | 2.17                     | 0.44              |
| 6:WH:181:GLU:O     | 6:WH:182:PRO:C     | 2.60                     | 0.44              |
| 6:WH:219:LEU:HG    | 6:WH:221:THR:H     | 1.82                     | 0.44              |
| 6:WS:168:GLU:O     | 6:WS:169:GLN:HB3   | 2.18                     | 0.44              |
| 6:WW:219:LEU:HG    | 6:WW:221:THR:H     | 1.82                     | 0.44              |
| 12:BE:119:LEU:HD23 | 12:BE:119:LEU:HA   | 1.67                     | 0.44              |
| 1:H:90:LYS:HA      | 1:I:142:ASN:HA     | 1.98                     | 0.44              |
| 1:H:126:ALA:HB3    | 1:J:232:MET:HE1    | 1.99                     | 0.44              |
| 1:I:50:SER:HB3     | 2:f:32:ARG:HH11    | 1.81                     | 0.44              |
| 1:K:63:GLN:OE1     | 2:i:131:SER:CB     | 2.65                     | 0.44              |
| 1:N:102:THR:HG23   | 1:O:130:ASN:HD22   | 1.82                     | 0.44              |
| 1:O:232:MET:HE3    | 1:O:232:MET:HB2    | 1.90                     | 0.44              |
| 1:P:50:SER:HB3     | 2:m:32:ARG:HH11    | 1.81                     | 0.44              |
| 1:R:102:THR:HG23   | 1:S:130:ASN:HD22   | 1.82                     | 0.44              |
| 1:T:102:THR:HG23   | 1:U:130:ASN:HD22   | 1.82                     | 0.44              |
| 2:c:78:ASN:CG      | 3:AG:145:ASN:HD21  | 2.24                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:f:21:ARG:HA     | 2:f:21:ARG:HD2    | 1.75                     | 0.44              |
| 3:1:238:ARG:O     | 3:1:242:ILE:HG12  | 2.17                     | 0.44              |
| 3:2:95:VAL:O      | 3:2:118:GLY:HA3   | 2.18                     | 0.44              |
| 3:3:167:PRO:HG3   | 3:ZE:196:GLN:HG2  | 2.00                     | 0.44              |
| 3:3:256:LYS:HG2   | 3:AM:241:GLU:HG2  | 1.99                     | 0.44              |
| 3:4:86:LEU:CD1    | 4:ZF:42:MET:HE1   | 2.42                     | 0.44              |
| 3:4:251:ASP:OD1   | 3:AM:238:ARG:NE   | 2.48                     | 0.44              |
| 3:5:95:VAL:O      | 3:5:118:GLY:HA3   | 2.18                     | 0.44              |
| 3:6:1:MET:HE3     | 3:AJ:29:VAL:HG11  | 1.99                     | 0.44              |
| 3:8:256:LYS:HD3   | 3:8:256:LYS:HA    | 1.77                     | 0.44              |
| 3:9:140:ILE:HD12  | 3:9:171:GLY:HA3   | 1.99                     | 0.44              |
| 3:ZA:77:THR:N     | 4:ZF:47:LYS:HD2   | 2.24                     | 0.44              |
| 3:ZB:233:MET:SD   | 4:ZG:388:THR:CA   | 3.02                     | 0.44              |
| 3:ZC:184:LEU:HB3  | 3:ZC:192:TYR:HB3  | 2.00                     | 0.44              |
| 3:ZD:175:LEU:HD12 | 3:ZD:206:PRO:HB3  | 1.99                     | 0.44              |
| 4:ZL:382:TYR:CD2  | 4:ZQ:395:ILE:HD13 | 2.53                     | 0.44              |
| 4:ZP:10:LEU:HD21  | 4:ZU:399:LEU:HD21 | 1.99                     | 0.44              |
| 4:ZP:71:ARG:NH1   | 4:ZP:74:ASP:OD1   | 2.51                     | 0.44              |
| 4:ZP:346:GLY:HA3  | 4:ZP:353:PHE:CE2  | 2.53                     | 0.44              |
| 4:ZQ:27:SER:OG    | 4:ZV:381:ASN:CG   | 2.60                     | 0.44              |
| 4:ZR:316:VAL:HG21 | 4:ZR:345:LEU:HD23 | 1.98                     | 0.44              |
| 4:ZS:181:LYS:CD   | 4:Zd:129:GLN:NE2  | 2.81                     | 0.44              |
| 4:ZS:181:LYS:CE   | 4:Zd:129:GLN:NE2  | 2.81                     | 0.44              |
| 4:ZV:103:ASP:OD1  | 4:ZV:107:ASN:N    | 2.41                     | 0.44              |
| 4:ZV:264:LEU:HD12 | 4:ZV:264:LEU:HA   | 1.88                     | 0.44              |
| 4:ZW:71:ARG:NH1   | 4:ZW:74:ASP:OD2   | 2.49                     | 0.44              |
| 4:ZX:307:GLU:O    | 4:ZX:308:GLN:HG2  | 2.18                     | 0.44              |
| 4:ZY:101:LYS:CD   | 4:Zd:324:GLU:OE2  | 2.59                     | 0.44              |
| 4:ZY:146:ALA:HB2  | 4:ZY:286:PRO:HD3  | 1.98                     | 0.44              |
| 4:ZZ:396:LEU:HD23 | 4:ZZ:396:LEU:HA   | 1.80                     | 0.44              |
| 5:AB:26:LEU:CD1   | 3:AG:242:ILE:CG2  | 2.92                     | 0.44              |
| 5:AC:227:PHE:O    | 5:AC:231:MET:HG2  | 2.17                     | 0.44              |
| 5:AD:105:ILE:HG12 | 5:AD:115:ILE:HD11 | 2.00                     | 0.44              |
| 5:AE:228:GLU:C    | 3:AK:258:THR:HG21 | 2.39                     | 0.44              |
| 3:AL:187:ILE:HD11 | 3:AL:193:ILE:HG13 | 1.99                     | 0.44              |
| 6:AY:235:LEU:HD13 | 6:AZ:244:ARG:HH22 | 1.81                     | 0.44              |
| 6:Ad:235:LEU:HD13 | 6:Ae:244:ARG:HH22 | 1.81                     | 0.44              |
| 6:Ae:374:HIS:CB   | 10:A2:4:ILE:CD1   | 2.93                     | 0.44              |
| 7:As:60:ILE:O     | 7:As:64:VAL:HG22  | 2.16                     | 0.44              |
| 9:Ax:159:LEU:CD2  | 6:WE:165:PHE:CD1  | 3.01                     | 0.44              |
| 10:A2:57:GLU:HG2  | 11:A7:11:PHE:CD2  | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A5:14:LEU:HD21 | 6:BR:370:ARG:HH21 | 1.83                     | 0.44              |
| 11:A7:51:LYS:HE2  | 11:A7:55:ARG:NH2  | 2.09                     | 0.44              |
| 6:UK:88:VAL:O     | 6:UK:89:PRO:C     | 2.60                     | 0.44              |
| 6:UM:55:PHE:O     | 6:UM:85:ALA:HA    | 2.18                     | 0.44              |
| 6:UO:52:ARG:O     | 6:UO:88:VAL:N     | 2.38                     | 0.44              |
| 6:UO:75:ILE:HG21  | 6:UO:96:LEU:HD11  | 2.00                     | 0.44              |
| 6:UP:55:PHE:O     | 6:UP:85:ALA:HA    | 2.18                     | 0.44              |
| 12:BA:122:VAL:O   | 12:BA:126:MET:HG2 | 2.18                     | 0.44              |
| 6:WC:131:ASN:O    | 6:WC:134:ARG:N    | 2.51                     | 0.44              |
| 6:WG:181:GLU:O    | 6:WG:182:PRO:C    | 2.60                     | 0.44              |
| 6:WQ:187:ASP:OD1  | 6:WQ:188:GLU:N    | 2.51                     | 0.44              |
| 6:BT:429:THR:OG1  | 6:BU:418:GLU:OE2  | 2.36                     | 0.44              |
| 1:C:102:THR:HG23  | 1:D:130:ASN:HD22  | 1.83                     | 0.44              |
| 1:L:63:GLN:OE1    | 2:j:131:SER:CB    | 2.65                     | 0.44              |
| 1:L:102:THR:HG23  | 1:M:130:ASN:HD22  | 1.83                     | 0.44              |
| 1:N:232:MET:HE3   | 1:N:232:MET:HB2   | 1.90                     | 0.44              |
| 1:O:181:SER:HB2   | 1:P:31:VAL:CG1    | 2.45                     | 0.44              |
| 1:P:102:THR:HG23  | 1:Q:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:T:63:GLN:OE1    | 2:r:131:SER:CB    | 2.65                     | 0.44              |
| 1:V:90:LYS:HA     | 1:W:142:ASN:HA    | 1.98                     | 0.44              |
| 1:W:47:ALA:HB1    | 2:t:178:GLN:HG3   | 1.97                     | 0.44              |
| 2:a:78:ASN:OD1    | 2:a:78:ASN:N      | 2.51                     | 0.44              |
| 2:c:129:VAL:HG21  | 2:d:136:LEU:HD13  | 1.98                     | 0.44              |
| 2:e:130:ASP:N     | 2:e:130:ASP:OD1   | 2.47                     | 0.44              |
| 2:p:47:GLY:H      | 2:p:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:s:319:LEU:HD21  | 2:t:264:MET:HE1   | 1.97                     | 0.44              |
| 2:u:47:GLY:H      | 2:u:83:ASN:HD22   | 1.64                     | 0.44              |
| 3:1:35:LYS:HD2    | 3:1:81:HIS:HA     | 1.99                     | 0.44              |
| 3:2:189:GLU:HA    | 3:7:42:GLU:HB2    | 1.98                     | 0.44              |
| 3:5:1:MET:O       | 3:AI:226:VAL:CG2  | 2.66                     | 0.44              |
| 3:5:79:ARG:NH2    | 3:5:184:LEU:O     | 2.50                     | 0.44              |
| 3:ZB:164:GLN:C    | 3:ZB:166:ALA:H    | 2.26                     | 0.44              |
| 3:ZC:95:VAL:O     | 3:ZC:118:GLY:HA3  | 2.17                     | 0.44              |
| 3:ZD:3:SER:O      | 3:ZD:6:TRP:N      | 2.51                     | 0.44              |
| 3:ZE:70:THR:HG22  | 3:ZE:71:GLY:N     | 2.33                     | 0.44              |
| 4:ZI:87:ASP:OD1   | 4:ZI:87:ASP:N     | 2.37                     | 0.44              |
| 4:ZM:30:TYR:HD1   | 4:ZM:363:ALA:HA   | 1.83                     | 0.44              |
| 4:ZN:112:GLN:HE22 | 4:ZS:55:ALA:HB1   | 1.83                     | 0.44              |
| 4:ZO:161:THR:HA   | 4:ZU:252:ASN:HD22 | 1.81                     | 0.44              |
| 4:ZQ:125:PRO:HA   | 4:ZQ:126:PRO:HD3  | 1.92                     | 0.44              |
| 4:ZR:179:ASN:N    | 4:ZR:200:PHE:O    | 2.45                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZU:112:GLN:NE2  | 4:ZZ:40:ALA:HB2   | 2.33                     | 0.44              |
| 4:Zf:196:MET:HE1  | 4:Zf:259:PHE:CZ   | 2.52                     | 0.44              |
| 4:Zh:69:THR:OG1   | 4:Zh:74:ASP:OD1   | 2.30                     | 0.44              |
| 5:AA:71:LEU:HD12  | 3:AL:70:THR:HG21  | 2.00                     | 0.44              |
| 5:AA:171:VAL:HG13 | 5:AA:179:PHE:HB3  | 1.98                     | 0.44              |
| 5:AC:62:PRO:CA    | 3:AH:63:PRO:CG    | 2.77                     | 0.44              |
| 3:AI:257:LEU:HD11 | 12:BD:99:VAL:HA   | 2.00                     | 0.44              |
| 3:AM:95:VAL:O     | 3:AM:118:GLY:HA3  | 2.18                     | 0.44              |
| 7:Ab:8:MET:HE3    | 6:WS:124:SER:CB   | 2.37                     | 0.44              |
| 6:Aj:235:LEU:HD13 | 6:Ak:244:ARG:HH22 | 1.81                     | 0.44              |
| 6:Ak:370:ARG:HH21 | 10:A1:7:ILE:CG1   | 2.26                     | 0.44              |
| 7:Ar:27:VAL:HG22  | 7:Ar:57:ALA:HB1   | 1.98                     | 0.44              |
| 8:At:88:MET:HA    | 8:At:247:ILE:HG21 | 1.99                     | 0.44              |
| 8:At:242:HIS:HB2  | 6:WJ:125:GLN:CB   | 2.48                     | 0.44              |
| 9:Au:214:PRO:HG2  | 9:Av:212:VAL:HG22 | 1.99                     | 0.44              |
| 10:Az:67:ALA:HB2  | 12:BA:2:ALA:HA    | 2.00                     | 0.44              |
| 6:UK:55:PHE:O     | 6:UK:85:ALA:HA    | 2.18                     | 0.44              |
| 6:UL:160:PRO:HG2  | 6:UL:170:LYS:HB3  | 2.00                     | 0.44              |
| 6:UL:216:SER:C    | 6:UL:218:HIS:N    | 2.75                     | 0.44              |
| 6:UO:80:ALA:N     | 6:UO:85:ALA:O     | 2.49                     | 0.44              |
| 6:WD:191:ILE:O    | 6:WD:195:VAL:HG23 | 2.18                     | 0.44              |
| 6:WE:197:LEU:HD12 | 6:WF:175:SER:HB3  | 1.99                     | 0.44              |
| 6:WP:163:SER:C    | 6:WP:165:PHE:N    | 2.76                     | 0.44              |
| 6:WV:192:SER:O    | 6:WV:195:VAL:HB   | 2.18                     | 0.44              |
| 12:BF:36:GLY:O    | 12:BF:37:PRO:C    | 2.60                     | 0.44              |
| 1:C:126:ALA:HB3   | 1:E:232:MET:HE1   | 1.99                     | 0.44              |
| 1:I:47:ALA:HB1    | 2:f:178:GLN:HG3   | 1.96                     | 0.44              |
| 1:I:90:LYS:HA     | 1:J:142:ASN:HA    | 1.98                     | 0.44              |
| 1:J:102:THR:HG23  | 1:K:130:ASN:HD22  | 1.82                     | 0.44              |
| 1:J:165:GLY:C     | 1:K:35:THR:HG21   | 2.40                     | 0.44              |
| 1:M:63:GLN:OE1    | 2:k:131:SER:CB    | 2.65                     | 0.44              |
| 1:P:62:TYR:CE1    | 2:n:129:VAL:HG13  | 2.47                     | 0.44              |
| 1:Q:62:TYR:CE1    | 2:o:129:VAL:HG13  | 2.47                     | 0.44              |
| 1:R:63:GLN:OE1    | 2:p:131:SER:CB    | 2.65                     | 0.44              |
| 1:R:232:MET:HE3   | 1:R:232:MET:HB2   | 1.90                     | 0.44              |
| 1:S:63:GLN:OE1    | 2:q:131:SER:CB    | 2.65                     | 0.44              |
| 2:g:21:ARG:HD2    | 2:g:21:ARG:HA     | 1.75                     | 0.44              |
| 2:h:78:ASN:OD1    | 2:h:78:ASN:N      | 2.51                     | 0.44              |
| 2:r:188:GLN:HE21  | 2:r:188:GLN:HB2   | 1.63                     | 0.44              |
| 2:v:56:PRO:CD     | 2:w:79:MET:HG2    | 2.45                     | 0.44              |
| 3:2:255:GLN:HE21  | 3:2:259:GLN:NE2   | 2.16                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:3:218:TYR:OH    | 3:ZE:73:ARG:HD2    | 2.17                     | 0.44              |
| 3:8:70:THR:HG22   | 3:8:71:GLY:N       | 2.31                     | 0.44              |
| 3:9:35:LYS:NZ     | 3:9:220:GLU:OE2    | 2.48                     | 0.44              |
| 3:ZC:44:LEU:HD23  | 3:ZC:44:LEU:HA     | 1.82                     | 0.44              |
| 3:ZE:19:MET:HE2   | 3:ZE:236:VAL:HG12  | 2.00                     | 0.44              |
| 3:ZE:121:GLN:NE2  | 3:ZE:131:ALA:HA    | 2.33                     | 0.44              |
| 4:ZH:41:ASP:OD2   | 4:ZH:41:ASP:N      | 2.48                     | 0.44              |
| 4:ZI:154:MET:HE2  | 4:ZI:276:ILE:HD13  | 1.98                     | 0.44              |
| 4:ZJ:93:PHE:HB3   | 4:ZJ:333:VAL:HG13  | 1.99                     | 0.44              |
| 4:ZL:373:VAL:O    | 4:ZL:374:ASN:C     | 2.60                     | 0.44              |
| 4:ZR:295:ASN:HB2  | 4:ZR:297:ASP:OD2   | 2.18                     | 0.44              |
| 4:ZS:379:GLN:CD   | 4:ZX:391:THR:HG23  | 2.42                     | 0.44              |
| 4:ZX:285:LYS:HB3  | 4:ZX:285:LYS:HE2   | 1.76                     | 0.44              |
| 4:ZX:382:TYR:CZ   | 4:Zc:395:ILE:HG23  | 2.53                     | 0.44              |
| 4:ZZ:269:GLN:CG   | 4:Zf:286:PRO:CG    | 2.91                     | 0.44              |
| 4:Zb:80:ASN:OD1   | 4:Zb:80:ASN:C      | 2.61                     | 0.44              |
| 4:Ze:117:THR:HA   | 4:Ze:136:PRO:HA    | 2.00                     | 0.44              |
| 5:AA:53:THR:OG1   | 11:A6:92:GLN:OE1   | 2.30                     | 0.44              |
| 5:AC:241:GLU:HG2  | 12:BC:110:ARG:HB3  | 2.00                     | 0.44              |
| 5:AE:53:THR:OG1   | 11:A0:92:GLN:HG2   | 2.18                     | 0.44              |
| 6:AR:278:THR:HG21 | 10:A2:21:ALA:HB3   | 1.97                     | 0.44              |
| 6:Af:365:ASN:ND2  | 11:A8:65:LEU:HD11  | 2.32                     | 0.44              |
| 6:AO:429:THR:OG1  | 6:AP:418:GLU:OE2   | 2.36                     | 0.44              |
| 6:AQ:429:THR:OG1  | 6:BR:418:GLU:OE2   | 2.36                     | 0.44              |
| 7:As:7:MET:HG3    | 8:At:234:PRO:HA    | 1.99                     | 0.44              |
| 11:A6:78:VAL:HG11 | 12:BA:57:GLN:HA    | 2.00                     | 0.44              |
| 11:A0:109:PHE:CZ  | 12:BE:118:VAL:HG13 | 2.53                     | 0.44              |
| 6:UJ:55:PHE:O     | 6:UJ:85:ALA:HA     | 2.18                     | 0.44              |
| 6:UN:75:ILE:HG21  | 6:UN:96:LEU:HD11   | 2.00                     | 0.44              |
| 6:UO:160:PRO:HG2  | 6:UO:170:LYS:HB3   | 2.00                     | 0.44              |
| 6:WA:160:PRO:O    | 6:WA:161:LYS:C     | 2.61                     | 0.44              |
| 6:WF:181:GLU:O    | 6:WF:182:PRO:C     | 2.60                     | 0.44              |
| 6:WJ:145:GLU:HG2  | 6:WJ:153:ALA:N     | 2.33                     | 0.44              |
| 6:WQ:171:SER:HB3  | 6:WQ:206:PRO:HD3   | 2.00                     | 0.44              |
| 1:A:90:LYS:HA     | 1:B:142:ASN:HA     | 1.98                     | 0.44              |
| 1:B:62:TYR:CE1    | 2:z:129:VAL:HG13   | 2.48                     | 0.44              |
| 1:B:106:PHE:HB3   | 1:B:109:VAL:HG22   | 2.00                     | 0.44              |
| 1:F:126:ALA:HB3   | 1:H:232:MET:HE1    | 1.99                     | 0.44              |
| 1:H:165:GLY:C     | 1:I:35:THR:HG21    | 2.40                     | 0.44              |
| 1:I:165:GLY:C     | 1:J:35:THR:HG21    | 2.41                     | 0.44              |
| 1:J:90:LYS:HA     | 1:K:142:ASN:HA     | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:126:ALA:HB3   | 1:M:232:MET:HE1   | 1.99                     | 0.44              |
| 1:K:165:GLY:C     | 1:L:35:THR:HG21   | 2.41                     | 0.44              |
| 1:N:63:GLN:OE1    | 2:l:131:SER:CB    | 2.65                     | 0.44              |
| 1:P:63:GLN:OE1    | 2:n:131:SER:CB    | 2.65                     | 0.44              |
| 1:P:68:ASP:OD1    | 2:o:64:ASN:ND2    | 2.48                     | 0.44              |
| 1:Q:63:GLN:OE1    | 2:o:131:SER:CB    | 2.65                     | 0.44              |
| 1:Q:181:SER:HB2   | 1:R:31:VAL:CG1    | 2.45                     | 0.44              |
| 1:U:68:ASP:OD1    | 2:t:64:ASN:ND2    | 2.47                     | 0.44              |
| 2:b:47:GLY:H      | 2:b:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:h:159:GLN:OE1   | 2:i:44:GLY:O      | 2.36                     | 0.44              |
| 2:i:159:GLN:OE1   | 2:j:44:GLY:O      | 2.36                     | 0.44              |
| 2:j:188:GLN:HE21  | 2:j:188:GLN:HB2   | 1.63                     | 0.44              |
| 2:s:47:GLY:H      | 2:s:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:t:47:GLY:H      | 2:t:83:ASN:HD22   | 1.64                     | 0.44              |
| 2:x:78:ASN:OD1    | 2:x:78:ASN:N      | 2.51                     | 0.44              |
| 3:4:47:GLN:N      | 3:4:68:ILE:O      | 2.50                     | 0.44              |
| 3:5:24:ASN:HA     | 3:ZA:7:ILE:HG21   | 1.99                     | 0.44              |
| 3:6:7:ILE:HG23    | 3:6:71:GLY:HA2    | 1.99                     | 0.44              |
| 3:8:45:LEU:HD12   | 3:AL:83:GLN:NE2   | 2.33                     | 0.44              |
| 3:ZA:88:GLN:HG2   | 3:ZA:90:ASN:OD1   | 2.18                     | 0.44              |
| 4:ZI:324:GLU:C    | 4:ZI:326:LEU:H    | 2.25                     | 0.44              |
| 4:ZK:27:SER:HA    | 4:ZK:366:VAL:CG2  | 2.48                     | 0.44              |
| 4:ZM:228:THR:HB   | 4:ZM:244:VAL:HG11 | 2.00                     | 0.44              |
| 4:ZM:246:ILE:HD13 | 4:ZM:246:ILE:HA   | 1.88                     | 0.44              |
| 4:ZU:369:SER:HB3  | 4:Za:382:TYR:OH   | 2.17                     | 0.44              |
| 4:ZV:14:ALA:HB2   | 4:ZV:382:TYR:HE2  | 1.83                     | 0.44              |
| 4:ZV:42:MET:SD    | 4:ZV:53:LYS:HB3   | 2.58                     | 0.44              |
| 4:ZW:70:GLY:O     | 4:ZW:71:ARG:C     | 2.61                     | 0.44              |
| 4:ZY:270:ASN:H    | 4:Ze:286:PRO:HG2  | 1.82                     | 0.44              |
| 4:Zf:210:VAL:HB   | 4:Zf:228:THR:HG22 | 2.00                     | 0.44              |
| 4:Zg:73:LEU:HB3   | 4:Zg:100:PHE:HB2  | 2.00                     | 0.44              |
| 4:Zg:269:GLN:HG2  | 4:Zg:270:ASN:H    | 1.83                     | 0.44              |
| 5:AB:9:MET:HG2    | 12:BB:99:VAL:HG12 | 1.99                     | 0.44              |
| 5:AB:29:ALA:HB1   | 3:AM:1:MET:HE3    | 1.99                     | 0.44              |
| 5:AD:19:GLN:HE22  | 5:AD:220:MET:HG2  | 1.83                     | 0.44              |
| 3:AH:6:TRP:HE1    | 12:BC:77:VAL:HB   | 1.81                     | 0.44              |
| 3:AM:102:PHE:HB3  | 3:AM:114:TYR:HB3  | 2.00                     | 0.44              |
| 7:Ab:15:LYS:HE2   | 7:Ab:15:LYS:HB3   | 1.88                     | 0.44              |
| 7:Ab:84:LEU:HB3   | 7:Ab:85:PRO:HD2   | 1.98                     | 0.44              |
| 6:Aj:370:ARG:NH2  | 10:A1:14:LEU:CD2  | 2.67                     | 0.44              |
| 6:An:429:THR:OG1  | 6:Ao:418:GLU:OE2  | 2.36                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:Aw:135:ARG:O     | 9:Aw:136:ALA:C    | 2.59                     | 0.44              |
| 9:Aw:171:LEU:HD23  | 9:Ax:95:PHE:CZ    | 2.53                     | 0.44              |
| 9:Ax:40:LEU:HD13   | 11:A9:4:ARG:HG2   | 1.98                     | 0.44              |
| 11:A8:67:LEU:HD21  | 11:A8:74:PRO:HA   | 2.00                     | 0.44              |
| 11:A9:117:GLN:HE22 | 12:BD:125:MET:HG2 | 1.83                     | 0.44              |
| 6:U1:75:ILE:HG21   | 6:U1:96:LEU:HD11  | 2.00                     | 0.44              |
| 6:UM:160:PRO:HG2   | 6:UM:170:LYS:HB3  | 2.00                     | 0.44              |
| 6:UN:98:LEU:HD11   | 6:UN:143:THR:O    | 2.17                     | 0.44              |
| 6:UN:160:PRO:HG2   | 6:UN:170:LYS:HB3  | 2.00                     | 0.44              |
| 6:UP:98:LEU:HD11   | 6:UP:143:THR:O    | 2.16                     | 0.44              |
| 12:BB:4:LEU:HD23   | 12:BB:7:PHE:HD1   | 1.82                     | 0.44              |
| 6:WE:164:LEU:HD13  | 6:WE:165:PHE:H    | 1.82                     | 0.44              |
| 6:WS:142:ARG:O     | 6:WS:146:THR:HG23 | 2.17                     | 0.44              |
| 6:WT:192:SER:O     | 6:WT:195:VAL:HB   | 2.18                     | 0.44              |
| 6:WV:130:VAL:HG12  | 6:WV:134:ARG:HD2  | 1.99                     | 0.44              |
| 12:BD:56:GLY:O     | 12:BD:57:GLN:HG2  | 2.18                     | 0.44              |
| 6:BW:429:THR:OG1   | 6:BX:418:GLU:OE2  | 2.36                     | 0.44              |
| 1:F:90:LYS:HA      | 1:G:142:ASN:HA    | 1.98                     | 0.43              |
| 1:I:62:TYR:CE1     | 2:g:129:VAL:HG13  | 2.48                     | 0.43              |
| 1:N:126:ALA:HB3    | 1:P:232:MET:HE1   | 1.99                     | 0.43              |
| 1:O:63:GLN:OE1     | 2:m:131:SER:CB    | 2.65                     | 0.43              |
| 1:W:102:THR:HG23   | 1:X:130:ASN:HD22  | 1.82                     | 0.43              |
| 2:e:93:TYR:OH      | 2:e:173:ARG:O     | 2.25                     | 0.43              |
| 2:f:159:GLN:OE1    | 2:g:44:GLY:O      | 2.36                     | 0.43              |
| 2:g:159:GLN:OE1    | 2:h:44:GLY:O      | 2.36                     | 0.43              |
| 2:g:258:ARG:HH12   | 2:i:140:ASN:HD21  | 1.64                     | 0.43              |
| 2:k:159:GLN:OE1    | 2:l:44:GLY:O      | 2.36                     | 0.43              |
| 2:p:346:MET:HE2    | 2:r:142:LEU:HD11  | 1.95                     | 0.43              |
| 2:v:346:MET:HE2    | 2:x:142:LEU:HD11  | 1.95                     | 0.43              |
| 3:0:1:MET:HG3      | 5:AD:213:PRO:CG   | 2.12                     | 0.43              |
| 3:0:16:GLN:NE2     | 3:5:2:ILE:HD11    | 2.33                     | 0.43              |
| 3:0:83:GLN:CG      | 3:ZB:45:LEU:HD13  | 2.46                     | 0.43              |
| 3:0:95:VAL:O       | 3:0:118:GLY:HA3   | 2.18                     | 0.43              |
| 3:3:123:ASP:OD1    | 3:3:127:GLN:N     | 2.49                     | 0.43              |
| 3:5:55:GLN:HA      | 3:5:55:GLN:HE21   | 1.82                     | 0.43              |
| 3:ZA:230:LEU:CD1   | 4:ZL:399:LEU:HB3  | 2.48                     | 0.43              |
| 3:ZB:215:TYR:HB3   | 3:ZB:218:TYR:CD2  | 2.53                     | 0.43              |
| 4:ZF:380:ARG:HH21  | 4:ZL:397:ASN:HB2  | 1.83                     | 0.43              |
| 4:ZG:288:ASP:N     | 4:ZG:288:ASP:OD1  | 2.51                     | 0.43              |
| 4:ZJ:139:ILE:HG12  | 4:ZJ:312:LEU:HD13 | 1.99                     | 0.43              |
| 4:ZK:112:GLN:HG2   | 4:ZK:331:ASP:HB3  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZM:307:GLU:OE1  | 4:ZM:307:GLU:O     | 2.35                     | 0.43              |
| 4:ZP:22:ASN:N     | 4:ZU:5:GLN:HE21    | 2.15                     | 0.43              |
| 4:ZR:86:VAL:HG13  | 4:ZR:117:THR:HG21  | 2.00                     | 0.43              |
| 4:ZX:380:ARG:HH21 | 4:Zd:393:ASP:CG    | 2.26                     | 0.43              |
| 4:ZY:137:ILE:HG21 | 4:ZY:300:VAL:HG21  | 2.00                     | 0.43              |
| 4:ZZ:233:ASN:HD21 | 4:ZZ:237:ILE:HB    | 1.83                     | 0.43              |
| 4:Ze:100:PHE:CE2  | 4:Ze:116:LEU:HD13  | 2.53                     | 0.43              |
| 4:Ze:396:LEU:HD12 | 4:Ze:396:LEU:HA    | 1.81                     | 0.43              |
| 5:AA:9:MET:CG     | 12:BA:103:VAL:HG21 | 2.47                     | 0.43              |
| 5:AC:51:LEU:HD23  | 12:BD:67:VAL:HG23  | 1.99                     | 0.43              |
| 5:AD:26:LEU:HD21  | 5:AD:216:ALA:CB    | 2.48                     | 0.43              |
| 5:AE:20:ALA:CA    | 3:AJ:4:SER:HB3     | 2.48                     | 0.43              |
| 3:AH:97:ILE:HB    | 3:AH:116:ARG:HH21  | 1.82                     | 0.43              |
| 3:AI:46:TYR:HB3   | 3:AI:67:GLN:HG2    | 1.99                     | 0.43              |
| 3:AM:123:ASP:OD2  | 3:AM:127:GLN:NE2   | 2.51                     | 0.43              |
| 6:Ae:429:THR:OG1  | 6:Af:418:GLU:OE2   | 2.36                     | 0.43              |
| 10:A4:61:LEU:HD13 | 11:A9:50:LYS:HE3   | 2.00                     | 0.43              |
| 6:UI:80:ALA:N     | 6:UI:85:ALA:O      | 2.49                     | 0.43              |
| 6:UI:125:GLN:C    | 6:UI:128:GLU:H     | 2.26                     | 0.43              |
| 6:UI:160:PRO:HG2  | 6:UI:170:LYS:HB3   | 2.00                     | 0.43              |
| 6:UJ:103:GLN:CB   | 6:WD:182:PRO:HA    | 2.48                     | 0.43              |
| 6:UK:160:PRO:HG2  | 6:UK:170:LYS:HB3   | 2.00                     | 0.43              |
| 6:UL:55:PHE:O     | 6:UL:85:ALA:HA     | 2.18                     | 0.43              |
| 6:UP:160:PRO:HG2  | 6:UP:170:LYS:HB3   | 2.00                     | 0.43              |
| 6:WA:196:HIS:NE2  | 6:WB:219:LEU:HD22  | 2.33                     | 0.43              |
| 6:WJ:160:PRO:HG2  | 6:WJ:170:LYS:O     | 2.18                     | 0.43              |
| 6:WR:190:GLN:HG2  | 6:WS:217:GLY:HA3   | 2.00                     | 0.43              |
| 6:WT:131:ASN:HA   | 6:WT:134:ARG:HD3   | 1.99                     | 0.43              |
| 1:A:106:PHE:HB3   | 1:A:109:VAL:HG22   | 2.00                     | 0.43              |
| 1:I:71:PRO:HB2    | 1:I:152:VAL:HG21   | 2.01                     | 0.43              |
| 1:K:71:PRO:HB2    | 1:K:152:VAL:HG21   | 2.01                     | 0.43              |
| 1:L:71:PRO:HB2    | 1:L:152:VAL:HG21   | 2.01                     | 0.43              |
| 1:L:165:GLY:C     | 1:M:35:THR:HG21    | 2.41                     | 0.43              |
| 1:S:62:TYR:CE1    | 2:q:129:VAL:HG13   | 2.48                     | 0.43              |
| 1:S:126:ALA:HB3   | 1:U:232:MET:HE1    | 1.99                     | 0.43              |
| 1:W:71:PRO:HB2    | 1:W:152:VAL:HG21   | 2.00                     | 0.43              |
| 1:X:71:PRO:HB2    | 1:X:152:VAL:HG21   | 2.01                     | 0.43              |
| 1:Z:71:PRO:HB2    | 1:Z:152:VAL:HG21   | 2.00                     | 0.43              |
| 2:a:140:ASN:HD21  | 2:y:258:ARG:HH12   | 1.64                     | 0.43              |
| 2:a:258:ARG:HH12  | 2:c:140:ASN:HD21   | 1.64                     | 0.43              |
| 2:d:78:ASN:OD1    | 2:d:78:ASN:N       | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:21:ARG:HA     | 2:e:21:ARG:HD2    | 1.74                     | 0.43              |
| 2:e:159:GLN:OE1   | 2:f:44:GLY:O      | 2.36                     | 0.43              |
| 2:f:56:PRO:CD     | 2:g:79:MET:HG2    | 2.45                     | 0.43              |
| 2:f:346:MET:HE2   | 2:h:142:LEU:HD11  | 1.95                     | 0.43              |
| 2:l:78:ASN:OD1    | 2:l:78:ASN:N      | 2.51                     | 0.43              |
| 2:v:188:GLN:HE21  | 2:v:188:GLN:HB2   | 1.63                     | 0.43              |
| 3:0:6:TRP:HD1     | 5:AD:70:GLN:HB2   | 1.83                     | 0.43              |
| 3:2:251:ASP:OD1   | 3:AK:238:ARG:NH2  | 2.51                     | 0.43              |
| 3:6:55:GLN:C      | 5:AE:138:ALA:HB2  | 2.38                     | 0.43              |
| 3:7:225:ASN:O     | 3:7:229:GLU:HG2   | 2.18                     | 0.43              |
| 3:9:257:LEU:O     | 3:9:258:THR:C     | 2.61                     | 0.43              |
| 3:ZD:42:GLU:HG2   | 3:ZD:75:VAL:HG23  | 2.00                     | 0.43              |
| 3:ZD:189:GLU:OE1  | 4:ZI:53:LYS:NZ    | 2.47                     | 0.43              |
| 3:ZE:89:THR:HG23  | 3:ZE:91:ASN:HB2   | 1.99                     | 0.43              |
| 4:ZJ:78:SER:O     | 4:ZJ:354:GLY:HA3  | 2.18                     | 0.43              |
| 4:ZL:28:ALA:O     | 4:ZQ:39:PHE:CD2   | 2.71                     | 0.43              |
| 4:ZP:77:ILE:HD13  | 4:ZP:356:LEU:HG   | 2.00                     | 0.43              |
| 4:ZQ:75:VAL:O     | 4:ZQ:98:GLY:HA3   | 2.18                     | 0.43              |
| 4:ZR:211:TYR:CE1  | 4:ZR:226:ALA:HA   | 2.53                     | 0.43              |
| 4:ZS:170:PHE:CE2  | 4:ZS:223:PRO:HG2  | 2.52                     | 0.43              |
| 4:ZS:202:LYS:HG3  | 4:ZS:208:TRP:CE2  | 2.53                     | 0.43              |
| 4:ZT:186:VAL:C    | 4:ZT:187:TYR:HD1  | 2.26                     | 0.43              |
| 4:ZW:2:SER:O      | 4:ZW:2:SER:OG     | 2.36                     | 0.43              |
| 4:ZY:212:THR:HG21 | 4:ZY:246:ILE:HD12 | 1.99                     | 0.43              |
| 5:AB:73:TYR:HD1   | 5:AB:205:VAL:HG12 | 1.83                     | 0.43              |
| 5:AC:215:GLU:HG2  | 3:AI:9:LYS:CE     | 2.40                     | 0.43              |
| 3:AF:137:GLN:HA   | 3:AF:139:ALA:N    | 2.33                     | 0.43              |
| 3:AI:16:GLN:HE22  | 3:AN:2:ILE:CD1    | 2.31                     | 0.43              |
| 7:Ab:3:PRO:HG3    | 9:Aw:228:LEU:HD12 | 1.99                     | 0.43              |
| 6:Ac:429:THR:OG1  | 6:Ad:418:GLU:OE2  | 2.36                     | 0.43              |
| 6:Ak:421:GLY:O    | 6:Ak:426:ARG:NH2  | 2.51                     | 0.43              |
| 7:Ar:29:LEU:CB    | 7:As:52:ILE:HG21  | 2.44                     | 0.43              |
| 7:Ar:52:ILE:O     | 7:Ar:55:ILE:HG22  | 2.18                     | 0.43              |
| 8:At:12:TRP:CZ3   | 10:A5:34:PHE:HB2  | 2.53                     | 0.43              |
| 9:Ax:212:VAL:HG21 | 9:Ax:217:ILE:HD11 | 2.00                     | 0.43              |
| 11:A9:19:ARG:NH2  | 11:A9:115:LYS:HD3 | 2.33                     | 0.43              |
| 11:A0:63:VAL:H    | 6:BX:297:GLN:NE2  | 2.16                     | 0.43              |
| 6:UJ:80:ALA:N     | 6:UJ:85:ALA:O     | 2.49                     | 0.43              |
| 6:UO:125:GLN:C    | 6:UO:128:GLU:H    | 2.26                     | 0.43              |
| 12:BE:97:ASP:O    | 12:BE:101:GLU:HG2 | 2.18                     | 0.43              |
| 6:BR:429:THR:OG1  | 6:BS:418:GLU:OE2  | 2.36                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:71:PRO:HB2    | 1:A:152:VAL:HG21   | 2.01                     | 0.43              |
| 1:M:232:MET:HE3   | 1:M:232:MET:HB2    | 1.90                     | 0.43              |
| 1:R:62:TYR:CE1    | 2:p:129:VAL:HG13   | 2.48                     | 0.43              |
| 1:T:126:ALA:HB3   | 1:V:232:MET:HE1    | 1.99                     | 0.43              |
| 1:U:90:LYS:HA     | 1:V:142:ASN:HA     | 1.98                     | 0.43              |
| 1:Z:106:PHE:HB3   | 1:Z:109:VAL:HG22   | 2.00                     | 0.43              |
| 2:b:56:PRO:CD     | 2:c:79:MET:HG2     | 2.45                     | 0.43              |
| 2:c:258:ARG:HH12  | 2:e:140:ASN:HD21   | 1.64                     | 0.43              |
| 2:d:159:GLN:OE1   | 2:e:44:GLY:O       | 2.36                     | 0.43              |
| 2:e:56:PRO:CD     | 2:f:79:MET:HG2     | 2.45                     | 0.43              |
| 2:e:258:ARG:HH12  | 2:g:140:ASN:HD21   | 1.64                     | 0.43              |
| 2:j:159:GLN:OE1   | 2:k:44:GLY:O       | 2.36                     | 0.43              |
| 2:r:47:GLY:H      | 2:r:83:ASN:HD22    | 1.64                     | 0.43              |
| 3:1:3:SER:O       | 5:AE:70:GLN:HG3    | 2.18                     | 0.43              |
| 3:4:50:ARG:HH12   | 3:AN:75:VAL:HG13   | 1.83                     | 0.43              |
| 3:8:185:GLU:HG3   | 3:ZD:67:GLN:HE22   | 1.84                     | 0.43              |
| 3:ZA:50:ARG:O     | 3:ZA:65:GLY:HA3    | 2.18                     | 0.43              |
| 3:ZE:24:ASN:ND2   | 4:ZJ:49:GLY:HA3    | 2.33                     | 0.43              |
| 3:ZE:70:THR:HG22  | 3:ZE:71:GLY:H      | 1.82                     | 0.43              |
| 4:ZH:205:ASP:CG   | 4:ZN:252:ASN:HA    | 2.37                     | 0.43              |
| 4:ZJ:178:TYR:HA   | 4:ZJ:201:VAL:HG22  | 2.00                     | 0.43              |
| 4:ZK:317:LEU:HD11 | 4:ZK:356:LEU:HD11  | 2.00                     | 0.43              |
| 4:ZK:349:GLY:O    | 4:ZQ:89:ASN:ND2    | 2.51                     | 0.43              |
| 4:ZM:6:ALA:HB1    | 4:ZM:389:ILE:HG13  | 2.00                     | 0.43              |
| 4:ZO:95:SER:HB2   | 4:ZO:333:VAL:HG22  | 2.00                     | 0.43              |
| 4:ZP:25:ALA:HB1   | 4:ZU:52:VAL:HG12   | 2.00                     | 0.43              |
| 4:ZT:14:ALA:HB2   | 4:ZT:382:TYR:HE2   | 1.82                     | 0.43              |
| 4:ZT:34:SER:HB3   | 4:ZT:366:VAL:HG22  | 2.01                     | 0.43              |
| 4:ZU:235:ASN:OD1  | 4:Za:189:SER:HB2   | 2.17                     | 0.43              |
| 4:ZU:367:ASP:O    | 4:ZU:371:GLU:HG2   | 2.18                     | 0.43              |
| 4:ZU:383:GLN:HG2  | 4:ZZ:398:THR:HG21  | 2.00                     | 0.43              |
| 4:ZV:267:MET:HE1  | 4:Zb:145:ALA:CB    | 2.48                     | 0.43              |
| 4:ZX:17:LEU:HD13  | 4:Zc:395:ILE:CD1   | 2.46                     | 0.43              |
| 4:ZX:210:VAL:O    | 4:ZX:227:SER:HB2   | 2.18                     | 0.43              |
| 4:Za:17:LEU:HD21  | 4:Zf:391:THR:HG21  | 2.00                     | 0.43              |
| 4:Zd:10:LEU:HD23  | 4:Zd:10:LEU:HA     | 1.80                     | 0.43              |
| 4:Zf:114:MET:HE3  | 4:Zf:333:VAL:HG21  | 2.00                     | 0.43              |
| 5:AA:9:MET:HG3    | 12:BA:103:VAL:CG2  | 2.47                     | 0.43              |
| 5:AA:15:THR:OG1   | 5:AA:226:ARG:NH1   | 2.51                     | 0.43              |
| 5:AA:84:GLN:CD    | 3:AL:48:THR:H      | 2.27                     | 0.43              |
| 5:AE:9:MET:CG     | 12:BE:103:VAL:HG21 | 2.48                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:AE:51:LEU:HG    | 5:AE:51:LEU:H    | 1.20                     | 0.43              |
| 3:AH:140:ILE:CG2  | 3:AH:171:GLY:HA3 | 2.46                     | 0.43              |
| 3:AJ:188:GLY:O    | 3:AJ:190:ASN:N   | 2.45                     | 0.43              |
| 3:AK:47:GLN:NE2   | 12:BF:74:GLU:O   | 2.52                     | 0.43              |
| 3:AK:73:ARG:HD3   | 12:BF:78:TYR:CG  | 2.53                     | 0.43              |
| 3:AM:17:THR:O     | 3:AM:19:MET:N    | 2.51                     | 0.43              |
| 6:AR:429:THR:OG1  | 6:Ac:418:GLU:OE2 | 2.36                     | 0.43              |
| 6:Ap:429:THR:OG1  | 6:AO:418:GLU:OE2 | 2.36                     | 0.43              |
| 9:Au:100:ILE:HG23 | 9:Au:101:MET:CE  | 2.47                     | 0.43              |
| 11:A8:35:THR:HG22 | 12:BC:49:PHE:CB  | 2.23                     | 0.43              |
| 6:UJ:88:VAL:O     | 6:UJ:89:PRO:C    | 2.60                     | 0.43              |
| 6:UJ:160:PRO:HG2  | 6:UJ:170:LYS:HB3 | 2.00                     | 0.43              |
| 6:UP:125:GLN:C    | 6:UP:128:GLU:H   | 2.27                     | 0.43              |
| 6:WB:113:PHE:HB3  | 6:WC:134:ARG:CZ  | 2.48                     | 0.43              |
| 6:WE:132:TYR:HB2  | 6:WF:126:PHE:HZ  | 1.83                     | 0.43              |
| 6:WM:219:LEU:HG   | 6:WM:221:THR:H   | 1.82                     | 0.43              |
| 6:WS:197:LEU:CD1  | 6:WT:175:SER:OG  | 2.64                     | 0.43              |
| 6:BV:429:THR:OG1  | 6:BW:418:GLU:OE2 | 2.36                     | 0.43              |
| 1:G:165:GLY:C     | 1:H:35:THR:HG21  | 2.40                     | 0.43              |
| 1:H:71:PRO:HB2    | 1:H:152:VAL:HG21 | 2.01                     | 0.43              |
| 1:H:102:THR:HG23  | 1:I:130:ASN:HD22 | 1.82                     | 0.43              |
| 1:M:71:PRO:HB2    | 1:M:152:VAL:HG21 | 2.01                     | 0.43              |
| 1:O:71:PRO:HB2    | 1:O:152:VAL:HG21 | 2.01                     | 0.43              |
| 1:O:126:ALA:HB3   | 1:Q:232:MET:HE1  | 2.00                     | 0.43              |
| 1:S:232:MET:HE3   | 1:S:232:MET:HB2  | 1.90                     | 0.43              |
| 1:T:71:PRO:HB2    | 1:T:152:VAL:HG21 | 2.00                     | 0.43              |
| 1:U:126:ALA:HB3   | 1:W:232:MET:HE1  | 1.99                     | 0.43              |
| 1:V:126:ALA:HB3   | 1:X:232:MET:HE1  | 2.00                     | 0.43              |
| 1:W:50:SER:HB3    | 2:t:32:ARG:HH11  | 1.80                     | 0.43              |
| 2:c:159:GLN:OE1   | 2:d:44:GLY:O     | 2.36                     | 0.43              |
| 2:e:47:GLY:H      | 2:e:83:ASN:HD22  | 1.64                     | 0.43              |
| 2:l:159:GLN:OE1   | 2:m:44:GLY:O     | 2.36                     | 0.43              |
| 2:p:192:GLU:H     | 2:p:192:GLU:HG3  | 1.52                     | 0.43              |
| 2:p:258:ARG:HH12  | 2:r:140:ASN:HD21 | 1.64                     | 0.43              |
| 2:q:80:GLN:OE1    | 3:AI:209:ASN:HA  | 2.18                     | 0.43              |
| 2:q:319:LEU:HD21  | 2:r:264:MET:HE1  | 1.98                     | 0.43              |
| 3:1:188:GLY:O     | 3:1:190:ASN:N    | 2.47                     | 0.43              |
| 3:3:35:LYS:NZ     | 3:3:220:GLU:OE2  | 2.48                     | 0.43              |
| 3:4:162:GLN:H     | 3:4:162:GLN:CD   | 2.23                     | 0.43              |
| 3:5:49:ILE:HG21   | 3:5:66:LEU:HD23  | 2.00                     | 0.43              |
| 3:9:57:SER:CA     | 3:AH:154:ASP:HB2 | 2.41                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZJ:370:LYS:HB2  | 4:ZJ:370:LYS:HE3  | 1.86                     | 0.43              |
| 4:ZJ:380:ARG:HD3  | 4:ZJ:380:ARG:HA   | 1.71                     | 0.43              |
| 4:ZK:138:THR:HG22 | 4:ZK:140:PRO:HD3  | 2.00                     | 0.43              |
| 4:ZM:14:ALA:HB2   | 4:ZM:382:TYR:HE2  | 1.82                     | 0.43              |
| 4:ZM:233:ASN:OD1  | 4:ZM:237:ILE:N    | 2.51                     | 0.43              |
| 4:ZQ:112:GLN:HE21 | 4:ZQ:331:ASP:HB3  | 1.82                     | 0.43              |
| 4:ZX:388:THR:O    | 4:ZX:392:GLN:HG2  | 2.18                     | 0.43              |
| 4:ZY:53:LYS:HE3   | 4:ZY:53:LYS:HB2   | 1.86                     | 0.43              |
| 4:ZZ:56:GLY:C     | 4:ZZ:57:ILE:HD12  | 2.44                     | 0.43              |
| 4:ZZ:144:MET:HE2  | 4:ZZ:144:MET:HB3  | 1.83                     | 0.43              |
| 5:AB:34:PHE:O     | 5:AB:210:ASN:ND2  | 2.51                     | 0.43              |
| 5:AB:243:ARG:O    | 5:AB:244:ALA:C    | 2.61                     | 0.43              |
| 5:AD:82:LEU:N     | 5:AD:82:LEU:HD12  | 2.33                     | 0.43              |
| 5:AD:165:LYS:O    | 5:AD:189:ARG:NH2  | 2.51                     | 0.43              |
| 3:AM:195:THR:HG22 | 3:AM:197:SER:H    | 1.83                     | 0.43              |
| 6:AS:429:THR:OG1  | 6:AT:418:GLU:OE2  | 2.36                     | 0.43              |
| 8:At:205:ASN:ND2  | 9:Au:211:MET:HB2  | 2.33                     | 0.43              |
| 9:Au:59:LEU:HD12  | 9:Av:88:VAL:HG23  | 2.00                     | 0.43              |
| 9:Aw:59:LEU:O     | 9:Aw:65:THR:OG1   | 2.30                     | 0.43              |
| 10:A5:99:VAL:O    | 10:A5:102:MET:HB2 | 2.18                     | 0.43              |
| 6:UJ:125:GLN:C    | 6:UJ:128:GLU:H    | 2.27                     | 0.43              |
| 6:UJ:164:LEU:HD22 | 6:UJ:164:LEU:H    | 1.81                     | 0.43              |
| 6:UK:125:GLN:C    | 6:UK:128:GLU:H    | 2.27                     | 0.43              |
| 6:UL:125:GLN:C    | 6:UL:128:GLU:H    | 2.27                     | 0.43              |
| 6:UM:94:HIS:HB2   | 6:UM:146:THR:HG21 | 1.97                     | 0.43              |
| 12:BA:68:ILE:HD11 | 6:BH:312:VAL:HG21 | 2.00                     | 0.43              |
| 12:BB:82:ASN:HD22 | 12:BB:91:VAL:HG21 | 1.83                     | 0.43              |
| 6:WC:142:ARG:O    | 6:WC:146:THR:HG23 | 2.18                     | 0.43              |
| 6:WD:181:GLU:O    | 6:WD:182:PRO:C    | 2.60                     | 0.43              |
| 6:WE:113:PHE:CE2  | 6:WE:139:GLU:HG3  | 2.54                     | 0.43              |
| 6:WL:172:PRO:HD2  | 6:WL:204:GLY:O    | 2.19                     | 0.43              |
| 6:WM:142:ARG:O    | 6:WM:146:THR:HG23 | 2.18                     | 0.43              |
| 6:WQ:145:GLU:C    | 6:WQ:147:LEU:N    | 2.75                     | 0.43              |
| 6:WR:192:SER:O    | 6:WR:195:VAL:HB   | 2.19                     | 0.43              |
| 6:WS:145:GLU:C    | 6:WS:147:LEU:N    | 2.75                     | 0.43              |
| 6:WT:134:ARG:HH21 | 6:WT:134:ARG:HB3  | 1.83                     | 0.43              |
| 1:C:50:SER:HB3    | 2:z:32:ARG:HH11   | 1.81                     | 0.43              |
| 1:C:71:PRO:HB2    | 1:C:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:C:106:PHE:HB3   | 1:C:109:VAL:HG22  | 2.00                     | 0.43              |
| 1:D:71:PRO:HB2    | 1:D:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:D:102:THR:HG23  | 1:E:130:ASN:HD22  | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:71:PRO:HB2    | 1:F:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:G:71:PRO:HB2    | 1:G:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:H:47:ALA:HB1    | 2:e:178:GLN:HG3   | 1.96                     | 0.43              |
| 1:I:166:GLU:HB2   | 1:J:35:THR:CG2    | 2.30                     | 0.43              |
| 1:J:71:PRO:HB2    | 1:J:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:M:165:GLY:C     | 1:N:35:THR:HG21   | 2.40                     | 0.43              |
| 1:P:71:PRO:HB2    | 1:P:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:S:71:PRO:HB2    | 1:S:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:U:106:PHE:HB3   | 1:U:109:VAL:HG22  | 2.00                     | 0.43              |
| 1:Y:71:PRO:HB2    | 1:Y:152:VAL:HG21  | 2.01                     | 0.43              |
| 2:g:250:ASP:OD1   | 2:h:23:ARG:NE     | 2.51                     | 0.43              |
| 2:m:159:GLN:OE1   | 2:n:44:GLY:O      | 2.36                     | 0.43              |
| 2:p:319:LEU:HD21  | 2:q:264:MET:HE1   | 1.98                     | 0.43              |
| 2:r:319:LEU:HD21  | 2:s:264:MET:HE1   | 1.98                     | 0.43              |
| 2:v:159:GLN:OE1   | 2:w:44:GLY:O      | 2.36                     | 0.43              |
| 2:w:56:PRO:CD     | 2:x:79:MET:HG2    | 2.45                     | 0.43              |
| 3:1:136:VAL:O     | 3:1:137:GLN:C     | 2.61                     | 0.43              |
| 3:1:218:TYR:HE1   | 3:ZC:73:ARG:CD    | 2.32                     | 0.43              |
| 3:2:36:ARG:HE     | 3:2:80:LEU:HD22   | 1.82                     | 0.43              |
| 3:2:42:GLU:HG3    | 3:2:43:ASP:O      | 2.18                     | 0.43              |
| 3:3:240:TYR:CG    | 3:8:253:MET:HE3   | 2.53                     | 0.43              |
| 3:4:194:GLU:OE1   | 3:AH:165:ALA:HB1  | 2.19                     | 0.43              |
| 3:5:249:THR:O     | 3:5:253:MET:HG3   | 2.19                     | 0.43              |
| 3:ZC:85:ASN:HD22  | 4:ZN:4:SER:CB     | 2.31                     | 0.43              |
| 3:ZC:240:TYR:CE2  | 4:ZH:395:ILE:HG21 | 2.48                     | 0.43              |
| 4:ZF:386:ALA:HB1  | 4:ZK:402:LEU:HD21 | 1.99                     | 0.43              |
| 4:ZL:84:ARG:HG3   | 4:ZL:84:ARG:HH11  | 1.83                     | 0.43              |
| 4:ZM:129:GLN:NE2  | 4:ZM:132:ALA:HB2  | 2.32                     | 0.43              |
| 4:ZN:9:GLY:C      | 4:ZN:385:ASN:HD22 | 2.25                     | 0.43              |
| 4:ZO:125:PRO:HA   | 4:ZO:126:PRO:HD3  | 1.94                     | 0.43              |
| 4:ZQ:128:ILE:HD13 | 4:ZQ:314:GLN:HB2  | 2.01                     | 0.43              |
| 4:ZQ:352:ASN:OD1  | 4:ZQ:352:ASN:O    | 2.37                     | 0.43              |
| 4:ZS:103:ASP:OD2  | 4:ZS:103:ASP:C    | 2.62                     | 0.43              |
| 4:ZT:185:THR:HG22 | 4:ZT:187:TYR:HE1  | 1.84                     | 0.43              |
| 4:ZT:375:MET:HE1  | 4:ZY:388:THR:HG23 | 1.99                     | 0.43              |
| 4:ZU:297:ASP:OD2  | 4:ZU:297:ASP:N    | 2.41                     | 0.43              |
| 4:ZW:390:LYS:O    | 4:ZW:394:GLN:HG3  | 2.18                     | 0.43              |
| 4:ZX:18:ASP:OD1   | 4:Zc:2:SER:N      | 2.52                     | 0.43              |
| 4:ZZ:307:GLU:O    | 4:ZZ:307:GLU:HG2  | 2.18                     | 0.43              |
| 4:Zf:380:ARG:HA   | 4:Zf:380:ARG:HD3  | 1.78                     | 0.43              |
| 4:Zg:322:ASN:HB3  | 4:Zg:340:SER:HA   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AA:70:GLN:HG3   | 3:AL:3:SER:C      | 2.36                     | 0.43              |
| 5:AB:72:ASP:OD1   | 5:AB:74:THR:HG23  | 2.18                     | 0.43              |
| 5:AC:51:LEU:O     | 5:AC:53:THR:HG23  | 2.19                     | 0.43              |
| 5:AD:34:PHE:HB3   | 5:AD:209:SER:HB2  | 2.00                     | 0.43              |
| 3:AF:35:LYS:HA    | 3:AF:35:LYS:HD3   | 1.92                     | 0.43              |
| 3:AF:242:ILE:HG12 | 3:AL:258:THR:HG22 | 2.01                     | 0.43              |
| 3:AH:127:GLN:N    | 3:AH:141:THR:HG23 | 2.33                     | 0.43              |
| 3:AL:98:LYS:O     | 3:AL:98:LYS:HG2   | 2.19                     | 0.43              |
| 3:AN:140:ILE:HG23 | 3:AN:170:VAL:HG12 | 1.99                     | 0.43              |
| 6:AZ:429:THR:OG1  | 6:Aa:418:GLU:OE2  | 2.36                     | 0.43              |
| 6:Ag:429:THR:OG1  | 6:Ah:418:GLU:OE2  | 2.36                     | 0.43              |
| 7:As:45:ASN:OD1   | 7:As:45:ASN:N     | 2.50                     | 0.43              |
| 9:Av:82:SER:HA    | 10:Az:103:GLN:NE2 | 2.33                     | 0.43              |
| 9:Av:114:GLN:HB3  | 9:Av:115:PRO:HD3  | 2.01                     | 0.43              |
| 9:Aw:42:VAL:HG13  | 10:A3:42:LEU:HD22 | 2.01                     | 0.43              |
| 9:Aw:82:SER:HB2   | 10:A1:103:GLN:O   | 2.18                     | 0.43              |
| 9:Ax:146:ASP:OD1  | 9:Ay:233:GLN:NE2  | 2.51                     | 0.43              |
| 9:Ay:204:LEU:HD11 | 9:Ay:217:ILE:HD12 | 1.99                     | 0.43              |
| 6:UN:99:ARG:O     | 6:UN:103:GLN:HG3  | 2.18                     | 0.43              |
| 6:UP:88:VAL:O     | 6:UP:89:PRO:C     | 2.60                     | 0.43              |
| 6:WG:166:VAL:HG12 | 6:WG:168:GLU:H    | 1.83                     | 0.43              |
| 6:BS:429:THR:OG1  | 6:BT:418:GLU:OE2  | 2.36                     | 0.43              |
| 6:BU:429:THR:OG1  | 6:BV:418:GLU:OE2  | 2.36                     | 0.43              |
| 1:A:102:THR:HG23  | 1:B:130:ASN:HD22  | 1.82                     | 0.43              |
| 1:B:50:SER:HB3    | 2:y:32:ARG:HH11   | 1.81                     | 0.43              |
| 1:B:126:ALA:HB3   | 1:D:232:MET:HE1   | 1.99                     | 0.43              |
| 1:G:126:ALA:HB3   | 1:I:232:MET:HE1   | 1.99                     | 0.43              |
| 1:J:136:GLY:CA    | 1:L:213:ILE:HG23  | 2.42                     | 0.43              |
| 1:M:126:ALA:HB3   | 1:O:232:MET:HE1   | 1.99                     | 0.43              |
| 1:M:181:SER:HB2   | 1:N:31:VAL:CG1    | 2.45                     | 0.43              |
| 1:N:71:PRO:HB2    | 1:N:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:N:232:MET:HG3   | 1:O:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:R:126:ALA:HB3   | 1:T:232:MET:HE1   | 1.99                     | 0.43              |
| 1:T:106:PHE:HB3   | 1:T:109:VAL:HG22  | 2.00                     | 0.43              |
| 1:U:71:PRO:HB2    | 1:U:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:W:126:ALA:HB3   | 1:Y:232:MET:HE1   | 1.99                     | 0.43              |
| 1:X:126:ALA:HB3   | 1:Z:232:MET:HE1   | 1.99                     | 0.43              |
| 2:a:159:GLN:OE1   | 2:b:44:GLY:O      | 2.36                     | 0.43              |
| 2:c:47:GLY:H      | 2:c:83:ASN:HD22   | 1.64                     | 0.43              |
| 2:d:319:LEU:HD21  | 2:e:264:MET:HE1   | 1.98                     | 0.43              |
| 2:i:253:VAL:HG11  | 2:i:349:LEU:HD13  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:r:21:ARG:HD2    | 2:r:21:ARG:HA      | 1.75                     | 0.43              |
| 2:r:78:ASN:OD1    | 2:r:78:ASN:N       | 2.51                     | 0.43              |
| 2:s:159:GLN:OE1   | 2:t:44:GLY:O       | 2.36                     | 0.43              |
| 3:0:85:ASN:O      | 3:0:221:THR:OG1    | 2.34                     | 0.43              |
| 3:0:260:LEU:C     | 3:AI:245:LYS:HE2   | 2.44                     | 0.43              |
| 3:4:140:ILE:HD13  | 3:4:157:VAL:HG21   | 2.00                     | 0.43              |
| 3:7:19:MET:HB2    | 3:7:236:VAL:HG11   | 2.00                     | 0.43              |
| 3:8:249:THR:O     | 3:8:253:MET:HG3    | 2.18                     | 0.43              |
| 3:9:92:SER:O      | 3:9:216:GLN:NE2    | 2.45                     | 0.43              |
| 4:ZK:374:ASN:O    | 4:ZK:376:ILE:N     | 2.51                     | 0.43              |
| 4:ZP:188:ASP:OD2  | 4:ZP:192:ASN:N     | 2.51                     | 0.43              |
| 4:ZR:271:THR:HG22 | 4:ZX:286:PRO:CB    | 2.48                     | 0.43              |
| 4:ZS:6:ALA:C      | 4:ZS:8:SER:N       | 2.76                     | 0.43              |
| 4:ZU:180:LYS:HB3  | 4:ZU:200:PHE:HD1   | 1.83                     | 0.43              |
| 4:ZV:346:GLY:HA3  | 4:ZV:353:PHE:CE2   | 2.54                     | 0.43              |
| 4:ZX:37:ALA:HA    | 4:ZX:57:ILE:HD13   | 2.00                     | 0.43              |
| 4:Zc:10:LEU:HD12  | 4:Zc:10:LEU:HA     | 1.71                     | 0.43              |
| 4:Zc:381:ASN:O    | 4:Zc:385:ASN:ND2   | 2.51                     | 0.43              |
| 4:Zf:396:LEU:HD23 | 4:Zf:396:LEU:HA    | 1.83                     | 0.43              |
| 5:AB:29:ALA:O     | 5:AB:209:SER:OG    | 2.36                     | 0.43              |
| 3:AG:260:LEU:CD2  | 12:BB:106:MET:SD   | 3.03                     | 0.43              |
| 3:AH:6:TRP:CE2    | 12:BC:77:VAL:HB    | 2.54                     | 0.43              |
| 3:AH:188:GLY:O    | 3:AH:190:ASN:N     | 2.51                     | 0.43              |
| 3:AI:187:ILE:HG23 | 3:AI:193:ILE:HG12  | 2.00                     | 0.43              |
| 3:AK:9:LYS:O      | 3:AK:10:THR:C      | 2.61                     | 0.43              |
| 6:AT:429:THR:OG1  | 6:AU:418:GLU:OE2   | 2.36                     | 0.43              |
| 6:AX:429:THR:OG1  | 6:AY:418:GLU:OE2   | 2.36                     | 0.43              |
| 6:Ai:421:GLY:O    | 6:Ai:426:ARG:NH2   | 2.51                     | 0.43              |
| 8:At:104:LEU:HD12 | 8:At:104:LEU:HA    | 1.78                     | 0.43              |
| 9:Ay:66:ARG:NH2   | 9:Ay:181:THR:HG21  | 2.33                     | 0.43              |
| 12:BB:7:PHE:CD2   | 12:BB:119:LEU:HD11 | 2.54                     | 0.43              |
| 6:WA:115:LEU:HD22 | 6:WA:134:ARG:HD2   | 2.01                     | 0.43              |
| 6:WI:136:LEU:O    | 6:WI:137:GLU:C     | 2.62                     | 0.43              |
| 6:WL:147:LEU:O    | 6:WL:148:GLY:C     | 2.61                     | 0.43              |
| 6:WN:147:LEU:O    | 6:WN:148:GLY:C     | 2.60                     | 0.43              |
| 6:WU:158:ALA:O    | 6:WU:160:PRO:HD3   | 2.18                     | 0.43              |
| 6:WV:113:PHE:HB3  | 6:WW:134:ARG:NH1   | 2.33                     | 0.43              |
| 6:WV:117:ASP:OD1  | 6:WW:120:LYS:NZ    | 2.51                     | 0.43              |
| 12:BD:54:ALA:CB   | 12:BD:55:PRO:CD    | 2.97                     | 0.43              |
| 1:B:71:PRO:HB2    | 1:B:152:VAL:HG21   | 2.01                     | 0.43              |
| 1:E:71:PRO:HB2    | 1:E:152:VAL:HG21   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:H:214:ASN:ND2   | 1:I:173:GLN:NE2    | 2.67                     | 0.43              |
| 1:K:232:MET:HG3   | 1:L:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:L:232:MET:HG3   | 1:M:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:M:232:MET:HG3   | 1:N:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:O:232:MET:HG3   | 1:P:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:Q:126:ALA:HB3   | 1:S:232:MET:HE1    | 1.99                     | 0.43              |
| 1:R:71:PRO:HB2    | 1:R:152:VAL:HG21   | 2.00                     | 0.43              |
| 1:T:136:GLY:CA    | 1:V:213:ILE:HG23   | 2.42                     | 0.43              |
| 1:T:232:MET:HE3   | 1:T:232:MET:HB2    | 1.90                     | 0.43              |
| 1:V:71:PRO:HB2    | 1:V:152:VAL:HG21   | 2.01                     | 0.43              |
| 2:d:56:PRO:CD     | 2:e:79:MET:HG2     | 2.45                     | 0.43              |
| 2:n:159:GLN:OE1   | 2:o:44:GLY:O       | 2.36                     | 0.43              |
| 2:o:93:TYR:OH     | 2:o:173:ARG:O      | 2.25                     | 0.43              |
| 2:v:93:TYR:OH     | 2:v:173:ARG:O      | 2.25                     | 0.43              |
| 3:ZA:140:ILE:HD12 | 3:ZA:171:GLY:HA3   | 2.00                     | 0.43              |
| 3:ZA:208:LEU:C    | 3:ZA:210:GLY:H     | 2.26                     | 0.43              |
| 4:ZI:80:ASN:OD1   | 4:ZI:81:GLY:N      | 2.52                     | 0.43              |
| 4:ZI:382:TYR:CE1  | 4:ZN:395:ILE:CG2   | 2.91                     | 0.43              |
| 4:ZJ:248:THR:HG23 | 4:ZJ:257:ALA:O     | 2.19                     | 0.43              |
| 4:ZL:322:ASN:OD1  | 4:ZL:325:GLY:N     | 2.50                     | 0.43              |
| 4:ZN:380:ARG:HG3  | 4:ZT:396:LEU:HD12  | 2.01                     | 0.43              |
| 4:ZS:180:LYS:NZ   | 4:ZS:274:ASN:O     | 2.51                     | 0.43              |
| 4:ZT:382:TYR:OH   | 4:ZY:399:LEU:HD11  | 2.18                     | 0.43              |
| 4:Zf:103:ASP:OD2  | 4:Zf:104:GLU:N     | 2.48                     | 0.43              |
| 5:AB:146:LEU:HB2  | 5:AB:155:VAL:HG22  | 2.01                     | 0.43              |
| 5:AD:65:ASP:OD2   | 5:AD:212:LYS:NZ    | 2.52                     | 0.43              |
| 5:AD:169:ASN:OD1  | 5:AD:169:ASN:N     | 2.51                     | 0.43              |
| 3:AK:95:VAL:O     | 3:AK:118:GLY:HA3   | 2.19                     | 0.43              |
| 3:AL:2:ILE:CG1    | 3:AL:254:LEU:HD11  | 2.48                     | 0.43              |
| 3:AM:87:SER:OG    | 3:AM:219:VAL:HG23  | 2.19                     | 0.43              |
| 6:AR:418:GLU:OE2  | 6:Aa:429:THR:OG1   | 2.36                     | 0.43              |
| 6:Aj:421:GLY:O    | 6:Aj:426:ARG:NH2   | 2.51                     | 0.43              |
| 6:AQ:374:HIS:CG   | 10:A5:15:GLN:HB2   | 2.53                     | 0.43              |
| 7:Aq:89:GLY:O     | 6:WW:164:LEU:CB    | 2.65                     | 0.43              |
| 8:At:54:ILE:HD11  | 9:Ay:153:LEU:HB3   | 2.01                     | 0.43              |
| 9:Av:116:PHE:HE2  | 11:A7:4:ARG:NH1    | 2.12                     | 0.43              |
| 10:A3:77:LYS:NZ   | 11:A9:13:GLN:OE1   | 2.36                     | 0.43              |
| 10:A4:75:MET:SD   | 11:A9:122:VAL:HG22 | 2.59                     | 0.43              |
| 11:A8:32:ASN:ND2  | 12:BC:51:VAL:HG12  | 2.34                     | 0.43              |
| 11:A8:65:LEU:HD23 | 11:A8:75:ALA:CB    | 2.49                     | 0.43              |
| 6:UJ:100:LEU:HD23 | 6:UJ:103:GLN:HE21  | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UK:102:GLN:CG   | 6:UK:193:ALA:HB2  | 2.49                     | 0.43              |
| 6:WA:113:PHE:CE2  | 6:WA:139:GLU:HG3  | 2.54                     | 0.43              |
| 6:WB:190:GLN:O    | 6:WB:191:ILE:C    | 2.61                     | 0.43              |
| 6:WG:166:VAL:CG1  | 6:WG:168:GLU:HB3  | 2.49                     | 0.43              |
| 6:WL:219:LEU:HG   | 6:WL:221:THR:H    | 1.82                     | 0.43              |
| 6:WM:190:GLN:HA   | 6:WN:217:GLY:HA3  | 2.00                     | 0.43              |
| 12:BF:125:MET:HE3 | 6:BG:316:LEU:HD11 | 2.00                     | 0.43              |
| 1:B:232:MET:HE1   | 1:Z:126:ALA:HB3   | 1.99                     | 0.43              |
| 1:E:144:PHE:CE2   | 1:F:171:ILE:CD1   | 3.01                     | 0.43              |
| 1:H:62:TYR:CE1    | 2:f:129:VAL:HG13  | 2.48                     | 0.43              |
| 1:J:232:MET:HG3   | 1:K:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:K:214:ASN:ND2   | 1:L:173:GLN:NE2   | 2.67                     | 0.43              |
| 1:L:126:ALA:HB3   | 1:N:232:MET:HE1   | 1.99                     | 0.43              |
| 1:L:232:MET:HE3   | 1:L:232:MET:HB2   | 1.90                     | 0.43              |
| 1:N:165:GLY:C     | 1:O:35:THR:HG21   | 2.40                     | 0.43              |
| 1:P:126:ALA:HB3   | 1:R:232:MET:HE1   | 2.00                     | 0.43              |
| 1:P:232:MET:HG3   | 1:Q:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:Q:71:PRO:HB2    | 1:Q:152:VAL:HG21  | 2.01                     | 0.43              |
| 1:R:232:MET:HG3   | 1:S:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:S:214:ASN:ND2   | 1:T:173:GLN:NE2   | 2.67                     | 0.43              |
| 1:T:65:LEU:CG     | 2:s:65:MET:HG3    | 2.39                     | 0.43              |
| 1:V:106:PHE:HB3   | 1:V:109:VAL:HG22  | 2.00                     | 0.43              |
| 1:V:232:MET:HG3   | 1:W:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:Y:106:PHE:HB3   | 1:Y:109:VAL:HG22  | 2.00                     | 0.43              |
| 2:b:159:GLN:OE1   | 2:c:44:GLY:O      | 2.36                     | 0.43              |
| 2:c:250:ASP:OD1   | 2:d:23:ARG:NE     | 2.51                     | 0.43              |
| 2:f:250:ASP:OD1   | 2:g:23:ARG:NE     | 2.51                     | 0.43              |
| 2:k:78:ASN:OD1    | 2:k:78:ASN:N      | 2.51                     | 0.43              |
| 2:l:192:GLU:H     | 2:l:192:GLU:HG3   | 1.52                     | 0.43              |
| 2:o:319:LEU:HD21  | 2:p:264:MET:HE1   | 1.97                     | 0.43              |
| 2:t:159:GLN:OE1   | 2:u:44:GLY:O      | 2.36                     | 0.43              |
| 2:w:78:ASN:OD1    | 2:w:78:ASN:N      | 2.51                     | 0.43              |
| 2:w:258:ARG:HH12  | 2:y:140:ASN:HD21  | 1.64                     | 0.43              |
| 3:0:143:PRO:HG2   | 3:0:159:VAL:HG11  | 1.99                     | 0.43              |
| 3:2:209:ASN:CG    | 3:AL:145:ASN:HD22 | 2.26                     | 0.43              |
| 3:3:107:LEU:HD21  | 3:3:191:LEU:HD13  | 2.00                     | 0.43              |
| 3:6:42:GLU:HB3    | 3:6:75:VAL:HG22   | 2.01                     | 0.43              |
| 3:8:42:GLU:N      | 3:8:73:ARG:O      | 2.52                     | 0.43              |
| 4:ZJ:121:ALA:HB1  | 4:ZJ:126:PRO:HB2  | 2.00                     | 0.43              |
| 4:ZK:236:GLY:CA   | 4:ZQ:190:GLN:HE22 | 2.32                     | 0.43              |
| 4:ZN:397:ASN:O    | 4:ZN:398:THR:C    | 2.60                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZS:41:ASP:OD2   | 4:ZS:41:ASP:N      | 2.45                     | 0.43              |
| 4:ZT:2:SER:C      | 4:ZT:4:SER:H       | 2.27                     | 0.43              |
| 4:Za:112:GLN:N    | 4:Za:112:GLN:OE1   | 2.51                     | 0.43              |
| 4:Zb:194:HIS:CE1  | 4:Zb:251:ILE:HD12  | 2.53                     | 0.43              |
| 4:Zf:71:ARG:HB2   | 4:Zf:74:ASP:OD2    | 2.19                     | 0.43              |
| 4:Zf:78:SER:OG    | 4:Zf:355:LYS:O     | 2.29                     | 0.43              |
| 4:Zg:117:THR:HA   | 4:Zg:136:PRO:HA    | 2.01                     | 0.43              |
| 5:AA:173:ARG:CD   | 3:AF:46:TYR:CZ     | 3.02                     | 0.43              |
| 5:AD:86:GLY:HA2   | 5:AD:199:ILE:HD12  | 2.01                     | 0.43              |
| 5:AD:221:ILE:HG21 | 3:AJ:251:ASP:CG    | 2.43                     | 0.43              |
| 3:AG:95:VAL:O     | 3:AG:118:GLY:HA3   | 2.18                     | 0.43              |
| 3:AG:225:ASN:OD1  | 3:AG:226:VAL:N     | 2.52                     | 0.43              |
| 7:Ab:20:LEU:HD11  | 7:Ab:73:LEU:CD2    | 2.49                     | 0.43              |
| 6:Ad:429:THR:OG1  | 6:Ae:418:GLU:OE2   | 2.36                     | 0.43              |
| 6:Ah:421:GLY:O    | 6:Ah:426:ARG:NH2   | 2.51                     | 0.43              |
| 6:Ak:429:THR:OG1  | 6:Al:418:GLU:OE2   | 2.36                     | 0.43              |
| 6:Ao:429:THR:OG1  | 6:Ap:418:GLU:OE2   | 2.36                     | 0.43              |
| 9:Aw:142:THR:HG23 | 6:WW:166:VAL:HG23  | 2.00                     | 0.43              |
| 9:Ax:60:MET:HE3   | 9:Ax:60:MET:HB3    | 1.87                     | 0.43              |
| 9:Ay:68:ILE:O     | 9:Ay:70:VAL:N      | 2.52                     | 0.43              |
| 10:Az:74:ASP:OD2  | 10:Az:74:ASP:N     | 2.52                     | 0.43              |
| 10:A4:11:ILE:HG22 | 6:BX:372:ILE:CG2   | 2.47                     | 0.43              |
| 6:UN:125:GLN:C    | 6:UN:128:GLU:H     | 2.27                     | 0.43              |
| 6:WH:139:GLU:HB3  | 6:WI:154:ARG:NH2   | 2.33                     | 0.43              |
| 6:WH:186:LEU:HD22 | 6:WH:190:GLN:HG2   | 2.00                     | 0.43              |
| 6:WI:191:ILE:O    | 6:WI:195:VAL:HG23  | 2.19                     | 0.43              |
| 6:WK:165:PHE:O    | 6:WK:166:VAL:HB    | 2.19                     | 0.43              |
| 6:WK:181:GLU:O    | 6:WK:182:PRO:C     | 2.60                     | 0.43              |
| 6:WS:193:ALA:HB1  | 6:WT:213:VAL:CG1   | 2.48                     | 0.43              |
| 6:WT:113:PHE:CE1  | 6:WU:134:ARG:HG2   | 2.54                     | 0.43              |
| 12:BC:7:PHE:HA    | 12:BC:119:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:232:MET:HE1   | 1:Y:126:ALA:HB3    | 2.00                     | 0.43              |
| 1:F:214:ASN:ND2   | 1:G:173:GLN:NE2    | 2.67                     | 0.43              |
| 1:H:144:PHE:CE2   | 1:I:171:ILE:CD1    | 3.01                     | 0.43              |
| 1:I:232:MET:HG3   | 1:J:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:S:106:PHE:HB3   | 1:S:109:VAL:HG22   | 2.00                     | 0.43              |
| 1:T:232:MET:HG3   | 1:U:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:X:232:MET:HG3   | 1:Y:223:GLN:HB2    | 2.01                     | 0.43              |
| 1:Y:232:MET:HG3   | 1:Z:223:GLN:HB2    | 2.01                     | 0.43              |
| 2:g:78:ASN:OD1    | 2:g:78:ASN:N       | 2.51                     | 0.43              |
| 2:h:253:VAL:HG11  | 2:h:349:LEU:HD13   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:j:253:VAL:HG11  | 2:j:349:LEU:HD13  | 2.01                     | 0.43              |
| 2:k:250:ASP:OD1   | 2:l:23:ARG:NE     | 2.51                     | 0.43              |
| 2:o:130:ASP:OD1   | 2:o:130:ASP:N     | 2.47                     | 0.43              |
| 2:u:78:ASN:OD1    | 2:u:78:ASN:N      | 2.51                     | 0.43              |
| 2:z:78:ASN:OD1    | 2:z:78:ASN:N      | 2.51                     | 0.43              |
| 3:3:173:LEU:HD23  | 3:3:214:LEU:HD13  | 1.99                     | 0.43              |
| 3:4:253:MET:HE2   | 3:AN:240:TYR:CG   | 2.54                     | 0.43              |
| 3:5:28:ASN:OD1    | 3:ZA:72:VAL:CG2   | 2.67                     | 0.43              |
| 3:5:189:GLU:HG2   | 3:ZA:42:GLU:OE1   | 2.18                     | 0.43              |
| 3:7:142:ILE:HD13  | 3:7:170:VAL:HG21  | 2.00                     | 0.43              |
| 3:ZA:227:ALA:HB1  | 4:ZL:399:LEU:CD2  | 2.49                     | 0.43              |
| 3:ZD:167:PRO:HG3  | 4:ZO:338:GLN:CD   | 2.44                     | 0.43              |
| 4:ZF:355:LYS:H    | 4:ZF:355:LYS:HG2  | 1.66                     | 0.43              |
| 4:ZK:102:LEU:HD21 | 4:ZK:106:ARG:HA   | 2.00                     | 0.43              |
| 4:ZQ:265:ASN:C    | 4:ZQ:267:MET:HE2  | 2.42                     | 0.43              |
| 4:ZR:157:ASN:HD21 | 4:ZX:143:LEU:HD13 | 1.82                     | 0.43              |
| 4:ZR:387:GLN:O    | 4:ZR:391:THR:HG23 | 2.19                     | 0.43              |
| 4:ZV:44:ALA:HB3   | 4:ZV:50:LEU:HD22  | 2.01                     | 0.43              |
| 4:ZV:144:MET:HB3  | 4:ZV:304:TYR:CE2  | 2.54                     | 0.43              |
| 4:ZY:5:GLN:HG2    | 4:ZY:50:LEU:O     | 2.19                     | 0.43              |
| 4:ZZ:2:SER:OG     | 4:ZZ:3:PHE:N      | 2.48                     | 0.43              |
| 4:ZZ:373:VAL:HG13 | 4:Zf:389:ILE:HD13 | 2.00                     | 0.43              |
| 4:Zc:60:ASP:O     | 4:Zc:365:ASN:ND2  | 2.52                     | 0.43              |
| 4:Ze:397:ASN:O    | 4:Ze:400:VAL:N    | 2.52                     | 0.43              |
| 4:Zg:42:MET:SD    | 4:Zg:53:LYS:HB3   | 2.58                     | 0.43              |
| 5:AA:217:MET:HE3  | 3:AL:257:LEU:O    | 2.06                     | 0.43              |
| 5:AC:51:LEU:O     | 5:AC:53:THR:N     | 2.52                     | 0.43              |
| 5:AD:48:GLY:HA2   | 6:BO:324:ASN:HB3  | 2.00                     | 0.43              |
| 5:AE:16:LEU:HA    | 3:AJ:253:MET:HE1  | 1.99                     | 0.43              |
| 3:AG:31:THR:HG23  | 3:AL:42:GLU:HA    | 2.01                     | 0.43              |
| 3:AH:44:LEU:CD2   | 12:BC:78:TYR:CG   | 3.02                     | 0.43              |
| 3:AN:138:PRO:HG2  | 3:AN:172:GLN:O    | 2.18                     | 0.43              |
| 3:AN:254:LEU:O    | 3:AN:258:THR:HG23 | 2.19                     | 0.43              |
| 6:Ah:429:THR:OG1  | 6:Ai:418:GLU:OE2  | 2.36                     | 0.43              |
| 6:Al:429:THR:OG1  | 6:Am:418:GLU:OE2  | 2.36                     | 0.43              |
| 6:Am:429:THR:OG1  | 6:An:418:GLU:OE2  | 2.36                     | 0.43              |
| 9:Au:37:SER:HA    | 9:Au:123:MET:HG3  | 2.01                     | 0.43              |
| 9:Au:171:LEU:HB3  | 9:Au:172:PRO:HD3  | 2.01                     | 0.43              |
| 10:A4:48:ARG:HH22 | 11:A0:6:ASP:CG    | 2.23                     | 0.43              |
| 11:A6:85:LEU:HD23 | 11:A6:85:LEU:HA   | 1.81                     | 0.43              |
| 6:WM:172:PRO:HD2  | 6:WM:204:GLY:O    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WS:113:PHE:HB3  | 6:WT:134:ARG:CZ   | 2.49                     | 0.43              |
| 1:A:136:GLY:CA    | 1:C:213:ILE:HG23  | 2.42                     | 0.43              |
| 1:A:223:GLN:HB2   | 1:Z:232:MET:HG3   | 2.01                     | 0.43              |
| 1:F:86:VAL:HB     | 1:F:142:ASN:ND2   | 2.34                     | 0.43              |
| 1:F:165:GLY:C     | 1:G:35:THR:HG21   | 2.40                     | 0.43              |
| 1:G:47:ALA:HB1    | 2:d:178:GLN:HG3   | 1.96                     | 0.43              |
| 1:M:166:GLU:HB2   | 1:N:35:THR:CG2    | 2.30                     | 0.43              |
| 1:O:50:SER:HB3    | 2:l:32:ARG:HH11   | 1.81                     | 0.43              |
| 1:O:166:GLU:HB2   | 1:P:35:THR:CG2    | 2.30                     | 0.43              |
| 1:Q:86:VAL:HB     | 1:Q:142:ASN:ND2   | 2.34                     | 0.43              |
| 1:S:232:MET:HG3   | 1:T:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:U:214:ASN:ND2   | 1:V:173:GLN:NE2   | 2.67                     | 0.43              |
| 1:V:214:ASN:ND2   | 1:W:173:GLN:NE2   | 2.67                     | 0.43              |
| 1:W:232:MET:HG3   | 1:X:223:GLN:HB2   | 2.01                     | 0.43              |
| 1:X:214:ASN:ND2   | 1:Y:173:GLN:NE2   | 2.67                     | 0.43              |
| 2:c:56:PRO:CD     | 2:d:79:MET:HG2    | 2.45                     | 0.43              |
| 2:g:253:VAL:HG11  | 2:g:349:LEU:HD13  | 2.01                     | 0.43              |
| 2:h:250:ASP:OD1   | 2:i:23:ARG:NE     | 2.51                     | 0.43              |
| 2:h:266:ARG:HA    | 2:h:328:LEU:HD22  | 2.01                     | 0.43              |
| 2:k:93:TYR:OH     | 2:k:173:ARG:O     | 2.25                     | 0.43              |
| 2:n:346:MET:HE2   | 2:p:142:LEU:HD11  | 1.95                     | 0.43              |
| 2:p:78:ASN:OD1    | 2:p:78:ASN:N      | 2.51                     | 0.43              |
| 2:p:159:GLN:OE1   | 2:q:44:GLY:O      | 2.36                     | 0.43              |
| 2:t:78:ASN:OD1    | 2:t:78:ASN:N      | 2.51                     | 0.43              |
| 2:y:159:GLN:OE1   | 2:z:44:GLY:O      | 2.36                     | 0.43              |
| 3:1:7:ILE:HG12    | 3:1:70:THR:O      | 2.18                     | 0.43              |
| 3:9:245:LYS:HB2   | 3:9:245:LYS:HE2   | 1.78                     | 0.43              |
| 4:ZG:154:MET:HE2  | 4:ZG:154:MET:HB3  | 1.73                     | 0.43              |
| 4:ZJ:199:TYR:O    | 4:ZJ:210:VAL:HA   | 2.19                     | 0.43              |
| 4:ZJ:380:ARG:CZ   | 4:ZP:393:ASP:OD1  | 2.67                     | 0.43              |
| 4:ZM:71:ARG:NH1   | 4:ZM:74:ASP:OD1   | 2.52                     | 0.43              |
| 4:ZN:269:GLN:HE22 | 4:ZT:146:ALA:H    | 1.66                     | 0.43              |
| 4:ZO:212:THR:O    | 4:ZO:223:PRO:HG3  | 2.19                     | 0.43              |
| 4:ZT:10:LEU:HD21  | 4:ZY:399:LEU:HD11 | 2.01                     | 0.43              |
| 4:ZT:146:ALA:HB2  | 4:ZT:286:PRO:HD3  | 1.99                     | 0.43              |
| 4:ZU:269:GLN:CG   | 4:Za:286:PRO:HG2  | 2.49                     | 0.43              |
| 4:ZV:188:ASP:OD2  | 4:ZV:194:HIS:NE2  | 2.52                     | 0.43              |
| 4:ZW:380:ARG:NH2  | 4:Zc:393:ASP:OD2  | 2.52                     | 0.43              |
| 4:ZY:298:GLY:HA3  | 4:ZY:315:ILE:HG22 | 2.01                     | 0.43              |
| 4:Za:149:THR:HG23 | 4:Za:259:PHE:HB3  | 2.01                     | 0.43              |
| 4:Zc:375:MET:HE1  | 4:Zh:388:THR:OG1  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zd:83:PHE:HB2   | 4:Zd:95:SER:O     | 2.19                     | 0.43              |
| 4:Zd:144:MET:HE3  | 4:Zd:145:ALA:H    | 1.84                     | 0.43              |
| 4:Zf:107:ASN:ND2  | 4:Zf:138:THR:HG22 | 2.34                     | 0.43              |
| 4:Zg:96:ARG:H     | 4:Zg:334:TRP:HZ3  | 1.67                     | 0.43              |
| 4:Zg:380:ARG:HD3  | 4:Zg:380:ARG:HA   | 1.45                     | 0.43              |
| 5:AA:245:ASN:OD1  | 5:AA:246:GLN:N    | 2.51                     | 0.43              |
| 5:AB:80:VAL:HB    | 5:AB:201:ILE:HD11 | 2.01                     | 0.43              |
| 5:AC:115:ILE:HG13 | 5:AC:120:VAL:HG22 | 2.01                     | 0.43              |
| 5:AD:214:VAL:CG1  | 3:AJ:12:LEU:CD1   | 2.95                     | 0.43              |
| 5:AE:165:LYS:HB2  | 5:AE:165:LYS:HE3  | 1.82                     | 0.43              |
| 3:AF:107:LEU:HD11 | 3:AF:191:LEU:HD13 | 2.01                     | 0.43              |
| 3:AG:2:ILE:HD13   | 3:AG:250:THR:HG23 | 2.01                     | 0.43              |
| 3:AL:6:TRP:O      | 3:AL:10:THR:HG23  | 2.18                     | 0.43              |
| 6:AT:421:GLY:O    | 6:AT:426:ARG:NH2  | 2.51                     | 0.43              |
| 6:AV:357:SER:OG   | 6:BO:318:ASN:CG   | 2.62                     | 0.43              |
| 6:AI:296:ARG:HG2  | 6:AI:296:ARG:NH1  | 2.34                     | 0.43              |
| 6:AL:294:ARG:HD2  | 11:A7:68:THR:CG2  | 2.49                     | 0.43              |
| 6:AN:290:LYS:HE3  | 6:AN:290:LYS:HB2  | 1.93                     | 0.43              |
| 8:AT:49:MET:HE2   | 8:AT:49:MET:HB2   | 1.86                     | 0.43              |
| 9:AV:161:GLY:O    | 9:AV:162:PRO:C    | 2.61                     | 0.43              |
| 9:AV:190:PHE:CD1  | 9:AW:220:PRO:HG3  | 2.54                     | 0.43              |
| 9:AX:138:MET:O    | 9:AX:142:THR:OG1  | 2.28                     | 0.43              |
| 9:AY:195:ILE:O    | 9:AY:199:VAL:HG13 | 2.18                     | 0.43              |
| 10:A1:75:MET:HE3  | 10:A1:75:MET:HB3  | 1.83                     | 0.43              |
| 10:A3:59:PHE:CD2  | 11:A8:118:MET:HE1 | 2.54                     | 0.43              |
| 6:UJ:75:ILE:HG21  | 6:UJ:96:LEU:HD11  | 2.00                     | 0.43              |
| 6:UK:75:ILE:HG21  | 6:UK:96:LEU:HD11  | 2.00                     | 0.43              |
| 6:UL:75:ILE:HG21  | 6:UL:96:LEU:HD11  | 2.00                     | 0.43              |
| 6:UM:125:GLN:C    | 6:UM:128:GLU:H    | 2.27                     | 0.43              |
| 6:UO:98:LEU:CD1   | 6:UO:146:THR:HG1  | 2.30                     | 0.43              |
| 6:WD:172:PRO:HD2  | 6:WD:204:GLY:O    | 2.18                     | 0.43              |
| 6:WG:145:GLU:O    | 6:WG:146:THR:C    | 2.62                     | 0.43              |
| 6:WR:143:THR:O    | 6:WR:146:THR:OG1  | 2.30                     | 0.43              |
| 6:BR:290:LYS:HE3  | 6:BR:290:LYS:HB2  | 1.93                     | 0.43              |
| 1:C:214:ASN:ND2   | 1:D:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:E:86:VAL:HB     | 1:E:142:ASN:ND2   | 2.34                     | 0.42              |
| 1:E:214:ASN:ND2   | 1:F:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:I:214:ASN:ND2   | 1:J:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:L:166:GLU:HB2   | 1:M:35:THR:CG2    | 2.30                     | 0.42              |
| 1:N:166:GLU:HB2   | 1:O:35:THR:CG2    | 2.30                     | 0.42              |
| 1:N:214:ASN:ND2   | 1:O:173:GLN:NE2   | 2.67                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:214:ASN:ND2   | 1:Q:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:Q:214:ASN:ND2   | 1:R:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:Q:232:MET:HG3   | 1:R:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:R:144:PHE:CE2   | 1:S:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:U:232:MET:HG3   | 1:V:223:GLN:HB2   | 2.01                     | 0.42              |
| 2:d:250:ASP:OD1   | 2:e:23:ARG:NE     | 2.51                     | 0.42              |
| 2:h:276:ALA:HB3   | 2:i:262:VAL:HB    | 2.01                     | 0.42              |
| 2:i:276:ALA:HB3   | 2:j:262:VAL:HB    | 2.01                     | 0.42              |
| 2:j:250:ASP:OD1   | 2:k:23:ARG:NE     | 2.52                     | 0.42              |
| 2:k:253:VAL:HG11  | 2:k:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:q:159:GLN:OE1   | 2:r:44:GLY:O      | 2.36                     | 0.42              |
| 2:u:159:GLN:OE1   | 2:v:44:GLY:O      | 2.36                     | 0.42              |
| 2:v:192:GLU:H     | 2:v:192:GLU:HG3   | 1.52                     | 0.42              |
| 2:w:188:GLN:HE21  | 2:w:188:GLN:HB2   | 1.63                     | 0.42              |
| 2:w:276:ALA:HB3   | 2:x:262:VAL:HB    | 2.01                     | 0.42              |
| 2:x:276:ALA:HB3   | 2:y:262:VAL:HB    | 2.01                     | 0.42              |
| 3:0:45:LEU:HD13   | 5:AD:83:GLN:HA    | 2.00                     | 0.42              |
| 3:1:44:LEU:HD23   | 5:AE:202:MET:SD   | 2.59                     | 0.42              |
| 3:1:73:ARG:NE     | 5:AE:202:MET:SD   | 2.92                     | 0.42              |
| 3:2:58:GLU:N      | 5:AA:140:ASP:OD2  | 2.52                     | 0.42              |
| 3:4:34:PHE:HB3    | 3:4:222:SER:HB3   | 2.01                     | 0.42              |
| 3:5:83:GLN:NE2    | 3:5:97:ILE:O      | 2.46                     | 0.42              |
| 3:5:245:LYS:HE2   | 3:5:245:LYS:HB2   | 1.52                     | 0.42              |
| 3:6:175:LEU:HG    | 3:6:206:PRO:HG3   | 2.00                     | 0.42              |
| 3:ZA:59:GLN:HG2   | 3:ZA:60:THR:HG23  | 2.01                     | 0.42              |
| 3:ZA:235:GLN:NE2  | 4:ZG:3:PHE:CB     | 2.80                     | 0.42              |
| 3:ZC:86:LEU:HD11  | 3:ZC:98:LYS:HD3   | 2.01                     | 0.42              |
| 3:ZE:137:GLN:HA   | 3:ZE:139:ALA:N    | 2.32                     | 0.42              |
| 3:ZE:255:GLN:O    | 3:ZE:259:GLN:HG2  | 2.19                     | 0.42              |
| 4:ZL:380:ARG:HD3  | 4:ZL:380:ARG:HA   | 1.66                     | 0.42              |
| 4:ZN:390:LYS:O    | 4:ZN:394:GLN:HG3  | 2.19                     | 0.42              |
| 4:ZP:175:ALA:HA   | 4:ZP:178:TYR:CZ   | 2.54                     | 0.42              |
| 4:ZR:26:ASN:CG    | 4:ZW:52:VAL:HG22  | 2.44                     | 0.42              |
| 4:ZR:246:ILE:HD13 | 4:ZR:246:ILE:HA   | 1.88                     | 0.42              |
| 4:ZS:288:ASP:O    | 4:ZS:305:SER:N    | 2.52                     | 0.42              |
| 4:ZU:159:ASN:HA   | 4:ZU:269:GLN:O    | 2.19                     | 0.42              |
| 4:ZW:159:ASN:ND2  | 4:ZW:162:ASP:OD1  | 2.45                     | 0.42              |
| 4:Zb:111:MET:N    | 4:Zb:111:MET:SD   | 2.92                     | 0.42              |
| 4:Zb:373:VAL:HG11 | 4:Zh:7:VAL:HG22   | 2.00                     | 0.42              |
| 4:Zf:99:GLN:HE21  | 4:Zf:361:LEU:HD11 | 1.84                     | 0.42              |
| 5:AB:181:LEU:HD11 | 5:AB:193:LEU:HD21 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AC:50:SER:CB    | 11:A8:91:ASP:O    | 2.67                     | 0.42              |
| 5:AD:189:ARG:HD2  | 5:AD:193:LEU:HD23 | 2.00                     | 0.42              |
| 5:AE:52:ALA:O     | 5:AE:54:ARG:N     | 2.51                     | 0.42              |
| 5:AE:55:THR:HB    | 12:BF:30:ASN:HD21 | 1.85                     | 0.42              |
| 6:AV:429:THR:OG1  | 6:AW:418:GLU:OE2  | 2.36                     | 0.42              |
| 6:AY:294:ARG:HD2  | 11:A9:68:THR:HG21 | 2.01                     | 0.42              |
| 6:Af:429:THR:OG1  | 6:Ag:418:GLU:OE2  | 2.36                     | 0.42              |
| 6:Ag:421:GLY:O    | 6:Ag:426:ARG:NH2  | 2.51                     | 0.42              |
| 8:At:166:SER:C    | 8:At:168:ALA:H    | 2.27                     | 0.42              |
| 9:Au:63:SER:O     | 9:Au:67:ILE:HD12  | 2.19                     | 0.42              |
| 9:Av:194:LEU:HD23 | 9:Av:194:LEU:HA   | 1.83                     | 0.42              |
| 9:Av:204:LEU:HD11 | 9:Av:217:ILE:HD12 | 2.01                     | 0.42              |
| 9:Aw:172:PRO:HG2  | 9:Ax:99:PHE:HE2   | 1.84                     | 0.42              |
| 11:A7:29:ASN:ND2  | 11:A7:40:ALA:HA   | 2.34                     | 0.42              |
| 6:UI:88:VAL:O     | 6:UI:89:PRO:C     | 2.60                     | 0.42              |
| 6:WD:113:PHE:HB3  | 6:WE:134:ARG:NH1  | 2.34                     | 0.42              |
| 6:WI:142:ARG:O    | 6:WI:146:THR:HG23 | 2.19                     | 0.42              |
| 6:WW:169:GLN:NE2  | 6:WW:170:LYS:O    | 2.52                     | 0.42              |
| 6:BX:421:GLY:O    | 6:BX:426:ARG:NH2  | 2.51                     | 0.42              |
| 1:A:232:MET:HG3   | 1:B:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:B:232:MET:HG3   | 1:C:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:D:106:PHE:HB3   | 1:D:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:H:50:SER:HB3    | 2:e:32:ARG:HH11   | 1.81                     | 0.42              |
| 1:H:232:MET:HG3   | 1:I:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:K:142:ASN:ND2   | 1:L:207:TYR:OH    | 2.28                     | 0.42              |
| 1:M:214:ASN:ND2   | 1:N:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:O:28:LYS:HD3    | 1:O:28:LYS:HA     | 1.89                     | 0.42              |
| 1:R:86:VAL:HB     | 1:R:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:S:86:VAL:HB     | 1:S:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:T:86:VAL:HB     | 1:T:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:Y:102:THR:HG23  | 1:Z:130:ASN:HD22  | 1.82                     | 0.42              |
| 2:a:276:ALA:HB3   | 2:b:262:VAL:HB    | 2.01                     | 0.42              |
| 2:c:276:ALA:HB3   | 2:d:262:VAL:HB    | 2.01                     | 0.42              |
| 2:d:21:ARG:HH21   | 2:d:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:e:21:ARG:HH21   | 2:e:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:f:266:ARG:HA    | 2:f:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:f:276:ALA:HB3   | 2:g:262:VAL:HB    | 2.02                     | 0.42              |
| 2:g:188:GLN:HE21  | 2:g:188:GLN:HB2   | 1.63                     | 0.42              |
| 2:h:130:ASP:N     | 2:h:130:ASP:OD1   | 2.47                     | 0.42              |
| 2:h:188:GLN:HE21  | 2:h:188:GLN:HB2   | 1.63                     | 0.42              |
| 2:i:266:ARG:HA    | 2:i:328:LEU:HD22  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:j:192:GLU:H     | 2:j:192:GLU:HG3   | 1.53                     | 0.42              |
| 2:o:78:ASN:OD1    | 2:o:78:ASN:N      | 2.51                     | 0.42              |
| 2:u:276:ALA:HB3   | 2:v:262:VAL:HB    | 2.02                     | 0.42              |
| 2:u:346:MET:HE2   | 2:w:142:LEU:HD11  | 1.95                     | 0.42              |
| 2:v:266:ARG:HA    | 2:v:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:w:159:GLN:OE1   | 2:x:44:GLY:O      | 2.36                     | 0.42              |
| 2:w:266:ARG:HA    | 2:w:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:x:159:GLN:OE1   | 2:y:44:GLY:O      | 2.36                     | 0.42              |
| 3:1:100:GLN:NE2   | 3:1:210:GLY:O     | 2.51                     | 0.42              |
| 3:1:238:ARG:HH21  | 3:7:251:ASP:CG    | 2.27                     | 0.42              |
| 3:3:36:ARG:HE     | 3:3:80:LEU:HD22   | 1.84                     | 0.42              |
| 3:3:231:VAL:HG11  | 3:9:9:LYS:HG3     | 2.01                     | 0.42              |
| 3:4:126:GLY:HA3   | 3:9:179:MET:HE3   | 2.01                     | 0.42              |
| 3:6:45:LEU:CD1    | 3:AJ:83:GLN:NE2   | 2.81                     | 0.42              |
| 3:6:70:THR:HG22   | 3:AJ:85:ASN:OD1   | 2.19                     | 0.42              |
| 3:8:179:MET:HE2   | 3:8:179:MET:HA    | 2.02                     | 0.42              |
| 3:ZA:103:PHE:HE1  | 3:ZA:214:LEU:HD21 | 1.83                     | 0.42              |
| 3:ZE:19:MET:HE2   | 3:ZE:19:MET:HB2   | 1.92                     | 0.42              |
| 4:ZL:3:PHE:HE1    | 4:ZL:396:LEU:HD12 | 1.84                     | 0.42              |
| 4:ZP:269:GLN:NE2  | 4:ZV:146:ALA:HB3  | 2.34                     | 0.42              |
| 4:ZS:233:ASN:OD1  | 4:ZS:237:ILE:N    | 2.49                     | 0.42              |
| 4:ZS:319:ASN:OD1  | 4:ZS:319:ASN:C    | 2.62                     | 0.42              |
| 4:ZT:106:ARG:HD3  | 4:ZY:321:ALA:HB1  | 2.01                     | 0.42              |
| 4:ZV:387:GLN:HG3  | 4:Zb:400:VAL:HG13 | 2.00                     | 0.42              |
| 4:ZW:380:ARG:NE   | 4:Zc:393:ASP:OD2  | 2.52                     | 0.42              |
| 4:ZZ:97:ASN:HD22  | 4:ZZ:332:ASN:ND2  | 2.17                     | 0.42              |
| 4:ZZ:119:TYR:HB2  | 4:ZZ:128:ILE:HD11 | 2.01                     | 0.42              |
| 4:ZZ:319:ASN:HB2  | 4:ZZ:353:PHE:CE1  | 2.54                     | 0.42              |
| 4:Ze:381:ASN:O    | 4:Ze:382:TYR:C    | 2.61                     | 0.42              |
| 4:Zh:392:GLN:HA   | 4:Zh:395:ILE:CG2  | 2.49                     | 0.42              |
| 5:AA:71:LEU:CG    | 3:AL:70:THR:HG21  | 2.49                     | 0.42              |
| 5:AB:72:ASP:OD1   | 5:AB:72:ASP:C     | 2.61                     | 0.42              |
| 5:AD:221:ILE:HD13 | 3:AJ:251:ASP:OD2  | 2.19                     | 0.42              |
| 3:AH:151:ILE:HG12 | 3:AH:157:VAL:HG22 | 2.01                     | 0.42              |
| 3:AN:198:SER:O    | 3:AN:198:SER:OG   | 2.31                     | 0.42              |
| 6:AU:421:GLY:O    | 6:AU:426:ARG:NH2  | 2.51                     | 0.42              |
| 6:Ai:429:THR:OG1  | 6:Aj:418:GLU:OE2  | 2.36                     | 0.42              |
| 8:At:186:LEU:HD11 | 8:At:236:ILE:HG22 | 2.01                     | 0.42              |
| 8:At:224:VAL:O    | 8:At:228:LEU:HB2  | 2.18                     | 0.42              |
| 8:At:251:LEU:HD23 | 8:At:251:LEU:HA   | 1.84                     | 0.42              |
| 9:Au:171:LEU:HD23 | 9:Av:95:PHE:CZ    | 2.54                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:A3:59:PHE:CD2   | 10:A3:59:PHE:C    | 2.97                     | 0.42              |
| 10:A5:7:ILE:CB     | 6:BR:278:THR:HG21 | 2.41                     | 0.42              |
| 6:UL:52:ARG:O      | 6:UL:88:VAL:N     | 2.38                     | 0.42              |
| 6:UM:52:ARG:O      | 6:UM:88:VAL:N     | 2.38                     | 0.42              |
| 6:WC:120:LYS:HE2   | 6:WC:120:LYS:HA   | 2.00                     | 0.42              |
| 6:WF:120:LYS:HB3   | 6:WF:121:PHE:H    | 1.66                     | 0.42              |
| 12:BC:127:LEU:HD23 | 12:BC:127:LEU:HA  | 1.89                     | 0.42              |
| 6:BG:318:ASN:O     | 6:BG:319:GLN:C    | 2.61                     | 0.42              |
| 1:A:126:ALA:HB3    | 1:C:232:MET:HE1   | 1.99                     | 0.42              |
| 1:A:214:ASN:ND2    | 1:B:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:C:232:MET:HG3    | 1:D:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:D:86:VAL:HB      | 1:D:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:F:102:THR:HG23   | 1:G:130:ASN:HD22  | 1.82                     | 0.42              |
| 1:G:232:MET:HG3    | 1:H:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:J:144:PHE:CE2    | 1:K:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:M:106:PHE:HB3    | 1:M:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:N:106:PHE:HB3    | 1:N:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:O:106:PHE:HB3    | 1:O:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:O:110:PRO:HD3    | 1:P:124:MET:CB    | 2.50                     | 0.42              |
| 1:P:86:VAL:HB      | 1:P:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:R:113:LEU:HD12   | 1:R:113:LEU:HA    | 1.90                     | 0.42              |
| 1:S:144:PHE:CE2    | 1:T:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:U:86:VAL:HB      | 1:U:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:U:232:MET:HE3    | 1:U:232:MET:HB2   | 1.90                     | 0.42              |
| 1:X:106:PHE:HB3    | 1:X:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:Z:86:VAL:HB      | 1:Z:142:ASN:ND2   | 2.34                     | 0.42              |
| 2:a:262:VAL:HB     | 2:z:276:ALA:HB3   | 2.02                     | 0.42              |
| 2:b:250:ASP:OD1    | 2:c:23:ARG:NE     | 2.51                     | 0.42              |
| 2:c:21:ARG:HH21    | 2:c:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:f:21:ARG:HH21    | 2:f:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:f:253:VAL:HG11   | 2:f:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:g:21:ARG:HH21    | 2:g:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:g:266:ARG:HA     | 2:g:328:LEU:HD22  | 2.02                     | 0.42              |
| 2:j:21:ARG:HA      | 2:j:21:ARG:HD2    | 1.74                     | 0.42              |
| 2:j:266:ARG:HA     | 2:j:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:j:276:ALA:HB3    | 2:k:262:VAL:HB    | 2.01                     | 0.42              |
| 2:l:253:VAL:HG11   | 2:l:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:o:159:GLN:OE1    | 2:p:44:GLY:O      | 2.36                     | 0.42              |
| 2:t:192:GLU:H      | 2:t:192:GLU:HG3   | 1.53                     | 0.42              |
| 2:x:266:ARG:HA     | 2:x:328:LEU:HD22  | 2.01                     | 0.42              |
| 3:2:57:SER:OG      | 3:AG:108:PRO:HG3  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:122:VAL:O     | 3:7:180:ASN:HB2   | 2.19                     | 0.42              |
| 3:7:49:ILE:HB     | 3:7:66:LEU:HB3    | 2.01                     | 0.42              |
| 3:7:145:ASN:HB2   | 3:ZC:209:ASN:O    | 2.19                     | 0.42              |
| 3:9:44:LEU:HB3    | 3:9:45:LEU:H      | 1.68                     | 0.42              |
| 3:ZB:225:ASN:O    | 3:ZB:229:GLU:HG2  | 2.19                     | 0.42              |
| 3:ZE:235:GLN:HE22 | 4:ZK:7:VAL:HG21   | 1.83                     | 0.42              |
| 3:ZE:245:LYS:HE2  | 4:ZK:400:VAL:O    | 2.19                     | 0.42              |
| 4:ZH:111:MET:HE2  | 4:ZM:58:THR:HG21  | 2.01                     | 0.42              |
| 4:ZI:66:THR:O     | 4:ZT:42:MET:HE1   | 2.20                     | 0.42              |
| 4:ZL:93:PHE:HE1   | 4:ZL:329:GLN:HG3  | 1.83                     | 0.42              |
| 4:ZM:396:LEU:HD23 | 4:ZM:396:LEU:HA   | 1.85                     | 0.42              |
| 4:ZN:165:PRO:HB3  | 4:ZN:176:ASP:O    | 2.19                     | 0.42              |
| 4:ZN:373:VAL:O    | 4:ZN:377:VAL:HG23 | 2.19                     | 0.42              |
| 4:ZP:352:ASN:O    | 4:ZP:352:ASN:OD1  | 2.37                     | 0.42              |
| 4:ZQ:34:SER:HB3   | 4:ZQ:366:VAL:HG12 | 2.01                     | 0.42              |
| 4:ZR:375:MET:HE1  | 4:ZW:388:THR:CB   | 2.49                     | 0.42              |
| 4:ZS:65:THR:HG22  | 4:Zd:50:LEU:HD12  | 2.00                     | 0.42              |
| 4:ZT:262:SER:OG   | 4:ZT:264:LEU:HG   | 2.18                     | 0.42              |
| 4:ZT:379:GLN:HB2  | 4:ZY:391:THR:HG23 | 2.00                     | 0.42              |
| 4:ZU:322:ASN:HB3  | 4:ZU:340:SER:HA   | 2.01                     | 0.42              |
| 4:ZW:18:ASP:OD1   | 4:Zb:2:SER:N      | 2.52                     | 0.42              |
| 4:ZX:99:GLN:HB3   | 4:ZX:111:MET:HE3  | 2.01                     | 0.42              |
| 4:ZX:104:GLU:OE2  | 4:Zc:339:ALA:HA   | 2.19                     | 0.42              |
| 4:Zf:94:TYR:CG    | 4:Zf:320:PHE:HZ   | 2.37                     | 0.42              |
| 4:Zf:187:TYR:HB3  | 4:Zf:191:GLY:HA2  | 2.00                     | 0.42              |
| 4:Zf:395:ILE:HD13 | 4:Zf:395:ILE:HA   | 1.86                     | 0.42              |
| 5:AD:181:LEU:HD11 | 5:AD:193:LEU:HG   | 2.00                     | 0.42              |
| 5:AE:5:ILE:HD11   | 12:BE:106:MET:CE  | 2.49                     | 0.42              |
| 3:AG:6:TRP:CH2    | 12:BB:77:VAL:HG11 | 2.55                     | 0.42              |
| 3:AH:5:LEU:HD23   | 3:AH:5:LEU:HA     | 1.90                     | 0.42              |
| 3:AH:195:THR:C    | 3:AH:197:SER:N    | 2.76                     | 0.42              |
| 3:AL:180:ASN:O    | 3:AL:198:SER:HB2  | 2.19                     | 0.42              |
| 6:AS:418:GLU:OE2  | 6:BX:429:THR:OG1  | 2.36                     | 0.42              |
| 6:AS:421:GLY:O    | 6:AS:426:ARG:NH2  | 2.51                     | 0.42              |
| 6:AV:421:GLY:O    | 6:AV:426:ARG:NH2  | 2.51                     | 0.42              |
| 6:Ap:296:ARG:HG2  | 6:Ap:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:AP:429:THR:OG1  | 6:AQ:418:GLU:OE2  | 2.36                     | 0.42              |
| 7:Ar:47:MET:HE3   | 9:Av:210:MET:HE1  | 2.01                     | 0.42              |
| 7:As:52:ILE:HD13  | 7:As:52:ILE:HA    | 1.83                     | 0.42              |
| 8:At:148:SER:HB2  | 9:Ay:149:LEU:HD11 | 2.01                     | 0.42              |
| 9:Av:87:GLN:HE22  | 10:Az:102:MET:HG3 | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Aw:114:GLN:O    | 9:Aw:118:GLU:HG2  | 2.19                     | 0.42              |
| 9:Ax:148:ALA:CB   | 6:WF:165:PHE:CD1  | 3.03                     | 0.42              |
| 10:A2:9:GLY:O     | 10:A2:13:GLN:HG3  | 2.18                     | 0.42              |
| 6:UN:69:GLN:HG3   | 6:UN:103:GLN:OE1  | 2.19                     | 0.42              |
| 6:WB:166:VAL:CG2  | 6:WB:169:GLN:HA   | 2.49                     | 0.42              |
| 6:WC:191:ILE:O    | 6:WC:195:VAL:HG23 | 2.20                     | 0.42              |
| 6:WI:161:LYS:HA   | 6:WI:162:PRO:HD3  | 1.89                     | 0.42              |
| 6:WN:172:PRO:HD2  | 6:WN:204:GLY:O    | 2.18                     | 0.42              |
| 6:WR:197:LEU:HA   | 6:WS:175:SER:CB   | 2.50                     | 0.42              |
| 6:WT:162:PRO:HB2  | 6:WT:163:SER:H    | 1.66                     | 0.42              |
| 6:WU:192:SER:O    | 6:WU:195:VAL:HB   | 2.20                     | 0.42              |
| 1:A:124:MET:CB    | 1:Z:110:PRO:HD3   | 2.50                     | 0.42              |
| 1:C:86:VAL:HB     | 1:C:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:G:86:VAL:HB     | 1:G:142:ASN:ND2   | 2.34                     | 0.42              |
| 1:G:106:PHE:HB3   | 1:G:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:H:106:PHE:HB3   | 1:H:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:J:106:PHE:HB3   | 1:J:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:J:214:ASN:ND2   | 1:K:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:L:106:PHE:HB3   | 1:L:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:O:165:GLY:C     | 1:P:35:THR:HG21   | 2.40                     | 0.42              |
| 1:Q:144:PHE:CE2   | 1:R:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:R:214:ASN:ND2   | 1:S:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:V:50:SER:HB3    | 2:s:32:ARG:HH11   | 1.81                     | 0.42              |
| 1:W:166:GLU:HB2   | 1:X:35:THR:CG2    | 2.30                     | 0.42              |
| 1:Y:86:VAL:HB     | 1:Y:142:ASN:ND2   | 2.34                     | 0.42              |
| 2:b:21:ARG:HH21   | 2:b:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:d:276:ALA:HB3   | 2:e:262:VAL:HB    | 2.02                     | 0.42              |
| 2:d:346:MET:HE2   | 2:f:142:LEU:HD11  | 1.95                     | 0.42              |
| 2:e:266:ARG:HA    | 2:e:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:e:276:ALA:HB3   | 2:f:262:VAL:HB    | 2.02                     | 0.42              |
| 2:g:276:ALA:HB3   | 2:h:262:VAL:HB    | 2.01                     | 0.42              |
| 2:r:159:GLN:OE1   | 2:s:44:GLY:O      | 2.36                     | 0.42              |
| 2:s:266:ARG:HA    | 2:s:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:t:266:ARG:HA    | 2:t:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:t:276:ALA:HB3   | 2:u:262:VAL:HB    | 2.02                     | 0.42              |
| 2:x:192:GLU:H     | 2:x:192:GLU:HG3   | 1.53                     | 0.42              |
| 3:0:42:GLU:OE2    | 3:AJ:189:GLU:CG   | 2.62                     | 0.42              |
| 3:4:122:VAL:HG13  | 3:4:126:GLY:HA2   | 2.01                     | 0.42              |
| 3:6:16:GLN:HE22   | 3:ZB:4:SER:HB3    | 1.84                     | 0.42              |
| 3:ZA:86:LEU:HD22  | 3:ZA:96:ALA:HB1   | 2.01                     | 0.42              |
| 4:ZF:158:LEU:HD22 | 4:ZF:208:TRP:CZ3  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZL:78:SER:O     | 4:ZL:354:GLY:HA3  | 2.19                     | 0.42              |
| 4:ZL:280:ASN:OD1  | 4:ZL:281:GLN:N    | 2.52                     | 0.42              |
| 4:ZM:269:GLN:OE1  | 4:ZS:286:PRO:HG3  | 2.19                     | 0.42              |
| 4:ZP:50:LEU:HD23  | 4:ZP:50:LEU:HA    | 1.89                     | 0.42              |
| 4:ZQ:319:ASN:OD1  | 4:ZQ:344:LEU:HB2  | 2.20                     | 0.42              |
| 4:ZS:109:VAL:HG12 | 4:ZS:115:GLN:HA   | 2.01                     | 0.42              |
| 4:ZS:160:SER:OG   | 4:ZY:192:ASN:ND2  | 2.52                     | 0.42              |
| 4:ZT:53:LYS:HE2   | 4:ZT:53:LYS:HB2   | 1.80                     | 0.42              |
| 4:ZY:116:LEU:HD11 | 4:ZY:315:ILE:HD11 | 2.02                     | 0.42              |
| 4:ZY:382:TYR:CZ   | 4:Zd:395:ILE:HG23 | 2.54                     | 0.42              |
| 4:Za:396:LEU:HD23 | 4:Za:396:LEU:HA   | 1.85                     | 0.42              |
| 4:Zc:213:HIS:HB2  | 4:Zc:223:PRO:HG3  | 2.01                     | 0.42              |
| 4:Ze:150:THR:OG1  | 4:Ze:282:ASN:ND2  | 2.51                     | 0.42              |
| 4:Zg:33:LYS:NZ    | 4:Zg:362:GLU:OE2  | 2.52                     | 0.42              |
| 3:AI:95:VAL:O     | 3:AI:118:GLY:HA3  | 2.20                     | 0.42              |
| 3:AM:189:GLU:O    | 3:AM:191:LEU:HG   | 2.19                     | 0.42              |
| 3:AN:7:ILE:HG12   | 3:AN:70:THR:O     | 2.19                     | 0.42              |
| 6:AS:295:SER:OG   | 11:A0:66:THR:O    | 2.36                     | 0.42              |
| 6:AW:278:THR:CG2  | 10:A3:14:LEU:HD23 | 2.49                     | 0.42              |
| 6:AY:372:ILE:HG21 | 10:A3:4:ILE:HG12  | 2.02                     | 0.42              |
| 6:Ah:296:ARG:HG2  | 6:Ah:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Aj:296:ARG:HG2  | 6:Aj:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Aj:429:THR:OG1  | 6:Ak:418:GLU:OE2  | 2.36                     | 0.42              |
| 6:Al:296:ARG:HG2  | 6:Al:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Am:294:ARG:HD3  | 11:A7:69:SER:OG   | 2.19                     | 0.42              |
| 6:Ao:296:ARG:HG2  | 6:Ao:296:ARG:NH1  | 2.35                     | 0.42              |
| 8:At:52:LEU:HD23  | 8:At:52:LEU:HA    | 1.87                     | 0.42              |
| 9:Av:217:ILE:O    | 9:Av:220:PRO:HD2  | 2.19                     | 0.42              |
| 9:Ay:138:MET:CE   | 9:Ay:171:LEU:HD23 | 2.41                     | 0.42              |
| 10:Az:73:ALA:CB   | 11:A6:13:GLN:NE2  | 2.82                     | 0.42              |
| 10:A4:69:ASN:OD1  | 10:A4:69:ASN:N    | 2.52                     | 0.42              |
| 12:BB:4:LEU:HD22  | 12:BB:126:MET:HE1 | 2.00                     | 0.42              |
| 6:WA:140:LEU:O    | 6:WA:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WB:135:ALA:O    | 6:WB:139:GLU:HG2  | 2.18                     | 0.42              |
| 6:WD:193:ALA:HB1  | 6:WE:213:VAL:HG21 | 2.00                     | 0.42              |
| 6:WF:140:LEU:O    | 6:WF:144:ILE:HG13 | 2.19                     | 0.42              |
| 6:WG:140:LEU:O    | 6:WG:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WJ:172:PRO:HD2  | 6:WJ:204:GLY:O    | 2.19                     | 0.42              |
| 6:WK:149:PRO:HD2  | 6:WK:190:GLN:HE22 | 1.84                     | 0.42              |
| 6:WL:214:ASP:OD1  | 6:WL:218:HIS:N    | 2.49                     | 0.42              |
| 6:WM:140:LEU:O    | 6:WM:144:ILE:HG13 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:WN:140:LEU:O   | 6:WN:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WQ:193:ALA:CB  | 6:WR:217:GLY:O    | 2.67                     | 0.42              |
| 6:WT:142:ARG:O   | 6:WT:146:THR:HG23 | 2.20                     | 0.42              |
| 6:WW:140:LEU:O   | 6:WW:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:BW:421:GLY:O   | 6:BW:426:ARG:NH2  | 2.51                     | 0.42              |
| 1:F:232:MET:HE3  | 1:F:232:MET:HB2   | 1.90                     | 0.42              |
| 1:G:144:PHE:CE2  | 1:H:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:K:106:PHE:HB3  | 1:K:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:L:86:VAL:HB    | 1:L:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:M:86:VAL:HB    | 1:M:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:N:86:VAL:HB    | 1:N:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:O:86:VAL:HB    | 1:O:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:O:144:PHE:CE2  | 1:P:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:P:106:PHE:HB3  | 1:P:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:T:214:ASN:ND2  | 1:U:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:U:110:PRO:HD3  | 1:V:124:MET:CB    | 2.50                     | 0.42              |
| 1:W:106:PHE:HB3  | 1:W:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:W:110:PRO:HD3  | 1:X:124:MET:CB    | 2.50                     | 0.42              |
| 2:b:273:CYS:CA   | 2:c:328:LEU:HD21  | 2.41                     | 0.42              |
| 2:b:346:MET:HE2  | 2:d:142:LEU:HD11  | 1.95                     | 0.42              |
| 2:h:53:THR:HB    | 3:AK:203:GLU:O    | 2.20                     | 0.42              |
| 2:l:276:ALA:HB3  | 2:m:262:VAL:HB    | 2.02                     | 0.42              |
| 2:n:319:LEU:HD21 | 2:o:264:MET:HE1   | 1.97                     | 0.42              |
| 2:s:346:MET:HE2  | 2:u:142:LEU:HD11  | 1.95                     | 0.42              |
| 2:u:266:ARG:HA   | 2:u:328:LEU:HD22  | 2.02                     | 0.42              |
| 2:v:276:ALA:HB3  | 2:w:262:VAL:HB    | 2.02                     | 0.42              |
| 2:x:188:GLN:HE21 | 2:x:188:GLN:HB2   | 1.63                     | 0.42              |
| 2:y:266:ARG:HA   | 2:y:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:y:276:ALA:HB3  | 2:z:262:VAL:HB    | 2.02                     | 0.42              |
| 3:0:231:VAL:HG11 | 3:6:9:LYS:HG3     | 2.01                     | 0.42              |
| 3:1:67:GLN:HE22  | 3:AK:186:SER:H    | 1.68                     | 0.42              |
| 3:6:77:THR:HG23  | 3:ZB:66:LEU:HD12  | 2.00                     | 0.42              |
| 3:7:44:LEU:HD23  | 3:7:44:LEU:HA     | 1.84                     | 0.42              |
| 3:ZB:164:GLN:C   | 3:ZB:166:ALA:N    | 2.78                     | 0.42              |
| 3:ZC:195:THR:O   | 3:ZC:196:GLN:C    | 2.63                     | 0.42              |
| 3:ZD:44:LEU:HD23 | 3:ZD:44:LEU:HA    | 1.88                     | 0.42              |
| 3:ZE:83:GLN:HG2  | 4:ZP:44:ALA:HB1   | 2.00                     | 0.42              |
| 4:ZF:93:PHE:HB3  | 4:ZF:333:VAL:HG13 | 2.00                     | 0.42              |
| 4:ZF:374:ASN:HA  | 4:ZF:377:VAL:HG22 | 2.00                     | 0.42              |
| 4:ZG:93:PHE:HB3  | 4:ZG:333:VAL:HG13 | 2.01                     | 0.42              |
| 4:ZH:269:GLN:CB  | 4:ZN:286:PRO:CG   | 2.97                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZK:14:ALA:HB2   | 4:ZK:382:TYR:HE2  | 1.85                     | 0.42              |
| 4:ZL:159:ASN:HD21 | 4:ZL:161:THR:HG23 | 1.84                     | 0.42              |
| 4:ZM:375:MET:SD   | 4:ZR:388:THR:OG1  | 2.72                     | 0.42              |
| 4:ZQ:368:LEU:HD13 | 4:ZV:384:SER:OG   | 2.19                     | 0.42              |
| 4:ZR:38:SER:O     | 4:ZR:55:ALA:N     | 2.51                     | 0.42              |
| 4:ZS:295:ASN:ND2  | 4:ZS:299:THR:HG1  | 2.17                     | 0.42              |
| 4:ZS:373:VAL:O    | 4:ZS:377:VAL:HG23 | 2.20                     | 0.42              |
| 4:ZV:401:ASN:O    | 4:ZV:402:LEU:C    | 2.62                     | 0.42              |
| 4:ZW:111:MET:HE2  | 4:ZW:111:MET:HA   | 2.00                     | 0.42              |
| 4:ZY:156:ILE:HD11 | 4:ZY:180:LYS:HG2  | 2.00                     | 0.42              |
| 4:Za:234:GLU:O    | 4:Zg:190:GLN:CG   | 2.67                     | 0.42              |
| 4:Za:375:MET:HE2  | 4:Za:375:MET:HB2  | 1.82                     | 0.42              |
| 4:Zc:5:GLN:HG2    | 4:Zc:50:LEU:O     | 2.20                     | 0.42              |
| 4:Zg:367:ASP:O    | 4:Zg:371:GLU:HG2  | 2.20                     | 0.42              |
| 4:Zg:385:ASN:O    | 4:Zg:386:ALA:C    | 2.63                     | 0.42              |
| 5:AB:116:GLN:HE22 | 3:AG:42:GLU:HG3   | 1.81                     | 0.42              |
| 5:AB:221:ILE:HG21 | 3:AH:251:ASP:OD1  | 2.20                     | 0.42              |
| 5:AE:35:ARG:NH1   | 5:AE:101:ARG:HG3  | 2.35                     | 0.42              |
| 5:AE:135:ILE:HG23 | 5:AE:143:ILE:HG23 | 2.01                     | 0.42              |
| 5:AE:240:ASN:CG   | 12:BF:109:SER:HG  | 2.27                     | 0.42              |
| 3:AH:95:VAL:O     | 3:AH:118:GLY:HA3  | 2.20                     | 0.42              |
| 3:AH:185:GLU:HB3  | 3:AH:193:ILE:HG22 | 2.02                     | 0.42              |
| 3:AK:260:LEU:CB   | 12:BF:106:MET:HE1 | 2.39                     | 0.42              |
| 6:AT:296:ARG:HG2  | 6:AT:296:ARG:NH1  | 2.35                     | 0.42              |
| 7:Ab:7:MET:HE3    | 7:Aq:66:GLY:HA3   | 2.00                     | 0.42              |
| 7:Ab:23:PRO:HG3   | 7:Ab:68:TRP:HZ3   | 1.84                     | 0.42              |
| 6:Ak:296:ARG:HG2  | 6:Ak:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Am:296:ARG:HG2  | 6:Am:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Am:404:LEU:HD22 | 6:Am:409:MET:HE3  | 2.02                     | 0.42              |
| 7:As:89:GLY:C     | 9:Ay:143:ARG:NE   | 2.77                     | 0.42              |
| 9:Aw:213:PRO:HA   | 9:Aw:214:PRO:HD3  | 1.93                     | 0.42              |
| 9:Ay:83:ALA:HB3   | 9:Ay:84:PRO:CD    | 2.50                     | 0.42              |
| 9:Ay:189:ILE:O    | 9:Ay:192:PRO:HD2  | 2.19                     | 0.42              |
| 10:A5:61:LEU:HD11 | 11:A0:50:LYS:HZ2  | 1.85                     | 0.42              |
| 6:UM:102:GLN:CG   | 6:UM:193:ALA:HB2  | 2.49                     | 0.42              |
| 6:UM:207:PRO:HD2  | 6:WP:187:ASP:HB3  | 2.02                     | 0.42              |
| 12:BA:13:ALA:HA   | 12:BA:62:VAL:HG12 | 2.02                     | 0.42              |
| 6:WB:196:HIS:HB3  | 6:WC:211:THR:HG21 | 2.01                     | 0.42              |
| 6:WJ:140:LEU:O    | 6:WJ:144:ILE:HG13 | 2.19                     | 0.42              |
| 6:WK:128:GLU:OE1  | 6:WL:126:PHE:CE2  | 2.73                     | 0.42              |
| 6:WO:140:LEU:O    | 6:WO:144:ILE:HG13 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:WQ:196:HIS:HB3 | 6:WR:211:THR:HG21 | 2.02                     | 0.42              |
| 6:WV:164:LEU:O   | 6:WV:166:VAL:N    | 2.49                     | 0.42              |
| 6:WW:172:PRO:HD2 | 6:WW:204:GLY:O    | 2.19                     | 0.42              |
| 12:BD:53:ALA:O   | 12:BD:54:ALA:C    | 2.63                     | 0.42              |
| 1:A:173:GLN:NE2  | 1:Z:214:ASN:ND2   | 2.67                     | 0.42              |
| 1:B:86:VAL:HB    | 1:B:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:D:214:ASN:ND2  | 1:E:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:F:232:MET:HG3  | 1:G:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:I:106:PHE:HB3  | 1:I:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:I:136:GLY:CA   | 1:K:213:ILE:HG23  | 2.42                     | 0.42              |
| 1:L:110:PRO:HD3  | 1:M:124:MET:CB    | 2.50                     | 0.42              |
| 1:V:110:PRO:HD3  | 1:W:124:MET:CB    | 2.50                     | 0.42              |
| 1:W:86:VAL:HB    | 1:W:142:ASN:ND2   | 2.34                     | 0.42              |
| 1:X:110:PRO:HD3  | 1:Y:124:MET:CB    | 2.50                     | 0.42              |
| 2:a:21:ARG:HH21  | 2:a:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:b:78:ASN:ND2   | 3:AG:169:GLN:OE1  | 2.53                     | 0.42              |
| 2:d:266:ARG:HA   | 2:d:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:e:250:ASP:OD1  | 2:f:23:ARG:NE     | 2.51                     | 0.42              |
| 2:e:253:VAL:HG11 | 2:e:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:h:346:MET:HE2  | 2:j:142:LEU:HD11  | 1.95                     | 0.42              |
| 2:k:276:ALA:HB3  | 2:l:262:VAL:HB    | 2.02                     | 0.42              |
| 2:l:250:ASP:OD1  | 2:m:23:ARG:NE     | 2.51                     | 0.42              |
| 2:m:276:ALA:HB3  | 2:n:262:VAL:HB    | 2.02                     | 0.42              |
| 2:r:266:ARG:HA   | 2:r:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:r:276:ALA:HB3  | 2:s:262:VAL:HB    | 2.01                     | 0.42              |
| 2:s:78:ASN:OD1   | 2:s:78:ASN:N      | 2.51                     | 0.42              |
| 2:y:253:VAL:HG11 | 2:y:349:LEU:HD13  | 2.01                     | 0.42              |
| 3:0:147:LEU:HD23 | 3:0:147:LEU:HA    | 1.84                     | 0.42              |
| 3:1:83:GLN:NE2   | 3:ZC:45:LEU:CD1   | 2.79                     | 0.42              |
| 3:1:258:THR:CA   | 5:AE:217:MET:HE1  | 2.33                     | 0.42              |
| 3:2:79:ARG:HG3   | 3:2:79:ARG:NH1    | 2.34                     | 0.42              |
| 3:5:74:PRO:HG2   | 3:ZA:66:LEU:HD21  | 2.00                     | 0.42              |
| 3:5:189:GLU:HA   | 3:ZA:42:GLU:HB2   | 2.00                     | 0.42              |
| 3:6:123:ASP:OD1  | 3:6:127:GLN:N     | 2.50                     | 0.42              |
| 3:8:100:GLN:HG3  | 3:8:210:GLY:O     | 2.20                     | 0.42              |
| 3:9:37:GLN:HE21  | 3:9:79:ARG:NH1    | 2.08                     | 0.42              |
| 3:ZD:89:THR:OG1  | 3:ZD:94:ASP:OD2   | 2.37                     | 0.42              |
| 4:ZH:281:GLN:OE1 | 4:ZH:281:GLN:C    | 2.63                     | 0.42              |
| 4:ZI:63:ASP:OD2  | 4:ZI:96:ARG:NH2   | 2.52                     | 0.42              |
| 4:ZK:153:SER:HB2 | 4:ZK:280:ASN:OD1  | 2.19                     | 0.42              |
| 4:ZP:382:TYR:CE1 | 4:ZU:395:ILE:HG23 | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZQ:337:THR:HG22 | 4:ZQ:339:ALA:H    | 1.84                     | 0.42              |
| 4:ZR:160:SER:OG   | 4:ZX:192:ASN:OD1  | 2.37                     | 0.42              |
| 4:ZT:380:ARG:NH2  | 4:ZZ:397:ASN:OD1  | 2.53                     | 0.42              |
| 4:ZW:65:THR:HG22  | 4:Zh:50:LEU:HB3   | 2.00                     | 0.42              |
| 4:Za:34:SER:HB3   | 4:Za:366:VAL:HG22 | 2.01                     | 0.42              |
| 4:Zd:296:ASN:OD1  | 4:Zd:355:LYS:HD2  | 2.20                     | 0.42              |
| 4:Zh:320:PHE:CD2  | 4:Zh:340:SER:HB2  | 2.54                     | 0.42              |
| 5:AA:109:PRO:CG   | 3:AF:197:SER:HA   | 2.50                     | 0.42              |
| 5:AB:47:ASP:O     | 6:BK:324:ASN:HB2  | 2.19                     | 0.42              |
| 3:AG:6:TRP:CZ2    | 12:BB:77:VAL:HG11 | 2.55                     | 0.42              |
| 3:AM:22:ILE:HG21  | 3:AM:233:MET:HG3  | 2.00                     | 0.42              |
| 6:AS:294:ARG:CD   | 11:A0:68:THR:HG22 | 2.36                     | 0.42              |
| 6:AS:296:ARG:HG2  | 6:AS:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:AS:374:HIS:HB2  | 10:A4:4:ILE:CD1   | 2.50                     | 0.42              |
| 6:AW:429:THR:OG1  | 6:AX:418:GLU:OE2  | 2.36                     | 0.42              |
| 6:AY:294:ARG:HD3  | 11:A9:68:THR:HG22 | 2.01                     | 0.42              |
| 6:AY:296:ARG:HG2  | 6:AY:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Ac:296:ARG:HG2  | 6:Ac:296:ARG:NH1  | 2.35                     | 0.42              |
| 8:At:125:LEU:O    | 8:At:129:MET:HG3  | 2.20                     | 0.42              |
| 9:Aw:40:LEU:HD21  | 11:A8:5:LEU:HA    | 2.01                     | 0.42              |
| 9:Aw:141:GLN:NE2  | 9:Aw:243:PHE:HA   | 2.34                     | 0.42              |
| 9:Ax:190:PHE:CD1  | 9:Ay:220:PRO:HG3  | 2.55                     | 0.42              |
| 9:Ay:92:LEU:HA    | 9:Ay:92:LEU:HD12  | 1.78                     | 0.42              |
| 9:Ay:121:ILE:HG23 | 9:Ay:125:GLU:HB3  | 2.02                     | 0.42              |
| 9:Ay:225:LEU:HD12 | 9:Ay:229:VAL:HG22 | 2.01                     | 0.42              |
| 11:A0:66:THR:HG23 | 6:BX:365:ASN:CG   | 2.44                     | 0.42              |
| 6:WB:140:LEU:O    | 6:WB:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WF:181:GLU:CB   | 6:WF:184:ARG:CG   | 2.85                     | 0.42              |
| 6:WW:131:ASN:HA   | 6:WW:134:ARG:HD3  | 2.01                     | 0.42              |
| 12:BF:16:ALA:HB1  | 12:BF:49:PHE:CE1  | 2.55                     | 0.42              |
| 6:BQ:312:VAL:HG12 | 6:BQ:315:ALA:HB2  | 2.01                     | 0.42              |
| 6:BR:296:ARG:HG2  | 6:BR:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:BS:296:ARG:HG2  | 6:BS:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:86:VAL:HB     | 1:A:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:B:110:PRO:HD3   | 1:C:124:MET:CB    | 2.50                     | 0.42              |
| 1:C:110:PRO:HD3   | 1:D:124:MET:CB    | 2.50                     | 0.42              |
| 1:D:232:MET:HG3   | 1:E:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:E:110:PRO:HD3   | 1:F:124:MET:CB    | 2.50                     | 0.42              |
| 1:E:165:GLY:C     | 1:F:35:THR:HG21   | 2.40                     | 0.42              |
| 1:H:86:VAL:HB     | 1:H:142:ASN:ND2   | 2.34                     | 0.42              |
| 1:Q:106:PHE:HB3   | 1:Q:109:VAL:HG22  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:110:PRO:HD3   | 1:T:124:MET:CB    | 2.50                     | 0.42              |
| 1:T:110:PRO:HD3   | 1:U:124:MET:CB    | 2.50                     | 0.42              |
| 1:W:169:ILE:HG22  | 1:W:171:ILE:HG12  | 2.02                     | 0.42              |
| 1:Y:214:ASN:ND2   | 1:Z:173:GLN:NE2   | 2.67                     | 0.42              |
| 2:a:44:GLY:O      | 2:z:159:GLN:OE1   | 2.36                     | 0.42              |
| 2:a:253:VAL:HG11  | 2:a:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:b:276:ALA:HB3   | 2:c:262:VAL:HB    | 2.01                     | 0.42              |
| 2:d:251:ALA:HB2   | 2:d:267:GLU:O     | 2.20                     | 0.42              |
| 2:i:250:ASP:OD1   | 2:j:23:ARG:NE     | 2.51                     | 0.42              |
| 2:k:266:ARG:HA    | 2:k:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:m:253:VAL:HG11  | 2:m:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:q:276:ALA:HB3   | 2:r:262:VAL:HB    | 2.02                     | 0.42              |
| 2:s:251:ALA:HB2   | 2:s:267:GLU:O     | 2.20                     | 0.42              |
| 2:t:251:ALA:HB2   | 2:t:267:GLU:O     | 2.20                     | 0.42              |
| 2:w:253:VAL:HG11  | 2:w:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:x:253:VAL:HG11  | 2:x:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:z:21:ARG:HH21   | 2:z:246:VAL:CG2   | 2.32                     | 0.42              |
| 2:z:253:VAL:HG11  | 2:z:349:LEU:HD13  | 2.01                     | 0.42              |
| 3:0:35:LYS:HD2    | 3:0:81:HIS:HA     | 2.01                     | 0.42              |
| 3:0:72:VAL:HB     | 3:AJ:28:ASN:OD1   | 2.19                     | 0.42              |
| 3:0:164:GLN:H     | 3:0:164:GLN:HG3   | 1.58                     | 0.42              |
| 3:0:257:LEU:CD2   | 5:AD:214:VAL:HG22 | 2.47                     | 0.42              |
| 3:1:100:GLN:HE22  | 3:AK:147:LEU:HD23 | 1.84                     | 0.42              |
| 3:2:238:ARG:HA    | 3:2:238:ARG:HD3   | 1.65                     | 0.42              |
| 3:3:109:ASP:OD2   | 3:3:111:THR:HG22  | 2.20                     | 0.42              |
| 3:5:185:GLU:HB3   | 3:5:193:ILE:HG12  | 2.02                     | 0.42              |
| 3:8:154:ASP:O     | 3:8:156:VAL:HG23  | 2.20                     | 0.42              |
| 3:ZC:260:LEU:HD23 | 3:ZC:260:LEU:HA   | 1.75                     | 0.42              |
| 4:ZM:59:GLN:NE2   | 4:ZM:334:TRP:HE1  | 2.18                     | 0.42              |
| 4:ZM:381:ASN:O    | 4:ZM:385:ASN:ND2  | 2.53                     | 0.42              |
| 4:ZN:6:ALA:HB1    | 4:ZN:389:ILE:HG12 | 2.02                     | 0.42              |
| 4:ZO:71:ARG:HB3   | 4:ZO:71:ARG:HH11  | 1.84                     | 0.42              |
| 4:ZO:380:ARG:HB3  | 4:ZU:396:LEU:HD13 | 2.02                     | 0.42              |
| 4:ZP:73:LEU:HD21  | 4:ZP:292:TYR:HE1  | 1.83                     | 0.42              |
| 4:ZS:233:ASN:HD21 | 4:ZS:237:ILE:HB   | 1.84                     | 0.42              |
| 4:ZW:83:PHE:HB2   | 4:ZW:95:SER:O     | 2.19                     | 0.42              |
| 4:Zd:16:ASN:HB2   | 4:Zd:39:PHE:HZ    | 1.85                     | 0.42              |
| 5:AA:35:ARG:NH2   | 5:AA:207:GLU:OE2  | 2.44                     | 0.42              |
| 5:AB:49:LEU:HD13  | 5:AB:49:LEU:O     | 2.19                     | 0.42              |
| 5:AD:1:MET:HG2    | 5:AD:241:GLU:CG   | 2.49                     | 0.42              |
| 5:AD:80:VAL:O     | 5:AD:103:GLY:HA3  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AE:228:GLU:OE2   | 3:AJ:256:LYS:CE   | 2.68                     | 0.42              |
| 5:AE:228:GLU:HG2   | 3:AJ:256:LYS:HG3  | 2.02                     | 0.42              |
| 3:AF:7:ILE:O       | 3:AF:10:THR:OG1   | 2.31                     | 0.42              |
| 3:AM:52:PRO:O      | 12:BC:87:ALA:O    | 2.35                     | 0.42              |
| 6:AU:296:ARG:HG2   | 6:AU:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:AU:429:THR:OG1   | 6:AV:418:GLU:OE2  | 2.36                     | 0.42              |
| 6:AW:421:GLY:O     | 6:AW:426:ARG:NH2  | 2.51                     | 0.42              |
| 6:AX:296:ARG:HG2   | 6:AX:296:ARG:NH1  | 2.35                     | 0.42              |
| 7:Ab:52:ILE:HD12   | 7:Ab:52:ILE:N     | 2.35                     | 0.42              |
| 6:Ad:296:ARG:HG2   | 6:Ad:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Ae:296:ARG:HG2   | 6:Ae:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Af:296:ARG:HG2   | 6:Af:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Al:404:LEU:HD22  | 6:Al:409:MET:HE3  | 2.02                     | 0.42              |
| 6:An:296:ARG:HG2   | 6:An:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:An:404:LEU:HD22  | 6:An:409:MET:HE3  | 2.02                     | 0.42              |
| 6:Ao:404:LEU:HD22  | 6:Ao:409:MET:HE3  | 2.02                     | 0.42              |
| 6:Ap:404:LEU:HD22  | 6:Ap:409:MET:HE3  | 2.02                     | 0.42              |
| 9:Au:63:SER:HB2    | 9:Au:66:ARG:HH21  | 1.84                     | 0.42              |
| 9:Av:45:LEU:O      | 9:Av:49:THR:OG1   | 2.30                     | 0.42              |
| 9:Aw:139:LEU:HD23  | 9:Aw:139:LEU:HA   | 1.86                     | 0.42              |
| 9:Ay:48:ILE:HD13   | 9:Ay:48:ILE:HA    | 1.83                     | 0.42              |
| 10:A3:69:ASN:HD21  | 11:A9:17:ASN:HA   | 1.84                     | 0.42              |
| 10:A4:59:PHE:CZ    | 12:BE:4:LEU:HD22  | 2.55                     | 0.42              |
| 10:A5:11:ILE:HG22  | 6:BR:372:ILE:CB   | 2.49                     | 0.42              |
| 11:A0:121:THR:HG23 | 12:BF:134:GLN:HG2 | 2.01                     | 0.42              |
| 6:UI:102:GLN:CG    | 6:UI:193:ALA:HB2  | 2.49                     | 0.42              |
| 6:WA:126:PHE:HD2   | 6:WW:128:GLU:HG2  | 1.84                     | 0.42              |
| 6:WC:140:LEU:O     | 6:WC:144:ILE:HG13 | 2.19                     | 0.42              |
| 6:WE:140:LEU:O     | 6:WE:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WG:170:LYS:HB2   | 6:WG:171:SER:H    | 1.78                     | 0.42              |
| 6:WG:193:ALA:HB1   | 6:WH:213:VAL:CG1  | 2.48                     | 0.42              |
| 6:WI:165:PHE:O     | 6:WI:165:PHE:CG   | 2.73                     | 0.42              |
| 6:WU:128:GLU:HG2   | 6:WV:126:PHE:CD2  | 2.48                     | 0.42              |
| 6:WV:112:GLY:HA2   | 6:WV:135:ALA:CA   | 2.28                     | 0.42              |
| 6:WW:187:ASP:H     | 6:WW:190:GLN:CD   | 2.26                     | 0.42              |
| 12:BF:34:VAL:HG13  | 12:BF:35:THR:HG22 | 2.02                     | 0.42              |
| 1:F:28:LYS:HD3     | 1:F:28:LYS:HA     | 1.89                     | 0.42              |
| 1:F:47:ALA:HB1     | 2:c:178:GLN:HG3   | 1.96                     | 0.42              |
| 1:G:142:ASN:ND2    | 1:H:207:TYR:OH    | 2.28                     | 0.42              |
| 1:H:136:GLY:CA     | 1:J:213:ILE:HG23  | 2.42                     | 0.42              |
| 1:K:86:VAL:HB      | 1:K:142:ASN:ND2   | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:232:MET:HE3   | 1:K:232:MET:HB2   | 1.90                     | 0.42              |
| 1:L:214:ASN:ND2   | 1:M:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:M:144:PHE:CE2   | 1:N:171:ILE:CD1   | 3.01                     | 0.42              |
| 1:O:169:ILE:HG22  | 1:O:171:ILE:HG12  | 2.02                     | 0.42              |
| 1:P:169:ILE:HG22  | 1:P:171:ILE:HG12  | 2.02                     | 0.42              |
| 1:Q:110:PRO:HD3   | 1:R:124:MET:CB    | 2.50                     | 0.42              |
| 1:R:110:PRO:HD3   | 1:S:124:MET:CB    | 2.50                     | 0.42              |
| 1:S:136:GLY:CA    | 1:U:213:ILE:HG23  | 2.42                     | 0.42              |
| 1:V:86:VAL:HB     | 1:V:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:X:169:ILE:HG22  | 1:X:171:ILE:HG12  | 2.02                     | 0.42              |
| 2:c:78:ASN:ND2    | 3:AG:145:ASN:HD22 | 2.13                     | 0.42              |
| 2:c:78:ASN:OD1    | 2:c:78:ASN:N      | 2.51                     | 0.42              |
| 2:c:251:ALA:HB2   | 2:c:267:GLU:O     | 2.20                     | 0.42              |
| 2:e:251:ALA:HB2   | 2:e:267:GLU:O     | 2.20                     | 0.42              |
| 2:h:251:ALA:HB2   | 2:h:267:GLU:O     | 2.20                     | 0.42              |
| 2:i:251:ALA:HB2   | 2:i:267:GLU:O     | 2.20                     | 0.42              |
| 2:u:258:ARG:HH12  | 2:w:140:ASN:HD21  | 1.64                     | 0.42              |
| 2:v:253:VAL:HG11  | 2:v:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:y:251:ALA:HB2   | 2:y:267:GLU:O     | 2.20                     | 0.42              |
| 2:z:266:ARG:HA    | 2:z:328:LEU:HD22  | 2.01                     | 0.42              |
| 3:2:43:ASP:HB2    | 3:AL:188:GLY:O    | 2.20                     | 0.42              |
| 3:5:175:LEU:HG    | 3:5:206:PRO:HG3   | 2.02                     | 0.42              |
| 3:6:1:MET:HB2     | 3:6:1:MET:HE3     | 1.86                     | 0.42              |
| 3:7:128:LEU:HD23  | 3:7:128:LEU:HA    | 1.82                     | 0.42              |
| 3:9:95:VAL:O      | 3:9:118:GLY:HA3   | 2.19                     | 0.42              |
| 3:ZD:122:VAL:O    | 4:ZI:322:ASN:HB2  | 2.20                     | 0.42              |
| 3:ZD:137:GLN:CA   | 3:ZD:139:ALA:H    | 2.31                     | 0.42              |
| 4:ZG:210:VAL:O    | 4:ZG:227:SER:N    | 2.52                     | 0.42              |
| 4:ZH:269:GLN:NE2  | 4:ZN:146:ALA:H    | 2.17                     | 0.42              |
| 4:ZH:379:GLN:NE2  | 4:ZM:391:THR:HA   | 2.35                     | 0.42              |
| 4:ZJ:373:VAL:CG1  | 4:ZP:7:VAL:HG22   | 2.49                     | 0.42              |
| 4:ZP:103:ASP:OD1  | 4:ZP:107:ASN:N    | 2.50                     | 0.42              |
| 4:ZR:204:LYS:HG2  | 4:ZR:205:ASP:H    | 1.84                     | 0.42              |
| 4:ZT:93:PHE:HB3   | 4:ZT:333:VAL:HG13 | 2.01                     | 0.42              |
| 4:ZV:213:HIS:HB2  | 4:ZV:223:PRO:HG3  | 2.02                     | 0.42              |
| 4:ZX:74:ASP:OD1   | 4:ZX:74:ASP:N     | 2.51                     | 0.42              |
| 4:ZX:361:LEU:HD12 | 4:ZX:361:LEU:HA   | 1.89                     | 0.42              |
| 4:ZY:60:ASP:OD2   | 4:ZY:365:ASN:ND2  | 2.53                     | 0.42              |
| 4:ZY:126:PRO:HG2  | 4:ZY:310:GLN:NE2  | 2.35                     | 0.42              |
| 5:AB:213:PRO:HG2  | 3:AM:2:ILE:HG12   | 2.01                     | 0.42              |
| 5:AB:221:ILE:HG23 | 5:AB:225:ARG:HH12 | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AB:225:ARG:HD3  | 5:AB:225:ARG:HA   | 1.35                     | 0.42              |
| 5:AC:143:ILE:HB   | 5:AC:159:GLY:O    | 2.18                     | 0.42              |
| 5:AD:76:ARG:HE    | 5:AD:78:LEU:HD12  | 1.84                     | 0.42              |
| 3:AL:2:ILE:O      | 3:AL:3:SER:HB3    | 2.18                     | 0.42              |
| 3:AN:185:GLU:HB3  | 3:AN:193:ILE:HG13 | 2.02                     | 0.42              |
| 6:AT:295:SER:CB   | 11:A0:73:ILE:HG13 | 2.43                     | 0.42              |
| 6:AX:361:ASN:ND2  | 11:A9:78:VAL:CG1  | 2.78                     | 0.42              |
| 6:Af:404:LEU:HD22 | 6:Af:409:MET:HE3  | 2.02                     | 0.42              |
| 6:Ag:296:ARG:HG2  | 6:Ag:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:Ag:404:LEU:HD22 | 6:Ag:409:MET:HE3  | 2.02                     | 0.42              |
| 6:Aj:278:THR:HG21 | 10:A1:7:ILE:HG22  | 2.01                     | 0.42              |
| 6:Ak:404:LEU:HD22 | 6:Ak:409:MET:HE3  | 2.02                     | 0.42              |
| 6:AO:404:LEU:HD22 | 6:AO:409:MET:HE3  | 2.02                     | 0.42              |
| 8:At:254:ILE:HD13 | 8:At:254:ILE:HA   | 1.86                     | 0.42              |
| 9:Av:121:ILE:HG12 | 9:Av:125:GLU:HB3  | 2.02                     | 0.42              |
| 9:Aw:152:ARG:CG   | 6:WB:166:VAL:O    | 2.67                     | 0.42              |
| 9:Ax:171:LEU:HB3  | 9:Ax:172:PRO:HD3  | 2.01                     | 0.42              |
| 12:BA:127:LEU:O   | 12:BA:128:LYS:C   | 2.57                     | 0.42              |
| 6:WD:140:LEU:O    | 6:WD:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WD:190:GLN:HA   | 6:WE:217:GLY:O    | 2.19                     | 0.42              |
| 6:WI:144:ILE:O    | 6:WI:147:LEU:HB2  | 2.20                     | 0.42              |
| 6:WI:187:ASP:H    | 6:WI:190:GLN:CD   | 2.28                     | 0.42              |
| 6:WP:140:LEU:O    | 6:WP:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WT:161:LYS:CB   | 6:WT:162:PRO:HD2  | 2.49                     | 0.42              |
| 6:WW:112:GLY:HA3  | 6:WW:135:ALA:HA   | 2.00                     | 0.42              |
| 1:A:110:PRO:HD3   | 1:B:124:MET:CB    | 2.50                     | 0.42              |
| 1:F:106:PHE:HB3   | 1:F:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:G:214:ASN:ND2   | 1:H:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:M:110:PRO:HD3   | 1:N:124:MET:CB    | 2.50                     | 0.42              |
| 1:N:110:PRO:HD3   | 1:O:124:MET:CB    | 2.50                     | 0.42              |
| 1:N:113:LEU:HD12  | 1:N:113:LEU:HA    | 1.90                     | 0.42              |
| 1:R:106:PHE:HB3   | 1:R:109:VAL:HG22  | 2.00                     | 0.42              |
| 1:V:169:ILE:HG22  | 1:V:171:ILE:HG12  | 2.02                     | 0.42              |
| 1:W:214:ASN:ND2   | 1:X:173:GLN:NE2   | 2.67                     | 0.42              |
| 1:X:86:VAL:HB     | 1:X:142:ASN:ND2   | 2.35                     | 0.42              |
| 1:Y:110:PRO:HD3   | 1:Z:124:MET:CB    | 2.50                     | 0.42              |
| 2:b:253:VAL:HG11  | 2:b:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:n:276:ALA:HB3   | 2:o:262:VAL:HB    | 2.02                     | 0.42              |
| 2:p:251:ALA:HB2   | 2:p:267:GLU:O     | 2.20                     | 0.42              |
| 2:p:266:ARG:HA    | 2:p:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:p:276:ALA:HB3   | 2:q:262:VAL:HB    | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:s:276:ALA:HB3   | 2:t:262:VAL:HB    | 2.02                     | 0.42              |
| 2:x:251:ALA:HB2   | 2:x:267:GLU:O     | 2.20                     | 0.42              |
| 3:5:237:GLN:HE22  | 3:ZA:256:LYS:HE2  | 1.85                     | 0.42              |
| 3:6:238:ARG:NE    | 3:ZC:251:ASP:OD1  | 2.50                     | 0.42              |
| 3:8:116:ARG:NH2   | 3:8:220:GLU:OE1   | 2.50                     | 0.42              |
| 3:9:116:ARG:HG3   | 3:9:116:ARG:O     | 2.20                     | 0.42              |
| 3:9:124:GLN:HB2   | 3:ZE:199:GLY:HA2  | 2.01                     | 0.42              |
| 3:ZB:124:GLN:NE2  | 4:ZG:338:GLN:HG2  | 2.35                     | 0.42              |
| 3:ZC:194:GLU:HG2  | 3:ZC:194:GLU:O    | 2.20                     | 0.42              |
| 3:ZD:95:VAL:O     | 3:ZD:118:GLY:HA3  | 2.20                     | 0.42              |
| 4:ZM:320:PHE:CE1  | 4:ZM:343:ALA:HB2  | 2.55                     | 0.42              |
| 4:ZO:380:ARG:HD3  | 4:ZO:380:ARG:HA   | 1.81                     | 0.42              |
| 4:ZP:47:LYS:HE2   | 4:ZP:47:LYS:HB2   | 1.91                     | 0.42              |
| 4:ZR:380:ARG:HD3  | 4:ZR:380:ARG:HA   | 1.75                     | 0.42              |
| 4:ZS:331:ASP:HA   | 4:ZX:40:ALA:HB1   | 2.01                     | 0.42              |
| 4:ZT:3:PHE:HB3    | 4:ZT:7:VAL:HG23   | 2.02                     | 0.42              |
| 4:ZU:185:THR:OG1  | 4:Zf:133:ASN:ND2  | 2.53                     | 0.42              |
| 4:ZV:212:THR:HG21 | 4:ZV:246:ILE:HD11 | 2.01                     | 0.42              |
| 4:Zb:77:ILE:HD12  | 4:Zb:96:ARG:HD2   | 2.01                     | 0.42              |
| 4:Zc:38:SER:O     | 4:Zc:55:ALA:N     | 2.52                     | 0.42              |
| 5:AC:193:LEU:HD23 | 5:AC:193:LEU:HA   | 1.92                     | 0.42              |
| 5:AD:214:VAL:HG13 | 3:AJ:12:LEU:HD12  | 2.01                     | 0.42              |
| 3:AI:50:ARG:HB2   | 6:BN:322:PRO:CG   | 2.49                     | 0.42              |
| 3:AL:193:ILE:HG22 | 3:AL:194:GLU:O    | 2.20                     | 0.42              |
| 3:AN:173:LEU:HD23 | 3:AN:173:LEU:HA   | 1.84                     | 0.42              |
| 6:AR:296:ARG:HG2  | 6:AR:296:ARG:NH1  | 2.35                     | 0.42              |
| 6:AX:278:THR:HG21 | 10:A3:7:ILE:CB    | 2.50                     | 0.42              |
| 6:AY:429:THR:OG1  | 6:AZ:418:GLU:OE2  | 2.36                     | 0.42              |
| 6:Aa:296:ARG:HG2  | 6:Aa:296:ARG:NH1  | 2.35                     | 0.42              |
| 7:Ab:24:LEU:HD22  | 9:Av:203:VAL:HG22 | 2.02                     | 0.42              |
| 6:Ad:290:LYS:HE3  | 6:Ad:290:LYS:HB2  | 1.93                     | 0.42              |
| 6:Aj:404:LEU:HD22 | 6:Aj:409:MET:HE3  | 2.02                     | 0.42              |
| 6:AO:296:ARG:HG2  | 6:AO:296:ARG:NH1  | 2.35                     | 0.42              |
| 8:At:138:LEU:HG   | 9:Ay:180:LYS:HG3  | 2.01                     | 0.42              |
| 9:Aw:180:LYS:HD2  | 9:Ax:230:ASP:OD1  | 2.20                     | 0.42              |
| 9:Ay:148:ALA:HB1  | 6:WI:164:LEU:HD13 | 2.01                     | 0.42              |
| 11:A9:3:ASP:O     | 11:A9:4:ARG:C     | 2.62                     | 0.42              |
| 6:UJ:52:ARG:O     | 6:UJ:88:VAL:N     | 2.38                     | 0.42              |
| 6:UJ:125:GLN:C    | 6:UJ:127:SER:N    | 2.77                     | 0.42              |
| 6:WB:166:VAL:HG21 | 6:WB:169:GLN:HA   | 2.01                     | 0.42              |
| 6:WF:187:ASP:HB3  | 6:WF:190:GLN:CG   | 2.44                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WI:140:LEU:O    | 6:WI:144:ILE:HG13 | 2.20                     | 0.42              |
| 6:WV:114:GLU:O    | 6:WV:118:GLN:HG3  | 2.20                     | 0.42              |
| 6:BX:296:ARG:HG2  | 6:BX:296:ARG:NH1  | 2.35                     | 0.42              |
| 1:D:165:GLY:C     | 1:E:35:THR:HG21   | 2.40                     | 0.42              |
| 1:E:232:MET:HG3   | 1:F:223:GLN:HB2   | 2.01                     | 0.42              |
| 1:I:86:VAL:HB     | 1:I:142:ASN:ND2   | 2.34                     | 0.42              |
| 1:J:110:PRO:HD3   | 1:K:124:MET:CB    | 2.50                     | 0.42              |
| 1:P:110:PRO:HD3   | 1:Q:124:MET:CB    | 2.50                     | 0.42              |
| 1:S:47:ALA:HB3    | 2:p:178:GLN:CD    | 2.45                     | 0.42              |
| 1:V:232:MET:HE3   | 1:V:232:MET:HB2   | 1.90                     | 0.42              |
| 1:W:28:LYS:HD3    | 1:W:28:LYS:HA     | 1.89                     | 0.42              |
| 1:Y:28:LYS:HA     | 1:Y:28:LYS:HD3    | 1.89                     | 0.42              |
| 2:a:23:ARG:NE     | 2:z:250:ASP:OD1   | 2.51                     | 0.42              |
| 2:c:266:ARG:HA    | 2:c:328:LEU:HD22  | 2.01                     | 0.42              |
| 2:n:250:ASP:OD1   | 2:o:23:ARG:NE     | 2.51                     | 0.42              |
| 2:n:258:ARG:HH12  | 2:p:140:ASN:HD21  | 1.64                     | 0.42              |
| 2:o:251:ALA:HB2   | 2:o:267:GLU:O     | 2.20                     | 0.42              |
| 2:o:276:ALA:HB3   | 2:p:262:VAL:HB    | 2.02                     | 0.42              |
| 2:q:266:ARG:HA    | 2:q:328:LEU:HD22  | 2.02                     | 0.42              |
| 2:t:188:GLN:HE21  | 2:t:188:GLN:HB2   | 1.63                     | 0.42              |
| 2:t:253:VAL:HG11  | 2:t:349:LEU:HD13  | 2.01                     | 0.42              |
| 2:u:253:VAL:HG11  | 2:u:349:LEU:HD13  | 2.01                     | 0.42              |
| 3:0:77:THR:HG23   | 3:5:66:LEU:HD12   | 2.02                     | 0.42              |
| 3:0:105:VAL:HG22  | 3:0:136:VAL:HG22  | 2.02                     | 0.42              |
| 3:1:129:VAL:HA    | 3:1:136:VAL:HG23  | 2.02                     | 0.42              |
| 3:3:143:PRO:HG2   | 3:3:159:VAL:HG21  | 2.02                     | 0.42              |
| 3:3:242:ILE:HD13  | 3:9:1:MET:HE1     | 2.00                     | 0.42              |
| 3:4:42:GLU:CD     | 3:AN:189:GLU:HG2  | 2.44                     | 0.42              |
| 3:5:208:LEU:HB3   | 3:5:209:ASN:H     | 1.64                     | 0.42              |
| 3:7:18:ASN:O      | 3:7:21:VAL:HB     | 2.20                     | 0.42              |
| 3:9:41:PHE:HA     | 3:9:74:PRO:HA     | 2.01                     | 0.42              |
| 3:ZA:104:GLN:HG2  | 3:ZA:137:GLN:HG3  | 2.01                     | 0.42              |
| 4:ZF:106:ARG:HB3  | 4:ZF:139:ILE:O    | 2.19                     | 0.42              |
| 4:ZI:42:MET:O     | 4:ZI:50:LEU:HB2   | 2.20                     | 0.42              |
| 4:ZK:71:ARG:O     | 4:ZK:359:GLY:HA2  | 2.20                     | 0.42              |
| 4:ZP:71:ARG:O     | 4:ZP:359:GLY:HA2  | 2.19                     | 0.42              |
| 4:ZP:170:PHE:HE2  | 4:ZP:223:PRO:HG2  | 1.85                     | 0.42              |
| 4:ZU:108:LEU:HD12 | 4:ZU:137:ILE:HG21 | 2.02                     | 0.42              |
| 4:ZU:386:ALA:O    | 4:ZU:389:ILE:HG22 | 2.20                     | 0.42              |
| 4:ZW:285:LYS:HB2  | 4:ZW:285:LYS:HE3  | 1.91                     | 0.42              |
| 4:ZX:396:LEU:HD23 | 4:ZX:396:LEU:HA   | 1.78                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:Zb:110:ASN:OD1  | 4:Zb:114:MET:N     | 2.50                     | 0.42              |
| 4:Zb:326:LEU:HD12 | 4:Zb:340:SER:HB2   | 2.01                     | 0.42              |
| 4:Zc:21:GLY:HA3   | 4:Zh:5:GLN:HE21    | 1.85                     | 0.42              |
| 4:Zh:154:MET:HE2  | 4:Zh:154:MET:HB3   | 1.99                     | 0.42              |
| 5:AC:82:LEU:HD11  | 5:AC:163:LEU:HD22  | 2.02                     | 0.42              |
| 5:AE:53:THR:O     | 12:BF:22:ASN:HB3   | 2.20                     | 0.42              |
| 3:AF:62:LEU:HG    | 12:BB:84:LEU:CD1   | 2.44                     | 0.42              |
| 3:AJ:140:ILE:HG21 | 3:AJ:157:VAL:HG11  | 2.01                     | 0.42              |
| 3:AM:17:THR:C     | 3:AM:19:MET:H      | 2.28                     | 0.42              |
| 3:AM:128:LEU:O    | 3:AM:136:VAL:HG23  | 2.20                     | 0.42              |
| 3:AN:85:ASN:O     | 3:AN:221:THR:OG1   | 2.33                     | 0.42              |
| 6:AS:372:ILE:HB   | 10:A4:4:ILE:HG12   | 2.01                     | 0.42              |
| 6:AZ:296:ARG:HG2  | 6:AZ:296:ARG:NH1   | 2.35                     | 0.42              |
| 6:Ae:404:LEU:HD22 | 6:Ae:409:MET:HE3   | 2.02                     | 0.42              |
| 6:Ah:404:LEU:HD22 | 6:Ah:409:MET:HE3   | 2.02                     | 0.42              |
| 7:Aq:36:SER:HB3   | 7:Ar:44:ILE:HG23   | 2.02                     | 0.42              |
| 9:Au:162:PRO:CD   | 9:Au:163:GLU:N     | 2.82                     | 0.42              |
| 10:Az:84:MET:HE2  | 11:A6:134:LEU:HD21 | 2.02                     | 0.42              |
| 10:A5:11:ILE:HG22 | 6:BR:372:ILE:HB    | 2.02                     | 0.42              |
| 10:A5:76:GLN:NE2  | 12:BA:7:PHE:HE1    | 2.18                     | 0.42              |
| 11:A7:34:ASP:OD1  | 12:BB:20:ARG:NH1   | 2.51                     | 0.42              |
| 6:UM:214:ASP:OD2  | 6:UM:218:HIS:HB2   | 2.20                     | 0.42              |
| 6:WB:164:LEU:HD23 | 6:WB:164:LEU:HA    | 1.75                     | 0.42              |
| 6:WG:121:PHE:CE2  | 6:WG:123:ILE:HA    | 2.55                     | 0.42              |
| 6:WH:190:GLN:HG3  | 6:WI:217:GLY:HA3   | 2.02                     | 0.42              |
| 6:WL:140:LEU:O    | 6:WL:144:ILE:HG13  | 2.19                     | 0.42              |
| 6:WU:140:LEU:O    | 6:WU:144:ILE:HG13  | 2.20                     | 0.42              |
| 6:WV:140:LEU:O    | 6:WV:144:ILE:HG13  | 2.20                     | 0.42              |
| 1:B:214:ASN:ND2   | 1:C:173:GLN:NE2    | 2.67                     | 0.41              |
| 1:G:28:LYS:HD3    | 1:G:28:LYS:HA      | 1.89                     | 0.41              |
| 1:K:144:PHE:CE2   | 1:L:171:ILE:CD1    | 3.01                     | 0.41              |
| 1:N:169:ILE:HG22  | 1:N:171:ILE:HG12   | 2.02                     | 0.41              |
| 1:P:144:PHE:CE2   | 1:Q:171:ILE:CD1    | 3.01                     | 0.41              |
| 2:b:21:ARG:HD2    | 2:b:21:ARG:HA      | 1.74                     | 0.41              |
| 2:e:78:ASN:ND2    | 3:AL:137:GLN:HG3   | 2.36                     | 0.41              |
| 2:r:253:VAL:HG11  | 2:r:349:LEU:HD13   | 2.01                     | 0.41              |
| 2:s:253:VAL:HG11  | 2:s:349:LEU:HD13   | 2.01                     | 0.41              |
| 2:u:362:LEU:HD23  | 2:w:166:THR:HG21   | 2.02                     | 0.41              |
| 2:y:21:ARG:HH21   | 2:y:246:VAL:CG2    | 2.32                     | 0.41              |
| 2:z:192:GLU:H     | 2:z:192:GLU:HG3    | 1.52                     | 0.41              |
| 2:z:251:ALA:HB2   | 2:z:267:GLU:O      | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:145:ASN:ND2   | 3:7:209:ASN:CG    | 2.78                     | 0.41              |
| 3:4:1:MET:HB2     | 3:AM:235:GLN:CG   | 2.50                     | 0.41              |
| 3:5:44:LEU:HD22   | 3:AI:86:LEU:CD1   | 2.39                     | 0.41              |
| 3:6:85:ASN:OD1    | 4:ZH:50:LEU:CD2   | 2.68                     | 0.41              |
| 3:6:128:LEU:HD23  | 3:6:128:LEU:HA    | 1.86                     | 0.41              |
| 3:7:56:SER:HB3    | 3:7:62:LEU:CB     | 2.50                     | 0.41              |
| 3:7:154:ASP:OD1   | 3:7:154:ASP:N     | 2.47                     | 0.41              |
| 3:9:44:LEU:HD21   | 3:9:73:ARG:HB2    | 2.02                     | 0.41              |
| 3:ZA:55:GLN:HG3   | 3:ZA:57:SER:O     | 2.19                     | 0.41              |
| 3:ZB:28:ASN:HD21  | 4:ZG:52:VAL:CB    | 2.33                     | 0.41              |
| 4:ZH:128:ILE:HD13 | 4:ZH:314:GLN:OE1  | 2.20                     | 0.41              |
| 4:ZH:280:ASN:OD1  | 4:ZH:281:GLN:N    | 2.53                     | 0.41              |
| 4:ZI:204:LYS:O    | 4:ZI:207:GLU:N    | 2.53                     | 0.41              |
| 4:ZP:372:LEU:HD21 | 4:ZU:384:SER:OG   | 2.20                     | 0.41              |
| 4:ZR:229:THR:O    | 4:ZR:241:GLY:HA3  | 2.19                     | 0.41              |
| 4:ZR:235:ASN:OD1  | 4:ZX:189:SER:HB2  | 2.19                     | 0.41              |
| 4:ZS:369:SER:HA   | 4:Zd:399:LEU:HD13 | 2.00                     | 0.41              |
| 4:ZU:78:SER:HB3   | 4:ZU:79:GLN:OE1   | 2.19                     | 0.41              |
| 4:ZU:197:ASN:HD21 | 4:ZU:215:SER:HB2  | 1.85                     | 0.41              |
| 4:ZX:106:ARG:CD   | 4:Zc:321:ALA:HB1  | 2.50                     | 0.41              |
| 4:ZZ:112:GLN:HG2  | 4:ZZ:331:ASP:HB3  | 2.02                     | 0.41              |
| 4:Zb:179:ASN:OD1  | 4:Zb:202:LYS:N    | 2.35                     | 0.41              |
| 4:Zc:388:THR:O    | 4:Zc:392:GLN:HG2  | 2.20                     | 0.41              |
| 4:Zd:397:ASN:C    | 4:Zd:399:LEU:H    | 2.28                     | 0.41              |
| 4:Zh:20:ILE:HG23  | 4:Zh:371:GLU:OE2  | 2.20                     | 0.41              |
| 6:AV:404:LEU:HD22 | 6:AV:409:MET:HE3  | 2.02                     | 0.41              |
| 6:AX:421:GLY:O    | 6:AX:426:ARG:NH2  | 2.51                     | 0.41              |
| 6:AI:404:LEU:HD22 | 6:AI:409:MET:HE3  | 2.02                     | 0.41              |
| 6:AP:404:LEU:HD22 | 6:AP:409:MET:HE3  | 2.02                     | 0.41              |
| 7:Ar:1:MET:HE2    | 7:Ar:1:MET:HB3    | 1.91                     | 0.41              |
| 7:As:18:LEU:CD2   | 8:At:227:MET:HB3  | 2.50                     | 0.41              |
| 9:Av:129:LYS:HD3  | 9:Av:129:LYS:HA   | 1.79                     | 0.41              |
| 9:Aw:68:ILE:HD12  | 9:Aw:68:ILE:HA    | 1.83                     | 0.41              |
| 10:Az:68:LEU:H    | 10:Az:68:LEU:HD12 | 1.85                     | 0.41              |
| 11:A7:24:GLU:HG2  | 12:BB:6:ILE:HD11  | 2.02                     | 0.41              |
| 11:A9:92:GLN:CD   | 12:BE:22:ASN:HD22 | 2.28                     | 0.41              |
| 11:A0:92:GLN:HE21 | 12:BF:19:LYS:HG2  | 1.85                     | 0.41              |
| 6:UK:214:ASP:OD2  | 6:UK:218:HIS:HB2  | 2.20                     | 0.41              |
| 6:UL:102:GLN:CG   | 6:UL:193:ALA:HB2  | 2.49                     | 0.41              |
| 6:UO:102:GLN:CG   | 6:UO:193:ALA:HB2  | 2.49                     | 0.41              |
| 6:UP:214:ASP:OD2  | 6:UP:218:HIS:HB2  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:BB:126:MET:HE3 | 12:BB:126:MET:HB3 | 1.80                     | 0.41              |
| 6:WD:197:LEU:HD11 | 6:WE:156:HIS:HD2  | 1.84                     | 0.41              |
| 6:WT:140:LEU:O    | 6:WT:144:ILE:HG13 | 2.20                     | 0.41              |
| 6:BT:296:ARG:HG2  | 6:BT:296:ARG:NH1  | 2.35                     | 0.41              |
| 6:BV:421:GLY:O    | 6:BV:426:ARG:NH2  | 2.51                     | 0.41              |
| 1:C:165:GLY:C     | 1:D:35:THR:HG21   | 2.40                     | 0.41              |
| 1:E:106:PHE:HB3   | 1:E:109:VAL:HG22  | 2.00                     | 0.41              |
| 1:L:144:PHE:CE2   | 1:M:171:ILE:CD1   | 3.01                     | 0.41              |
| 1:O:214:ASN:ND2   | 1:P:173:GLN:NE2   | 2.67                     | 0.41              |
| 1:P:165:GLY:C     | 1:Q:35:THR:HG21   | 2.40                     | 0.41              |
| 1:Q:169:ILE:HG22  | 1:Q:171:ILE:HG12  | 2.02                     | 0.41              |
| 2:c:253:VAL:HG11  | 2:c:349:LEU:HD13  | 2.01                     | 0.41              |
| 2:d:253:VAL:HG11  | 2:d:349:LEU:HD13  | 2.01                     | 0.41              |
| 2:j:78:ASN:OD1    | 2:j:78:ASN:N      | 2.51                     | 0.41              |
| 2:k:21:ARG:HD2    | 2:k:21:ARG:HA     | 1.75                     | 0.41              |
| 2:l:251:ALA:HB2   | 2:l:267:GLU:O     | 2.20                     | 0.41              |
| 2:n:253:VAL:HG11  | 2:n:349:LEU:HD13  | 2.01                     | 0.41              |
| 2:y:250:ASP:OD1   | 2:z:23:ARG:NE     | 2.51                     | 0.41              |
| 3:1:252:GLN:NE2   | 3:AK:237:GLN:HE22 | 2.18                     | 0.41              |
| 3:3:247:VAL:HG12  | 3:8:260:LEU:HD11  | 2.02                     | 0.41              |
| 3:5:10:THR:OG1    | 3:5:71:GLY:HA3    | 2.20                     | 0.41              |
| 3:ZB:26:LEU:HD22  | 4:ZG:384:SER:OG   | 2.20                     | 0.41              |
| 3:ZB:244:SER:OG   | 4:ZG:398:THR:HG22 | 2.19                     | 0.41              |
| 3:ZD:58:GLU:HB3   | 3:ZD:59:GLN:OE1   | 2.20                     | 0.41              |
| 3:ZE:167:PRO:HG2  | 4:ZP:338:GLN:HE22 | 1.83                     | 0.41              |
| 4:ZF:198:VAL:HG22 | 4:ZF:212:THR:HG22 | 2.02                     | 0.41              |
| 4:ZG:87:ASP:OD1   | 4:ZG:91:SER:N     | 2.48                     | 0.41              |
| 4:ZO:148:SER:HB3  | 4:ZO:188:ASP:C    | 2.45                     | 0.41              |
| 4:ZO:235:ASN:O    | 4:ZO:237:ILE:N    | 2.51                     | 0.41              |
| 4:ZT:24:ILE:HG22  | 4:ZY:385:ASN:OD1  | 2.20                     | 0.41              |
| 4:ZU:368:LEU:HA   | 4:ZU:368:LEU:HD23 | 1.80                     | 0.41              |
| 4:Zb:269:GLN:HG3  | 4:Zh:190:GLN:O    | 2.20                     | 0.41              |
| 4:Ze:85:LEU:HD23  | 4:Ze:114:MET:HB3  | 2.02                     | 0.41              |
| 4:Zf:298:GLY:O    | 4:Zf:315:ILE:HG13 | 2.20                     | 0.41              |
| 4:Zg:41:ASP:OD1   | 4:Zg:41:ASP:N     | 2.52                     | 0.41              |
| 5:AA:123:GLU:H    | 5:AA:123:GLU:HG3  | 1.53                     | 0.41              |
| 5:AD:80:VAL:HG11  | 5:AD:137:ILE:HG21 | 2.02                     | 0.41              |
| 3:AG:43:ASP:OD1   | 3:AG:43:ASP:N     | 2.53                     | 0.41              |
| 3:AG:158:SER:HB3  | 3:AG:169:GLN:HE21 | 1.85                     | 0.41              |
| 3:AH:247:VAL:HG11 | 3:AM:260:LEU:HD21 | 2.03                     | 0.41              |
| 3:AI:154:ASP:O    | 3:AI:154:ASP:OD2  | 2.38                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AK:223:ASN:OD1  | 3:AK:223:ASN:O    | 2.38                     | 0.41              |
| 3:AM:140:ILE:HD13 | 3:AM:157:VAL:HG21 | 2.01                     | 0.41              |
| 6:AV:296:ARG:HG2  | 6:AV:296:ARG:NH1  | 2.35                     | 0.41              |
| 6:AX:404:LEU:HD22 | 6:AX:409:MET:HE3  | 2.02                     | 0.41              |
| 6:Ak:370:ARG:HE   | 10:A1:7:ILE:HD11  | 1.79                     | 0.41              |
| 6:AQ:404:LEU:HD22 | 6:AQ:409:MET:HE3  | 2.02                     | 0.41              |
| 7:As:18:LEU:HD22  | 8:At:227:MET:HB3  | 2.01                     | 0.41              |
| 7:As:77:VAL:HG11  | 9:Ay:225:LEU:HD11 | 2.02                     | 0.41              |
| 9:Av:171:LEU:HD23 | 9:Aw:95:PHE:CZ    | 2.55                     | 0.41              |
| 9:Ay:143:ARG:CZ   | 9:Ay:180:LYS:HE2  | 2.50                     | 0.41              |
| 6:UO:125:GLN:C    | 6:UO:127:SER:N    | 2.77                     | 0.41              |
| 6:WK:190:GLN:HA   | 6:WL:217:GLY:O    | 2.20                     | 0.41              |
| 6:WR:165:PHE:O    | 6:WR:166:VAL:HG22 | 2.19                     | 0.41              |
| 6:WS:140:LEU:O    | 6:WS:144:ILE:HG13 | 2.19                     | 0.41              |
| 6:BU:296:ARG:HG2  | 6:BU:296:ARG:NH1  | 2.35                     | 0.41              |
| 6:BX:290:LYS:HE3  | 6:BX:290:LYS:HB2  | 1.93                     | 0.41              |
| 1:D:110:PRO:HD3   | 1:E:124:MET:CB    | 2.50                     | 0.41              |
| 1:E:113:LEU:HD12  | 1:E:113:LEU:HA    | 1.90                     | 0.41              |
| 1:G:136:GLY:CA    | 1:I:213:ILE:HG23  | 2.42                     | 0.41              |
| 1:H:110:PRO:HD3   | 1:I:124:MET:CB    | 2.50                     | 0.41              |
| 1:I:47:ALA:HB3    | 2:f:178:GLN:CD    | 2.45                     | 0.41              |
| 1:J:86:VAL:HB     | 1:J:142:ASN:ND2   | 2.35                     | 0.41              |
| 1:Q:165:GLY:C     | 1:R:35:THR:HG21   | 2.40                     | 0.41              |
| 1:U:169:ILE:HG22  | 1:U:171:ILE:HG12  | 2.02                     | 0.41              |
| 2:a:247:THR:O     | 2:a:248:PRO:C     | 2.64                     | 0.41              |
| 2:a:266:ARG:HA    | 2:a:328:LEU:HD22  | 2.01                     | 0.41              |
| 2:a:362:LEU:HD23  | 2:c:166:THR:HG21  | 2.03                     | 0.41              |
| 2:b:93:TYR:OH     | 2:b:173:ARG:O     | 2.25                     | 0.41              |
| 2:f:188:GLN:HE21  | 2:f:188:GLN:HB2   | 1.63                     | 0.41              |
| 2:h:192:GLU:H     | 2:h:192:GLU:HG3   | 1.53                     | 0.41              |
| 2:k:130:ASP:N     | 2:k:130:ASP:OD1   | 2.47                     | 0.41              |
| 2:l:266:ARG:HA    | 2:l:328:LEU:HD22  | 2.02                     | 0.41              |
| 2:o:266:ARG:HA    | 2:o:328:LEU:HD22  | 2.02                     | 0.41              |
| 2:q:253:VAL:HG11  | 2:q:349:LEU:HD13  | 2.01                     | 0.41              |
| 2:q:273:CYS:CA    | 2:r:328:LEU:HD21  | 2.41                     | 0.41              |
| 2:s:359:ARG:HE    | 2:t:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:u:251:ALA:HB2   | 2:u:267:GLU:O     | 2.20                     | 0.41              |
| 2:v:78:ASN:OD1    | 2:v:78:ASN:N      | 2.51                     | 0.41              |
| 2:x:362:LEU:HD23  | 2:z:166:THR:HG21  | 2.03                     | 0.41              |
| 3:3:20:ASP:OD1    | 3:8:4:SER:OG      | 2.28                     | 0.41              |
| 3:3:95:VAL:O      | 3:3:118:GLY:HA3   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:5:92:SER:O      | 3:5:216:GLN:NE2   | 2.42                     | 0.41              |
| 3:6:142:ILE:HD13  | 3:6:149:ILE:HD13  | 2.01                     | 0.41              |
| 3:6:145:ASN:HB2   | 3:ZB:209:ASN:O    | 2.19                     | 0.41              |
| 3:7:194:GLU:OE2   | 3:7:201:PRO:HD3   | 2.20                     | 0.41              |
| 3:9:85:ASN:CB     | 4:ZK:4:SER:CB     | 2.97                     | 0.41              |
| 3:ZB:29:VAL:HG11  | 4:ZG:381:ASN:ND2  | 2.36                     | 0.41              |
| 3:ZD:239:ALA:O    | 3:ZD:240:TYR:C    | 2.63                     | 0.41              |
| 4:ZI:105:ASN:OD1  | 4:ZI:105:ASN:N    | 2.53                     | 0.41              |
| 4:ZK:380:ARG:HD3  | 4:ZK:380:ARG:HA   | 1.53                     | 0.41              |
| 4:ZL:74:ASP:N     | 4:ZL:74:ASP:OD1   | 2.53                     | 0.41              |
| 4:ZN:73:LEU:HD21  | 4:ZN:292:TYR:HE2  | 1.86                     | 0.41              |
| 4:ZN:95:SER:OG    | 4:ZN:332:ASN:O    | 2.30                     | 0.41              |
| 4:ZN:184:VAL:HG13 | 4:ZN:196:MET:HB2  | 2.01                     | 0.41              |
| 4:ZO:49:GLY:O     | 4:ZO:50:LEU:C     | 2.63                     | 0.41              |
| 4:ZP:159:ASN:N    | 4:ZP:274:ASN:OD1  | 2.47                     | 0.41              |
| 4:ZR:10:LEU:HG    | 4:ZR:382:TYR:CE2  | 2.55                     | 0.41              |
| 4:ZT:121:ALA:HB2  | 4:ZT:128:ILE:HD13 | 2.03                     | 0.41              |
| 4:ZT:125:PRO:HA   | 4:ZT:126:PRO:HD3  | 1.96                     | 0.41              |
| 4:ZT:128:ILE:HD13 | 4:ZT:128:ILE:HA   | 1.83                     | 0.41              |
| 4:ZW:17:LEU:HD13  | 4:Zb:395:ILE:HD11 | 2.02                     | 0.41              |
| 4:ZX:16:ASN:HB2   | 4:ZX:39:PHE:HZ    | 1.85                     | 0.41              |
| 4:Za:53:LYS:HB2   | 4:Za:53:LYS:HE2   | 1.92                     | 0.41              |
| 4:Za:83:PHE:O     | 4:Za:94:TYR:HA    | 2.19                     | 0.41              |
| 4:Za:284:TYR:HB3  | 4:Za:308:GLN:HE22 | 1.84                     | 0.41              |
| 4:Za:328:SER:HB2  | 4:Zf:43:PHE:CD1   | 2.55                     | 0.41              |
| 4:Zc:25:ALA:HB1   | 4:Zh:52:VAL:HG12  | 2.02                     | 0.41              |
| 4:Zc:368:LEU:HD23 | 4:Zc:368:LEU:HA   | 1.87                     | 0.41              |
| 4:Zg:370:LYS:HB2  | 4:Zg:370:LYS:HE2  | 1.90                     | 0.41              |
| 4:Zh:380:ARG:HD3  | 4:Zh:380:ARG:HA   | 1.76                     | 0.41              |
| 5:AB:228:GLU:HB2  | 3:AH:258:THR:HB   | 2.02                     | 0.41              |
| 5:AD:89:VAL:HG22  | 5:AD:99:TYR:CD1   | 2.56                     | 0.41              |
| 3:AF:62:LEU:HD21  | 12:BB:83:PRO:HD2  | 2.01                     | 0.41              |
| 3:AG:77:THR:HG23  | 3:AL:66:LEU:HB2   | 2.01                     | 0.41              |
| 3:AI:146:ALA:O    | 3:AN:100:GLN:NE2  | 2.50                     | 0.41              |
| 6:AS:404:LEU:HD22 | 6:AS:409:MET:HE3  | 2.02                     | 0.41              |
| 6:Ad:404:LEU:HD22 | 6:Ad:409:MET:HE3  | 2.02                     | 0.41              |
| 8:At:101:PHE:CE2  | 9:Au:80:THR:HG21  | 2.55                     | 0.41              |
| 8:At:178:LEU:HD12 | 8:At:182:ASN:ND2  | 2.33                     | 0.41              |
| 9:Au:175:VAL:O    | 9:Au:179:LEU:HG   | 2.20                     | 0.41              |
| 10:Az:86:ILE:CD1  | 10:A5:98:GLU:HG3  | 2.47                     | 0.41              |
| 6:UJ:102:GLN:CG   | 6:UJ:193:ALA:HB2  | 2.49                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:UO:214:ASP:OD2  | 6:UO:218:HIS:HB2  | 2.20                     | 0.41              |
| 6:UP:102:GLN:CG   | 6:UP:193:ALA:HB2  | 2.49                     | 0.41              |
| 12:BB:47:VAL:O    | 6:BJ:313:PRO:CD   | 2.68                     | 0.41              |
| 12:BB:95:ASN:OD1  | 12:BB:95:ASN:N    | 2.43                     | 0.41              |
| 6:WI:129:GLN:HE22 | 6:WI:132:TYR:HD2  | 1.68                     | 0.41              |
| 6:WI:135:ALA:O    | 6:WI:139:GLU:HG2  | 2.21                     | 0.41              |
| 6:WL:181:GLU:CB   | 6:WL:184:ARG:CG   | 2.85                     | 0.41              |
| 6:WR:181:GLU:CB   | 6:WR:184:ARG:CG   | 2.85                     | 0.41              |
| 6:WR:192:SER:O    | 6:WR:195:VAL:N    | 2.53                     | 0.41              |
| 6:BU:421:GLY:O    | 6:BU:426:ARG:NH2  | 2.51                     | 0.41              |
| 6:BW:404:LEU:HD22 | 6:BW:409:MET:HE3  | 2.02                     | 0.41              |
| 1:G:110:PRO:HD3   | 1:H:124:MET:CB    | 2.50                     | 0.41              |
| 1:H:47:ALA:HB3    | 2:e:178:GLN:CD    | 2.45                     | 0.41              |
| 1:I:144:PHE:CE2   | 1:J:171:ILE:CD1   | 3.01                     | 0.41              |
| 1:J:47:ALA:HB3    | 2:g:178:GLN:CD    | 2.45                     | 0.41              |
| 1:K:47:ALA:HB3    | 2:h:178:GLN:CD    | 2.45                     | 0.41              |
| 1:L:142:ASN:ND2   | 1:M:207:TYR:OH    | 2.28                     | 0.41              |
| 1:N:50:SER:HB3    | 2:k:32:ARG:HH11   | 1.81                     | 0.41              |
| 1:N:142:ASN:ND2   | 1:O:207:TYR:OH    | 2.28                     | 0.41              |
| 1:Q:47:ALA:HB3    | 2:n:178:GLN:CD    | 2.45                     | 0.41              |
| 1:Y:169:ILE:HG22  | 1:Y:171:ILE:HG12  | 2.02                     | 0.41              |
| 2:b:166:THR:HG21  | 2:z:362:LEU:HD23  | 2.03                     | 0.41              |
| 2:b:192:GLU:H     | 2:b:192:GLU:HG3   | 1.52                     | 0.41              |
| 2:c:362:LEU:HD23  | 2:e:166:THR:HG21  | 2.03                     | 0.41              |
| 2:d:247:THR:O     | 2:d:248:PRO:C     | 2.64                     | 0.41              |
| 2:g:251:ALA:HB2   | 2:g:267:GLU:O     | 2.20                     | 0.41              |
| 2:k:251:ALA:HB2   | 2:k:267:GLU:O     | 2.20                     | 0.41              |
| 2:n:266:ARG:HA    | 2:n:328:LEU:HD22  | 2.01                     | 0.41              |
| 2:o:250:ASP:OD1   | 2:p:23:ARG:NE     | 2.51                     | 0.41              |
| 2:q:247:THR:O     | 2:q:248:PRO:C     | 2.64                     | 0.41              |
| 2:r:359:ARG:HE    | 2:s:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:t:359:ARG:HE    | 2:u:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:u:247:THR:O     | 2:u:248:PRO:C     | 2.64                     | 0.41              |
| 2:v:362:LEU:HD23  | 2:x:166:THR:HG21  | 2.03                     | 0.41              |
| 2:w:362:LEU:HD23  | 2:y:166:THR:HG21  | 2.03                     | 0.41              |
| 2:x:21:ARG:HH21   | 2:x:246:VAL:CG2   | 2.32                     | 0.41              |
| 2:y:78:ASN:OD1    | 2:y:78:ASN:N      | 2.51                     | 0.41              |
| 2:z:188:GLN:HE21  | 2:z:188:GLN:HB2   | 1.63                     | 0.41              |
| 3:1:124:GLN:HB2   | 3:6:199:GLY:N     | 2.35                     | 0.41              |
| 3:2:178:PHE:CE1   | 3:2:184:LEU:HD11  | 2.56                     | 0.41              |
| 3:2:209:ASN:HB2   | 3:AL:145:ASN:HD22 | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:2:ILE:HD13    | 3:4:250:THR:CG2   | 2.41                     | 0.41              |
| 3:4:67:GLN:NE2    | 3:AN:185:GLU:OE2  | 2.53                     | 0.41              |
| 3:5:24:ASN:CA     | 3:ZA:7:ILE:HG21   | 2.50                     | 0.41              |
| 3:ZD:77:THR:N     | 4:ZI:47:LYS:HE3   | 2.35                     | 0.41              |
| 4:ZF:181:LYS:HE3  | 4:ZF:181:LYS:HB2  | 1.85                     | 0.41              |
| 4:ZF:380:ARG:HD3  | 4:ZF:380:ARG:HA   | 1.69                     | 0.41              |
| 4:ZH:270:ASN:CB   | 4:ZN:191:GLY:O    | 2.68                     | 0.41              |
| 4:ZI:112:GLN:HG2  | 4:ZI:331:ASP:HB3  | 2.01                     | 0.41              |
| 4:ZI:183:THR:OG1  | 4:ZT:131:GLY:O    | 2.38                     | 0.41              |
| 4:ZI:324:GLU:C    | 4:ZI:326:LEU:N    | 2.78                     | 0.41              |
| 4:ZL:22:ASN:OD1   | 4:ZL:26:ASN:ND2   | 2.53                     | 0.41              |
| 4:ZP:107:ASN:ND2  | 4:ZP:138:THR:HG22 | 2.33                     | 0.41              |
| 4:ZQ:307:GLU:OE1  | 4:Zb:92:VAL:CG2   | 2.67                     | 0.41              |
| 4:ZU:3:PHE:O      | 4:ZU:7:VAL:HG23   | 2.20                     | 0.41              |
| 4:ZU:112:GLN:HE21 | 4:ZZ:40:ALA:HB2   | 1.85                     | 0.41              |
| 4:ZV:93:PHE:HB3   | 4:ZV:333:VAL:HG22 | 2.03                     | 0.41              |
| 4:ZW:376:ILE:HG23 | 4:Zc:393:ASP:OD1  | 2.20                     | 0.41              |
| 4:ZZ:107:ASN:ND2  | 4:ZZ:138:THR:HG22 | 2.35                     | 0.41              |
| 4:Za:108:LEU:HD23 | 4:Za:108:LEU:HA   | 1.83                     | 0.41              |
| 4:Zb:233:ASN:OD1  | 4:Zb:237:ILE:N    | 2.52                     | 0.41              |
| 4:Zc:348:ALA:HB2  | 4:Zc:356:LEU:HG   | 2.02                     | 0.41              |
| 5:AA:29:ALA:O     | 5:AA:209:SER:OG   | 2.37                     | 0.41              |
| 5:AA:46:VAL:CG1   | 11:A6:93:PRO:HB2  | 2.43                     | 0.41              |
| 5:AB:227:PHE:O    | 5:AB:228:GLU:C    | 2.62                     | 0.41              |
| 5:AE:231:MET:CE   | 3:AJ:257:LEU:HD13 | 2.41                     | 0.41              |
| 3:AL:19:MET:HE1   | 3:AL:233:MET:HG2  | 2.02                     | 0.41              |
| 3:AL:83:GLN:HE22  | 3:AL:86:LEU:HD21  | 1.85                     | 0.41              |
| 3:AM:6:TRP:O      | 3:AM:7:ILE:C      | 2.62                     | 0.41              |
| 3:AM:88:GLN:HB2   | 3:AM:218:TYR:CE1  | 2.55                     | 0.41              |
| 6:AT:236:LYS:NZ   | 6:UJ:167:ARG:NH1  | 2.60                     | 0.41              |
| 6:AQ:296:ARG:HG2  | 6:AQ:296:ARG:NH1  | 2.35                     | 0.41              |
| 7:Ar:40:ALA:CB    | 7:As:44:ILE:HD11  | 2.50                     | 0.41              |
| 7:As:14:MET:HG2   | 8:At:230:ALA:HB2  | 2.02                     | 0.41              |
| 9:Au:38:TRP:HB2   | 10:A1:46:SER:CB   | 2.46                     | 0.41              |
| 9:Au:194:LEU:HD12 | 9:Av:220:PRO:HG2  | 2.03                     | 0.41              |
| 9:Ay:124:GLN:H    | 9:Ay:124:GLN:HG2  | 1.67                     | 0.41              |
| 9:Ay:217:ILE:O    | 9:Ay:220:PRO:HD2  | 2.20                     | 0.41              |
| 11:A6:133:VAL:C   | 11:A6:135:GLN:N   | 2.78                     | 0.41              |
| 11:A8:16:LEU:HD11 | 11:A8:120:LEU:HG  | 2.02                     | 0.41              |
| 6:UK:52:ARG:O     | 6:UK:88:VAL:N     | 2.38                     | 0.41              |
| 6:WE:164:LEU:HD13 | 6:WE:165:PHE:N    | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:WH:140:LEU:O    | 6:WH:144:ILE:HG13 | 2.20                     | 0.41              |
| 6:WH:149:PRO:CD   | 6:WH:190:GLN:HE22 | 2.33                     | 0.41              |
| 6:WK:145:GLU:C    | 6:WK:147:LEU:N    | 2.76                     | 0.41              |
| 6:WL:135:ALA:O    | 6:WL:136:LEU:C    | 2.63                     | 0.41              |
| 6:WL:196:HIS:HB3  | 6:WM:211:THR:HG21 | 2.03                     | 0.41              |
| 6:WT:128:GLU:HG3  | 6:WU:126:PHE:CE2  | 2.55                     | 0.41              |
| 6:WT:147:LEU:O    | 6:WT:148:GLY:C    | 2.64                     | 0.41              |
| 6:BR:404:LEU:HD22 | 6:BR:409:MET:HE3  | 2.02                     | 0.41              |
| 1:C:169:ILE:HG22  | 1:C:171:ILE:HG12  | 2.02                     | 0.41              |
| 1:E:232:MET:HE3   | 1:E:232:MET:HB2   | 1.90                     | 0.41              |
| 1:L:47:ALA:HB3    | 2:i:178:GLN:CD    | 2.45                     | 0.41              |
| 1:Q:28:LYS:HD3    | 1:Q:28:LYS:HA     | 1.89                     | 0.41              |
| 1:V:47:ALA:HB3    | 2:s:178:GLN:CD    | 2.45                     | 0.41              |
| 2:b:266:ARG:HA    | 2:b:328:LEU:HD22  | 2.01                     | 0.41              |
| 2:b:362:LEU:HD23  | 2:d:166:THR:HG21  | 2.03                     | 0.41              |
| 2:c:78:ASN:CG     | 3:AG:145:ASN:ND2  | 2.77                     | 0.41              |
| 2:m:250:ASP:OD1   | 2:n:23:ARG:NE     | 2.51                     | 0.41              |
| 2:m:319:LEU:HD21  | 2:n:264:MET:HE1   | 1.98                     | 0.41              |
| 2:p:253:VAL:HG11  | 2:p:349:LEU:HD13  | 2.01                     | 0.41              |
| 2:q:359:ARG:HE    | 2:r:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:r:251:ALA:HB2   | 2:r:267:GLU:O     | 2.20                     | 0.41              |
| 2:s:362:LEU:HD23  | 2:u:166:THR:HG21  | 2.03                     | 0.41              |
| 2:t:247:THR:O     | 2:t:248:PRO:C     | 2.64                     | 0.41              |
| 2:w:247:THR:O     | 2:w:248:PRO:C     | 2.64                     | 0.41              |
| 2:w:251:ALA:HB2   | 2:w:267:GLU:O     | 2.20                     | 0.41              |
| 2:x:247:THR:O     | 2:x:248:PRO:C     | 2.64                     | 0.41              |
| 3:0:89:THR:HG23   | 3:0:91:ASN:H      | 1.86                     | 0.41              |
| 3:1:128:LEU:O     | 3:1:136:VAL:HG23  | 2.20                     | 0.41              |
| 3:2:50:ARG:HD3    | 3:2:66:LEU:HB2    | 2.03                     | 0.41              |
| 3:8:28:ASN:ND2    | 3:ZD:43:ASP:OD1   | 2.53                     | 0.41              |
| 3:8:153:ARG:HG2   | 3:8:214:LEU:O     | 2.21                     | 0.41              |
| 3:ZA:52:PRO:HA    | 3:ZA:65:GLY:H     | 1.86                     | 0.41              |
| 3:ZD:123:ASP:OD1  | 3:ZD:123:ASP:N    | 2.47                     | 0.41              |
| 3:ZE:70:THR:CG2   | 3:ZE:71:GLY:H     | 2.32                     | 0.41              |
| 4:ZH:306:ASN:C    | 4:ZH:307:GLU:HG2  | 2.45                     | 0.41              |
| 4:ZH:352:ASN:O    | 4:ZH:352:ASN:CG   | 2.64                     | 0.41              |
| 4:ZH:399:LEU:O    | 4:ZH:402:LEU:HG   | 2.21                     | 0.41              |
| 4:ZM:87:ASP:OD2   | 4:ZM:87:ASP:N     | 2.45                     | 0.41              |
| 4:ZM:237:ILE:H    | 4:ZM:237:ILE:HD12 | 1.85                     | 0.41              |
| 4:ZQ:99:GLN:HG2   | 4:ZQ:111:MET:HE3  | 2.02                     | 0.41              |
| 4:ZS:183:THR:CB   | 4:Zd:132:ALA:HA   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZS:245:ASN:OD1  | 4:ZS:245:ASN:N     | 2.53                     | 0.41              |
| 4:ZT:380:ARG:HD2  | 4:ZZ:396:LEU:HB3   | 2.01                     | 0.41              |
| 4:ZX:376:ILE:HG23 | 4:Zd:393:ASP:OD2   | 2.20                     | 0.41              |
| 4:ZY:171:SER:O    | 4:ZY:177:SER:OG    | 2.39                     | 0.41              |
| 4:ZZ:380:ARG:HB3  | 4:Zf:396:LEU:HD12  | 2.02                     | 0.41              |
| 4:Zc:71:ARG:O     | 4:Zc:359:GLY:HA2   | 2.20                     | 0.41              |
| 4:Zc:101:LYS:CE   | 4:Zh:322:ASN:HD21  | 2.27                     | 0.41              |
| 4:Zg:116:LEU:HD12 | 4:Zg:116:LEU:HA    | 1.90                     | 0.41              |
| 5:AB:68:PRO:HG3   | 3:AM:47:GLN:CB     | 2.50                     | 0.41              |
| 5:AB:71:LEU:HD23  | 3:AM:44:LEU:HD12   | 1.89                     | 0.41              |
| 5:AD:2:ASP:OD2    | 5:AD:3:HIS:N       | 2.54                     | 0.41              |
| 5:AD:15:THR:OG1   | 5:AD:226:ARG:NH1   | 2.53                     | 0.41              |
| 5:AE:146:LEU:O    | 5:AE:148:PRO:N     | 2.53                     | 0.41              |
| 5:AE:220:MET:HE2  | 3:AJ:246:ALA:HB2   | 2.02                     | 0.41              |
| 5:AE:231:MET:HE1  | 3:AJ:257:LEU:CG    | 2.45                     | 0.41              |
| 5:AE:244:ALA:HB2  | 12:BF:116:ILE:HD11 | 2.02                     | 0.41              |
| 3:AH:49:ILE:HD11  | 3:AH:68:ILE:HD11   | 2.03                     | 0.41              |
| 3:AI:98:LYS:HD3   | 3:AI:213:LEU:HD12  | 2.03                     | 0.41              |
| 3:AK:113:ALA:HB1  | 3:AK:191:LEU:HB3   | 2.02                     | 0.41              |
| 6:AU:404:LEU:HD22 | 6:AU:409:MET:HE3   | 2.02                     | 0.41              |
| 6:AW:296:ARG:HG2  | 6:AW:296:ARG:NH1   | 2.35                     | 0.41              |
| 9:Ax:153:LEU:CD2  | 6:WG:165:PHE:CZ    | 3.01                     | 0.41              |
| 9:Ay:237:GLY:HA2  | 6:WG:165:PHE:HZ    | 1.85                     | 0.41              |
| 6:UJ:103:GLN:H    | 6:UJ:103:GLN:HG2   | 1.74                     | 0.41              |
| 6:UL:125:GLN:C    | 6:UL:127:SER:N     | 2.77                     | 0.41              |
| 6:UP:94:HIS:HB2   | 6:UP:146:THR:HG21  | 1.97                     | 0.41              |
| 12:BB:126:MET:HG2 | 12:BB:126:MET:H    | 1.60                     | 0.41              |
| 6:WK:190:GLN:CG   | 6:WL:217:GLY:HA3   | 2.51                     | 0.41              |
| 6:WN:181:GLU:CB   | 6:WN:184:ARG:CG    | 2.85                     | 0.41              |
| 6:WQ:140:LEU:O    | 6:WQ:144:ILE:HG13  | 2.20                     | 0.41              |
| 6:WR:140:LEU:O    | 6:WR:144:ILE:HG13  | 2.20                     | 0.41              |
| 6:WV:187:ASP:O    | 6:WV:190:GLN:HB2   | 2.20                     | 0.41              |
| 12:BD:112:TYR:CE2 | 12:BD:116:ILE:HD11 | 2.55                     | 0.41              |
| 1:G:47:ALA:HB3    | 2:d:178:GLN:CD     | 2.45                     | 0.41              |
| 1:I:169:ILE:HG22  | 1:I:171:ILE:HG12   | 2.02                     | 0.41              |
| 1:O:106:PHE:CD1   | 1:P:126:ALA:HB2    | 2.56                     | 0.41              |
| 1:R:169:ILE:HG22  | 1:R:171:ILE:HG12   | 2.02                     | 0.41              |
| 1:T:166:GLU:HB2   | 1:U:35:THR:CG2     | 2.30                     | 0.41              |
| 1:T:169:ILE:HG22  | 1:T:171:ILE:HG12   | 2.02                     | 0.41              |
| 1:W:232:MET:HE3   | 1:W:232:MET:HB2    | 1.90                     | 0.41              |
| 1:X:47:ALA:HB3    | 2:u:178:GLN:CD     | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:166:THR:HG21  | 2:y:362:LEU:HD23  | 2.03                     | 0.41              |
| 2:a:250:ASP:OD1   | 2:b:23:ARG:NE     | 2.51                     | 0.41              |
| 2:b:251:ALA:HB2   | 2:b:267:GLU:O     | 2.20                     | 0.41              |
| 2:d:80:GLN:HE21   | 2:d:80:GLN:HB2    | 1.68                     | 0.41              |
| 2:d:362:LEU:HD23  | 2:f:166:THR:HG21  | 2.03                     | 0.41              |
| 2:n:78:ASN:OD1    | 2:n:78:ASN:N      | 2.51                     | 0.41              |
| 2:n:247:THR:O     | 2:n:248:PRO:C     | 2.64                     | 0.41              |
| 2:t:362:LEU:HD23  | 2:v:166:THR:HG21  | 2.03                     | 0.41              |
| 3:0:68:ILE:HD13   | 3:AJ:17:THR:HG23  | 2.01                     | 0.41              |
| 3:4:137:GLN:HA    | 3:4:138:PRO:HA    | 1.71                     | 0.41              |
| 3:ZB:44:LEU:HD23  | 3:ZB:44:LEU:HA    | 1.87                     | 0.41              |
| 3:ZD:77:THR:O     | 3:ZD:77:THR:OG1   | 2.32                     | 0.41              |
| 4:ZF:85:LEU:HD13  | 4:ZF:114:MET:HB2  | 2.02                     | 0.41              |
| 4:ZH:111:MET:SD   | 4:ZH:111:MET:N    | 2.94                     | 0.41              |
| 4:ZI:323:ASN:H    | 4:ZI:323:ASN:HD22 | 1.69                     | 0.41              |
| 4:ZL:157:ASN:ND2  | 4:ZR:143:LEU:HD13 | 2.36                     | 0.41              |
| 4:ZM:102:LEU:HD12 | 4:ZM:102:LEU:HA   | 1.88                     | 0.41              |
| 4:ZM:290:VAL:HA   | 4:ZR:352:ASN:ND2  | 2.35                     | 0.41              |
| 4:ZM:331:ASP:HA   | 4:ZR:40:ALA:HB1   | 2.02                     | 0.41              |
| 4:ZM:387:GLN:OE1  | 4:ZS:400:VAL:HG13 | 2.20                     | 0.41              |
| 4:ZN:167:LYS:NZ   | 4:ZN:168:THR:O    | 2.54                     | 0.41              |
| 4:ZO:112:GLN:HG2  | 4:ZO:331:ASP:HB3  | 2.02                     | 0.41              |
| 4:ZP:178:TYR:HA   | 4:ZP:201:VAL:CG1  | 2.51                     | 0.41              |
| 4:ZQ:22:ASN:HB2   | 4:ZV:5:GLN:NE2    | 2.35                     | 0.41              |
| 4:ZS:382:TYR:CZ   | 4:ZX:395:ILE:HG23 | 2.56                     | 0.41              |
| 4:ZT:367:ASP:HB3  | 4:ZT:370:LYS:HG3  | 2.03                     | 0.41              |
| 4:ZU:102:LEU:HD21 | 4:ZU:106:ARG:HA   | 2.02                     | 0.41              |
| 4:ZU:232:PHE:HE2  | 4:ZU:267:MET:HA   | 1.86                     | 0.41              |
| 4:ZW:212:THR:HG21 | 4:ZW:246:ILE:HG21 | 2.03                     | 0.41              |
| 4:ZX:267:MET:HE3  | 4:ZX:267:MET:HB3  | 1.95                     | 0.41              |
| 4:ZZ:269:GLN:HG3  | 4:Zf:190:GLN:O    | 2.20                     | 0.41              |
| 4:Zd:210:VAL:HG11 | 4:Zd:263:PHE:CZ   | 2.55                     | 0.41              |
| 5:AA:70:GLN:HB2   | 3:AL:6:TRP:CB     | 2.47                     | 0.41              |
| 5:AA:148:PRO:C    | 3:AF:210:GLY:HA2  | 2.46                     | 0.41              |
| 5:AB:51:LEU:HD12  | 12:BC:19:LYS:HD3  | 2.02                     | 0.41              |
| 5:AB:224:ALA:HA   | 3:AG:253:MET:HE2  | 2.02                     | 0.41              |
| 5:AE:54:ARG:NH1   | 12:BF:22:ASN:ND2  | 2.69                     | 0.41              |
| 3:AF:161:GLN:HA   | 3:AF:161:GLN:OE1  | 2.21                     | 0.41              |
| 3:AH:126:GLY:HA3  | 3:AH:141:THR:HG23 | 2.02                     | 0.41              |
| 6:AP:296:ARG:HG2  | 6:AP:296:ARG:NH1  | 2.35                     | 0.41              |
| 6:AP:299:ASN:ND2  | 12:BA:55:PRO:O    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:At:104:LEU:CD2 | 9:Au:80:THR:HG22  | 2.51                     | 0.41              |
| 9:Au:97:THR:HA   | 9:Au:100:ILE:HG22 | 2.01                     | 0.41              |
| 9:Ay:139:LEU:C   | 9:Ay:141:GLN:H    | 2.28                     | 0.41              |
| 10:A5:82:MET:HE2 | 10:A5:82:MET:HA   | 2.03                     | 0.41              |
| 6:UN:214:ASP:OD2 | 6:UN:218:HIS:HB2  | 2.21                     | 0.41              |
| 6:WC:125:GLN:O   | 6:WC:128:GLU:HG2  | 2.20                     | 0.41              |
| 6:WP:186:LEU:HA  | 6:WP:186:LEU:HD23 | 1.93                     | 0.41              |
| 6:BQ:319:GLN:NE2 | 6:BV:355:PRO:CB   | 2.83                     | 0.41              |
| 6:BW:296:ARG:HG2 | 6:BW:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:165:GLY:C    | 1:C:35:THR:HG21   | 2.40                     | 0.41              |
| 1:B:169:ILE:HG22 | 1:B:171:ILE:HG12  | 2.02                     | 0.41              |
| 1:C:166:GLU:HB2  | 1:D:35:THR:CG2    | 2.30                     | 0.41              |
| 1:F:47:ALA:HB3   | 2:c:178:GLN:CD    | 2.45                     | 0.41              |
| 1:I:110:PRO:HD3  | 1:J:124:MET:CB    | 2.50                     | 0.41              |
| 1:J:169:ILE:HG22 | 1:J:171:ILE:HG12  | 2.02                     | 0.41              |
| 1:J:232:MET:HE3  | 1:J:232:MET:HB2   | 1.90                     | 0.41              |
| 1:M:169:ILE:HG22 | 1:M:171:ILE:HG12  | 2.02                     | 0.41              |
| 1:Q:106:PHE:CD1  | 1:R:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:T:106:PHE:CD1  | 1:U:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:V:106:PHE:CD1  | 1:W:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:Z:28:LYS:HD3   | 1:Z:28:LYS:HA     | 1.89                     | 0.41              |
| 2:a:21:ARG:HA    | 2:a:21:ARG:HD2    | 1.74                     | 0.41              |
| 2:f:130:ASP:OD1  | 2:f:130:ASP:N     | 2.47                     | 0.41              |
| 2:g:247:THR:O    | 2:g:248:PRO:C     | 2.64                     | 0.41              |
| 2:m:251:ALA:HB2  | 2:m:267:GLU:O     | 2.20                     | 0.41              |
| 2:m:266:ARG:HA   | 2:m:328:LEU:HD22  | 2.01                     | 0.41              |
| 2:p:359:ARG:HE   | 2:q:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:r:247:THR:O    | 2:r:248:PRO:C     | 2.64                     | 0.41              |
| 2:r:273:CYS:CA   | 2:s:328:LEU:HD21  | 2.40                     | 0.41              |
| 2:r:362:LEU:HD23 | 2:t:166:THR:HG21  | 2.03                     | 0.41              |
| 2:u:359:ARG:HE   | 2:v:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:w:21:ARG:HH21  | 2:w:246:VAL:CG2   | 2.32                     | 0.41              |
| 2:z:247:THR:O    | 2:z:248:PRO:C     | 2.64                     | 0.41              |
| 3:0:242:ILE:HD12 | 3:AJ:230:LEU:CD1  | 2.45                     | 0.41              |
| 3:3:46:TYR:HA    | 3:3:69:GLY:HA2    | 2.02                     | 0.41              |
| 3:6:40:VAL:O     | 3:6:75:VAL:N      | 2.50                     | 0.41              |
| 3:7:109:ASP:OD2  | 3:7:109:ASP:C     | 2.63                     | 0.41              |
| 3:7:237:GLN:NE2  | 3:ZC:252:GLN:OE1  | 2.53                     | 0.41              |
| 3:8:58:GLU:HA    | 3:AG:156:VAL:HG21 | 2.02                     | 0.41              |
| 3:9:173:LEU:HD23 | 3:9:173:LEU:HA    | 1.94                     | 0.41              |
| 4:ZF:154:MET:HE3 | 4:ZF:184:VAL:HB   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:ZG:214:ASP:OD2  | 4:ZG:249:GLY:N    | 2.46                     | 0.41              |
| 4:ZG:369:SER:HB3  | 4:ZM:382:TYR:OH   | 2.21                     | 0.41              |
| 4:ZI:143:LEU:HD12 | 4:ZI:287:GLY:O    | 2.20                     | 0.41              |
| 4:ZJ:75:VAL:O     | 4:ZJ:98:GLY:HA3   | 2.21                     | 0.41              |
| 4:ZL:128:ILE:HD12 | 4:ZL:314:GLN:HB2  | 2.03                     | 0.41              |
| 4:ZM:99:GLN:HG2   | 4:ZM:361:LEU:HD11 | 2.02                     | 0.41              |
| 4:ZO:268:GLN:NE2  | 4:ZU:190:GLN:NE2  | 2.68                     | 0.41              |
| 4:ZR:20:ILE:HG21  | 4:ZR:375:MET:HB2  | 2.02                     | 0.41              |
| 4:ZS:118:GLY:HA3  | 4:ZS:314:GLN:O    | 2.21                     | 0.41              |
| 4:ZS:158:LEU:HD13 | 4:ZS:208:TRP:CD2  | 2.56                     | 0.41              |
| 4:ZS:232:PHE:HB3  | 4:ZS:236:GLY:HA2  | 2.01                     | 0.41              |
| 4:ZT:382:TYR:CD1  | 4:ZY:395:ILE:HG23 | 2.55                     | 0.41              |
| 4:ZV:198:VAL:HG12 | 4:ZV:212:THR:HG22 | 2.03                     | 0.41              |
| 4:ZX:290:VAL:HG12 | 4:ZX:303:ASN:O    | 2.20                     | 0.41              |
| 4:ZZ:369:SER:CB   | 4:Zf:382:TYR:OH   | 2.66                     | 0.41              |
| 4:Zc:304:TYR:HE1  | 4:Zc:310:GLN:HB3  | 1.86                     | 0.41              |
| 4:Ze:367:ASP:O    | 4:Ze:371:GLU:HG2  | 2.21                     | 0.41              |
| 5:AD:17:ASN:ND2   | 3:AI:66:LEU:HD21  | 2.35                     | 0.41              |
| 5:AD:49:LEU:HG    | 11:A9:90:PRO:HD2  | 2.03                     | 0.41              |
| 5:AE:14:GLN:OE1   | 5:AE:17:ASN:ND2   | 2.53                     | 0.41              |
| 3:AF:73:ARG:HD2   | 12:BA:78:TYR:OH   | 2.19                     | 0.41              |
| 3:AH:3:SER:O      | 3:AH:7:ILE:HD12   | 2.21                     | 0.41              |
| 3:AH:80:LEU:HD23  | 3:AH:80:LEU:HA    | 1.93                     | 0.41              |
| 3:AJ:38:ARG:HE    | 3:AJ:38:ARG:HB3   | 1.65                     | 0.41              |
| 3:AN:129:VAL:HA   | 3:AN:136:VAL:HG23 | 2.03                     | 0.41              |
| 3:AN:225:ASN:O    | 3:AN:229:GLU:HG2  | 2.20                     | 0.41              |
| 6:AT:404:LEU:HD22 | 6:AT:409:MET:HE3  | 2.02                     | 0.41              |
| 6:AV:235:LEU:HB3  | 6:AW:244:ARG:NH2  | 2.36                     | 0.41              |
| 7:Ab:69:MET:O     | 7:Ab:70:LEU:C     | 2.63                     | 0.41              |
| 6:Al:295:SER:CB   | 11:A7:65:LEU:HB3  | 2.50                     | 0.41              |
| 7:Ar:54:LYS:HZ1   | 9:Ax:207:LEU:HA   | 1.86                     | 0.41              |
| 8:At:172:LEU:O    | 8:At:175:ALA:HB3  | 2.21                     | 0.41              |
| 9:Av:49:THR:HG21  | 10:A2:89:ARG:HG3  | 2.02                     | 0.41              |
| 10:Az:86:ILE:HD11 | 10:A5:99:VAL:HG22 | 2.03                     | 0.41              |
| 11:A6:111:ASP:OD1 | 12:BB:3:LEU:HD23  | 2.21                     | 0.41              |
| 6:UI:214:ASP:OD2  | 6:UI:218:HIS:HB2  | 2.20                     | 0.41              |
| 6:UN:102:GLN:CG   | 6:UN:193:ALA:HB2  | 2.49                     | 0.41              |
| 6:WA:196:HIS:CD2  | 6:WB:219:LEU:HD13 | 2.56                     | 0.41              |
| 6:WB:114:GLU:O    | 6:WB:117:ASP:N    | 2.54                     | 0.41              |
| 6:WD:193:ALA:HB1  | 6:WE:213:VAL:CG2  | 2.50                     | 0.41              |
| 6:WV:145:GLU:C    | 6:WV:147:LEU:N    | 2.78                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:BV:296:ARG:HG2  | 6:BV:296:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:213:ILE:HG23  | 1:Z:136:GLY:CA    | 2.42                     | 0.41              |
| 1:D:169:ILE:HG22  | 1:D:171:ILE:HG12  | 2.02                     | 0.41              |
| 1:F:110:PRO:HD3   | 1:G:124:MET:CB    | 2.50                     | 0.41              |
| 1:H:169:ILE:HG22  | 1:H:171:ILE:HG12  | 2.02                     | 0.41              |
| 1:M:47:ALA:HB3    | 2:j:178:GLN:CD    | 2.45                     | 0.41              |
| 1:N:47:ALA:HB3    | 2:k:178:GLN:CD    | 2.45                     | 0.41              |
| 1:R:165:GLY:C     | 1:S:35:THR:HG21   | 2.40                     | 0.41              |
| 2:c:247:THR:O     | 2:c:248:PRO:C     | 2.64                     | 0.41              |
| 2:f:78:ASN:OD1    | 2:f:78:ASN:N      | 2.51                     | 0.41              |
| 2:f:251:ALA:HB2   | 2:f:267:GLU:O     | 2.20                     | 0.41              |
| 2:i:130:ASP:OD1   | 2:i:130:ASP:N     | 2.47                     | 0.41              |
| 2:o:253:VAL:HG11  | 2:o:349:LEU:HD13  | 2.01                     | 0.41              |
| 2:p:273:CYS:CA    | 2:q:328:LEU:HD21  | 2.41                     | 0.41              |
| 3:1:22:ILE:HD11   | 3:1:232:ASN:HB3   | 2.02                     | 0.41              |
| 3:1:52:PRO:CG     | 12:BF:89:GLY:HA3  | 2.50                     | 0.41              |
| 3:1:179:MET:CE    | 3:AK:126:GLY:HA2  | 2.50                     | 0.41              |
| 3:2:180:ASN:O     | 3:2:181:ASP:C     | 2.62                     | 0.41              |
| 3:6:225:ASN:O     | 3:6:229:GLU:HG2   | 2.20                     | 0.41              |
| 3:6:260:LEU:HD13  | 3:AJ:234:ILE:HD11 | 2.03                     | 0.41              |
| 3:7:57:SER:HB3    | 3:7:60:THR:HG22   | 2.03                     | 0.41              |
| 3:9:48:THR:O      | 3:9:49:ILE:C      | 2.63                     | 0.41              |
| 3:ZA:7:ILE:HG23   | 3:ZA:71:GLY:HA2   | 2.03                     | 0.41              |
| 3:ZB:231:VAL:HG11 | 4:ZH:7:VAL:CG2    | 2.51                     | 0.41              |
| 3:ZD:231:VAL:HG11 | 4:ZJ:7:VAL:HG22   | 2.02                     | 0.41              |
| 4:ZG:60:ASP:OD1   | 4:ZG:62:THR:HG23  | 2.21                     | 0.41              |
| 4:ZI:374:ASN:C    | 4:ZI:376:ILE:N    | 2.79                     | 0.41              |
| 4:ZP:328:SER:HB3  | 4:ZU:43:PHE:CD2   | 2.56                     | 0.41              |
| 4:ZQ:199:TYR:O    | 4:ZQ:210:VAL:HA   | 2.21                     | 0.41              |
| 4:ZQ:202:LYS:HB2  | 4:ZQ:202:LYS:HE2  | 1.97                     | 0.41              |
| 4:ZR:396:LEU:HD23 | 4:ZR:396:LEU:HA   | 1.76                     | 0.41              |
| 4:ZU:38:SER:O     | 4:ZU:55:ALA:N     | 2.54                     | 0.41              |
| 4:ZU:78:SER:O     | 4:ZU:354:GLY:HA3  | 2.20                     | 0.41              |
| 4:ZU:139:ILE:HA   | 4:ZU:312:LEU:HD22 | 2.03                     | 0.41              |
| 4:ZX:242:GLY:HA2  | 4:ZX:263:PHE:HB2  | 2.03                     | 0.41              |
| 4:ZZ:106:ARG:HD2  | 4:ZZ:106:ARG:HA   | 1.80                     | 0.41              |
| 4:Zd:33:LYS:O     | 4:Zd:59:GLN:NE2   | 2.54                     | 0.41              |
| 4:Zf:267:MET:HG3  | 4:Zf:268:GLN:N    | 2.35                     | 0.41              |
| 4:Zg:103:ASP:HB3  | 4:Zg:109:VAL:HG21 | 2.01                     | 0.41              |
| 3:AH:175:LEU:HD11 | 3:AH:214:LEU:HD21 | 2.02                     | 0.41              |
| 3:AI:62:LEU:HD21  | 12:BE:84:LEU:HD23 | 1.98                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AL:198:SER:O    | 3:AL:198:SER:OG   | 2.27                     | 0.41              |
| 3:AM:3:SER:O      | 3:AM:7:ILE:HG13   | 2.20                     | 0.41              |
| 6:AX:278:THR:HG21 | 10:A3:7:ILE:HB    | 2.02                     | 0.41              |
| 6:AY:404:LEU:HD22 | 6:AY:409:MET:HE3  | 2.02                     | 0.41              |
| 6:Ac:404:LEU:HD22 | 6:Ac:409:MET:HE3  | 2.02                     | 0.41              |
| 7:Ar:47:MET:CE    | 9:Av:210:MET:HE1  | 2.50                     | 0.41              |
| 8:At:179:ILE:H    | 8:At:179:ILE:HG13 | 1.69                     | 0.41              |
| 8:At:213:ILE:HG21 | 9:Au:211:MET:O    | 2.20                     | 0.41              |
| 9:Av:211:MET:HE1  | 9:Aw:210:MET:HE2  | 2.03                     | 0.41              |
| 10:A5:11:ILE:HG21 | 6:BR:372:ILE:CG2  | 2.49                     | 0.41              |
| 11:A6:96:ASP:OD1  | 11:A6:96:ASP:N    | 2.53                     | 0.41              |
| 11:A7:29:ASN:HD22 | 11:A7:38:TYR:HE2  | 1.69                     | 0.41              |
| 11:A8:92:GLN:NE2  | 12:BD:22:ASN:ND2  | 2.68                     | 0.41              |
| 11:A9:39:GLN:HA   | 11:A9:99:THR:HB   | 2.02                     | 0.41              |
| 6:UL:216:SER:HB2  | 6:UL:218:HIS:ND1  | 2.36                     | 0.41              |
| 6:WK:140:LEU:O    | 6:WK:144:ILE:HG13 | 2.20                     | 0.41              |
| 6:WR:165:PHE:O    | 6:WR:167:ARG:N    | 2.53                     | 0.41              |
| 12:BE:52:ASP:HB2  | 12:BE:63:LYS:HB3  | 2.03                     | 0.41              |
| 12:BE:54:ALA:HB3  | 12:BE:55:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:165:GLY:C     | 1:B:35:THR:HG21   | 2.40                     | 0.41              |
| 1:B:93:SER:OG     | 1:C:139:ASN:OD1   | 2.39                     | 0.41              |
| 1:D:106:PHE:CD1   | 1:E:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:E:47:ALA:HB3    | 2:b:178:GLN:CD    | 2.45                     | 0.41              |
| 1:E:93:SER:OG     | 1:F:139:ASN:OD1   | 2.39                     | 0.41              |
| 1:F:106:PHE:CD1   | 1:G:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:F:136:GLY:CA    | 1:H:213:ILE:HG23  | 2.42                     | 0.41              |
| 1:K:110:PRO:HD3   | 1:L:124:MET:CB    | 2.50                     | 0.41              |
| 1:L:106:PHE:CD1   | 1:M:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:M:106:PHE:CD1   | 1:N:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:R:106:PHE:CD1   | 1:S:126:ALA:HB2   | 2.56                     | 0.41              |
| 1:T:93:SER:OG     | 1:U:139:ASN:OD1   | 2.39                     | 0.41              |
| 1:X:106:PHE:CD1   | 1:Y:126:ALA:HB2   | 2.56                     | 0.41              |
| 2:b:39:TYR:CE2    | 2:b:61:THR:HG21   | 2.56                     | 0.41              |
| 2:c:273:CYS:CA    | 2:d:328:LEU:HD21  | 2.41                     | 0.41              |
| 2:d:188:GLN:HE21  | 2:d:188:GLN:HB2   | 1.63                     | 0.41              |
| 2:e:39:TYR:CE2    | 2:e:61:THR:HG21   | 2.56                     | 0.41              |
| 2:e:78:ASN:HD21   | 3:AL:137:GLN:HG3  | 1.85                     | 0.41              |
| 2:e:247:THR:O     | 2:e:248:PRO:C     | 2.64                     | 0.41              |
| 2:e:362:LEU:HD23  | 2:g:166:THR:HG21  | 2.03                     | 0.41              |
| 2:f:39:TYR:CE2    | 2:f:61:THR:HG21   | 2.56                     | 0.41              |
| 2:f:362:LEU:HD23  | 2:h:166:THR:HG21  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:362:LEU:HD23  | 2:i:166:THR:HG21  | 2.03                     | 0.41              |
| 2:i:273:CYS:CA    | 2:j:328:LEU:HD21  | 2.40                     | 0.41              |
| 2:j:251:ALA:HB2   | 2:j:267:GLU:O     | 2.20                     | 0.41              |
| 2:n:251:ALA:HB2   | 2:n:267:GLU:O     | 2.20                     | 0.41              |
| 2:o:359:ARG:HE    | 2:p:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:p:93:TYR:OH     | 2:p:173:ARG:O     | 2.25                     | 0.41              |
| 2:q:21:ARG:HD2    | 2:q:21:ARG:HA     | 1.75                     | 0.41              |
| 2:q:251:ALA:HB2   | 2:q:267:GLU:O     | 2.20                     | 0.41              |
| 2:v:359:ARG:HE    | 2:w:21:ARG:HH22   | 1.69                     | 0.41              |
| 2:x:250:ASP:OD1   | 2:y:23:ARG:NE     | 2.51                     | 0.41              |
| 3:0:73:ARG:NE     | 5:AD:202:MET:SD   | 2.93                     | 0.41              |
| 3:1:3:SER:C       | 3:1:5:LEU:H       | 2.28                     | 0.41              |
| 3:1:179:MET:HE1   | 3:AK:142:ILE:O    | 2.21                     | 0.41              |
| 3:3:138:PRO:O     | 3:3:139:ALA:HB3   | 2.21                     | 0.41              |
| 3:5:102:PHE:HE2   | 3:5:181:ASP:OD1   | 2.03                     | 0.41              |
| 3:ZA:241:GLU:HG2  | 4:ZF:398:THR:HG21 | 2.02                     | 0.41              |
| 3:ZD:77:THR:H     | 4:ZI:47:LYS:CE    | 2.33                     | 0.41              |
| 3:ZE:256:LYS:HD3  | 3:ZE:256:LYS:HA   | 1.89                     | 0.41              |
| 4:ZF:197:ASN:N    | 4:ZF:197:ASN:HD22 | 2.17                     | 0.41              |
| 4:ZG:144:MET:HE2  | 4:ZG:310:GLN:HE21 | 1.85                     | 0.41              |
| 4:ZH:269:GLN:HB2  | 4:ZN:286:PRO:CG   | 2.47                     | 0.41              |
| 4:ZJ:156:ILE:HG13 | 4:ZJ:276:ILE:HA   | 2.03                     | 0.41              |
| 4:ZJ:268:GLN:O    | 4:ZP:190:GLN:NE2  | 2.48                     | 0.41              |
| 4:ZJ:380:ARG:HD2  | 4:ZP:396:LEU:HB3  | 2.02                     | 0.41              |
| 4:ZL:16:ASN:HB2   | 4:ZL:39:PHE:HZ    | 1.85                     | 0.41              |
| 4:ZM:281:GLN:NE2  | 4:ZM:283:GLY:O    | 2.47                     | 0.41              |
| 4:ZN:222:ALA:HA   | 4:ZN:223:PRO:HD3  | 1.96                     | 0.41              |
| 4:ZN:233:ASN:ND2  | 4:ZN:237:ILE:HB   | 2.35                     | 0.41              |
| 4:ZO:160:SER:HA   | 4:ZO:268:GLN:HE21 | 1.85                     | 0.41              |
| 4:ZO:282:ASN:OD1  | 4:ZO:282:ASN:N    | 2.47                     | 0.41              |
| 4:ZP:104:GLU:H    | 4:ZP:104:GLU:CD   | 2.29                     | 0.41              |
| 4:ZR:79:GLN:HB3   | 4:ZR:80:ASN:H     | 1.75                     | 0.41              |
| 4:ZS:71:ARG:NH1   | 4:ZS:74:ASP:OD1   | 2.54                     | 0.41              |
| 4:ZS:381:ASN:O    | 4:ZS:385:ASN:ND2  | 2.54                     | 0.41              |
| 4:ZT:17:LEU:CD1   | 4:ZY:395:ILE:CD1  | 2.88                     | 0.41              |
| 4:ZT:103:ASP:OD1  | 4:ZT:105:ASN:N    | 2.52                     | 0.41              |
| 4:ZT:297:ASP:OD2  | 4:ZT:297:ASP:N    | 2.53                     | 0.41              |
| 4:ZU:188:ASP:OD1  | 4:ZU:192:ASN:N    | 2.54                     | 0.41              |
| 4:ZV:217:ASP:HA   | 4:ZV:251:ILE:HD11 | 2.01                     | 0.41              |
| 4:ZW:184:VAL:HG13 | 4:ZW:196:MET:HB2  | 2.02                     | 0.41              |
| 4:ZW:326:LEU:HD22 | 4:ZW:334:TRP:HB3  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:ZW:331:ASP:O    | 4:ZW:333:VAL:HG23  | 2.20                     | 0.41              |
| 4:Za:107:ASN:ND2  | 4:Za:138:THR:HG22  | 2.36                     | 0.41              |
| 4:Za:376:ILE:HG21 | 4:Zg:393:ASP:OD2   | 2.21                     | 0.41              |
| 4:Ze:86:VAL:HG23  | 4:Ze:117:THR:HG21  | 2.03                     | 0.41              |
| 4:Zf:41:ASP:OD1   | 4:Zf:41:ASP:N      | 2.47                     | 0.41              |
| 5:AA:26:LEU:HA    | 5:AA:26:LEU:HD23   | 1.86                     | 0.41              |
| 5:AA:70:GLN:NE2   | 3:AL:3:SER:HB2     | 2.36                     | 0.41              |
| 5:AB:5:ILE:HG12   | 12:BB:103:VAL:HG13 | 2.03                     | 0.41              |
| 5:AB:20:ALA:HB2   | 3:AG:3:SER:OG      | 2.20                     | 0.41              |
| 5:AB:74:THR:OG1   | 5:AB:79:ASP:OD2    | 2.34                     | 0.41              |
| 5:AC:59:ALA:CB    | 3:AH:66:LEU:CD2    | 2.95                     | 0.41              |
| 5:AE:41:LEU:O     | 12:BF:33:SER:HA    | 2.20                     | 0.41              |
| 5:AE:51:LEU:HD21  | 12:BF:19:LYS:HD3   | 2.03                     | 0.41              |
| 3:AG:155:GLY:HA2  | 3:AG:214:LEU:HD12  | 2.03                     | 0.41              |
| 3:AH:2:ILE:O      | 3:AH:3:SER:HB3     | 2.21                     | 0.41              |
| 3:AI:42:GLU:OE1   | 3:AI:73:ARG:NH2    | 2.54                     | 0.41              |
| 3:AJ:82:SER:OG    | 3:AJ:223:ASN:ND2   | 2.54                     | 0.41              |
| 3:AK:70:THR:CG2   | 12:BF:76:LEU:O     | 2.69                     | 0.41              |
| 3:AL:248:SER:O    | 3:AL:252:GLN:HG3   | 2.20                     | 0.41              |
| 3:AN:83:GLN:NE2   | 3:AN:97:ILE:O      | 2.36                     | 0.41              |
| 6:AS:235:LEU:HB3  | 6:AT:244:ARG:NH2   | 2.36                     | 0.41              |
| 6:AT:295:SER:HB3  | 11:A0:72:HIS:HA    | 2.02                     | 0.41              |
| 6:AX:290:LYS:HE3  | 6:AX:290:LYS:HB2   | 1.93                     | 0.41              |
| 6:AY:235:LEU:HB3  | 6:AZ:244:ARG:NH2   | 2.36                     | 0.41              |
| 6:AY:421:GLY:O    | 6:AY:426:ARG:NH2   | 2.51                     | 0.41              |
| 6:Aa:404:LEU:HD22 | 6:Aa:409:MET:HE3   | 2.02                     | 0.41              |
| 7:Ab:8:MET:HG2    | 6:WS:124:SER:HB2   | 2.03                     | 0.41              |
| 6:Ae:372:ILE:HD13 | 10:A2:3:ALA:HA     | 2.02                     | 0.41              |
| 6:Af:235:LEU:HB3  | 6:Ag:244:ARG:NH2   | 2.36                     | 0.41              |
| 6:An:276:GLU:CD   | 10:Az:11:ILE:HD13  | 2.46                     | 0.41              |
| 7:Ar:33:LEU:HD12  | 7:Ar:33:LEU:HA     | 1.95                     | 0.41              |
| 7:Ar:40:ALA:HB3   | 7:As:44:ILE:HD11   | 2.03                     | 0.41              |
| 8:At:44:LEU:CD2   | 10:A5:100:MET:HA   | 2.51                     | 0.41              |
| 8:At:214:PHE:CE1  | 9:Ax:210:MET:SD    | 3.14                     | 0.41              |
| 8:At:243:LEU:HD23 | 8:At:243:LEU:HA    | 1.81                     | 0.41              |
| 9:Av:171:LEU:O    | 9:Av:175:VAL:HG23  | 2.21                     | 0.41              |
| 9:Av:213:PRO:HA   | 9:Av:214:PRO:HD3   | 1.88                     | 0.41              |
| 9:Av:234:LEU:HD12 | 9:Av:234:LEU:HA    | 1.92                     | 0.41              |
| 9:Aw:86:ASN:HD22  | 10:A2:103:GLN:HA   | 1.84                     | 0.41              |
| 9:Ax:159:LEU:CD2  | 6:WE:165:PHE:HD1   | 2.33                     | 0.41              |
| 9:Ay:42:VAL:HG21  | 10:A5:46:SER:HB2   | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:Ay:147:LEU:CD1   | 6:WH:166:VAL:CG1   | 2.70                     | 0.41              |
| 10:A2:48:ARG:NH1   | 11:A8:5:LEU:HD23   | 2.35                     | 0.41              |
| 10:A2:86:ILE:HD11  | 11:A7:133:VAL:HG22 | 2.02                     | 0.41              |
| 10:A3:69:ASN:HB2   | 11:A9:16:LEU:HD23  | 2.02                     | 0.41              |
| 11:A9:117:GLN:NE2  | 12:BD:125:MET:HG2  | 2.36                     | 0.41              |
| 11:A0:121:THR:HG23 | 12:BF:134:GLN:CG   | 2.51                     | 0.41              |
| 6:UI:125:GLN:C     | 6:UI:127:SER:N     | 2.77                     | 0.41              |
| 6:UI:167:ARG:HA    | 6:UI:167:ARG:HD2   | 1.92                     | 0.41              |
| 6:UJ:51:TYR:HB2    | 6:UJ:78:ARG:CZ     | 2.51                     | 0.41              |
| 6:UK:51:TYR:HB2    | 6:UK:78:ARG:CZ     | 2.51                     | 0.41              |
| 6:UL:69:GLN:NE2    | 6:WH:182:PRO:CG    | 2.84                     | 0.41              |
| 6:UN:125:GLN:C     | 6:UN:127:SER:N     | 2.77                     | 0.41              |
| 6:WB:163:SER:CB    | 6:WB:166:VAL:HG22  | 2.45                     | 0.41              |
| 6:WR:128:GLU:HB3   | 6:WS:126:PHE:CE2   | 2.55                     | 0.41              |
| 6:WS:147:LEU:O     | 6:WS:148:GLY:C     | 2.63                     | 0.41              |
| 6:WS:164:LEU:HD23  | 6:WS:164:LEU:HA    | 1.87                     | 0.41              |
| 6:WU:163:SER:O     | 6:WU:166:VAL:HG22  | 2.20                     | 0.41              |
| 6:WU:181:GLU:CB    | 6:WU:184:ARG:CG    | 2.85                     | 0.41              |
| 6:WU:193:ALA:HB1   | 6:WV:213:VAL:HG11  | 2.03                     | 0.41              |
| 12:BD:49:PHE:CG    | 6:BN:313:PRO:HG3   | 2.56                     | 0.41              |
| 12:BE:126:MET:O    | 12:BE:129:THR:HG22 | 2.21                     | 0.41              |
| 12:BF:98:VAL:O     | 12:BF:102:MET:HG2  | 2.21                     | 0.41              |
| 1:A:47:ALA:HB3     | 2:x:178:GLN:CD     | 2.45                     | 0.41              |
| 1:A:139:ASN:OD1    | 1:Z:93:SER:OG      | 2.39                     | 0.41              |
| 1:A:167:LYS:HG3    | 1:Z:203:ALA:HB3    | 2.04                     | 0.41              |
| 1:C:93:SER:OG      | 1:D:139:ASN:OD1    | 2.39                     | 0.41              |
| 1:C:106:PHE:CD1    | 1:D:126:ALA:HB2    | 2.56                     | 0.41              |
| 1:F:93:SER:OG      | 1:G:139:ASN:OD1    | 2.39                     | 0.41              |
| 1:J:106:PHE:CD1    | 1:K:126:ALA:HB2    | 2.56                     | 0.41              |
| 1:N:144:PHE:CE2    | 1:O:171:ILE:CD1    | 3.01                     | 0.41              |
| 1:S:106:PHE:CD1    | 1:T:126:ALA:HB2    | 2.56                     | 0.41              |
| 1:S:169:ILE:HG22   | 1:S:171:ILE:HG12   | 2.02                     | 0.41              |
| 1:W:93:SER:OG      | 1:X:139:ASN:OD1    | 2.39                     | 0.41              |
| 1:X:232:MET:HE3    | 1:X:232:MET:HB2    | 1.90                     | 0.41              |
| 1:Y:47:ALA:HB3     | 2:v:178:GLN:CD     | 2.45                     | 0.41              |
| 1:Z:47:ALA:HB3     | 2:w:178:GLN:CD     | 2.45                     | 0.41              |
| 2:a:144:GLY:HA3    | 2:z:259:THR:HG22   | 2.03                     | 0.41              |
| 2:a:251:ALA:HB2    | 2:a:267:GLU:O      | 2.20                     | 0.41              |
| 2:b:247:THR:O      | 2:b:248:PRO:C      | 2.64                     | 0.41              |
| 2:d:39:TYR:CE2     | 2:d:61:THR:HG21    | 2.56                     | 0.41              |
| 2:g:39:TYR:CE2     | 2:g:61:THR:HG21    | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:h:259:THR:HG22  | 2:i:144:GLY:HA3   | 2.03                     | 0.41              |
| 2:i:259:THR:HG22  | 2:j:144:GLY:HA3   | 2.03                     | 0.41              |
| 2:j:39:TYR:CE2    | 2:j:61:THR:HG21   | 2.56                     | 0.41              |
| 2:p:247:THR:O     | 2:p:248:PRO:C     | 2.64                     | 0.41              |
| 2:q:362:LEU:HD23  | 2:s:166:THR:HG21  | 2.03                     | 0.41              |
| 2:v:250:ASP:OD1   | 2:w:23:ARG:NE     | 2.51                     | 0.41              |
| 2:v:259:THR:HG22  | 2:w:144:GLY:HA3   | 2.03                     | 0.41              |
| 2:y:259:THR:HG22  | 2:z:144:GLY:HA3   | 2.03                     | 0.41              |
| 3:1:5:LEU:HD23    | 3:1:5:LEU:HA      | 1.95                     | 0.41              |
| 3:4:106:MET:HE2   | 3:4:106:MET:HB3   | 1.81                     | 0.41              |
| 3:5:45:LEU:N      | 3:5:45:LEU:HD23   | 2.36                     | 0.41              |
| 3:8:208:LEU:C     | 3:8:210:GLY:H     | 2.28                     | 0.41              |
| 3:ZA:233:MET:SD   | 4:ZF:388:THR:CA   | 3.08                     | 0.41              |
| 3:ZD:122:VAL:HG13 | 4:ZI:322:ASN:HA   | 2.02                     | 0.41              |
| 3:ZD:205:THR:HA   | 3:ZD:206:PRO:HD3  | 1.94                     | 0.41              |
| 4:ZH:78:SER:HG    | 4:ZH:355:LYS:H    | 1.65                     | 0.41              |
| 4:ZJ:351:GLY:C    | 4:ZJ:353:PHE:H    | 2.29                     | 0.41              |
| 4:ZL:379:GLN:CG   | 4:ZQ:391:THR:HG23 | 2.51                     | 0.41              |
| 4:ZM:149:THR:O    | 4:ZM:259:PHE:HB3  | 2.21                     | 0.41              |
| 4:ZO:167:LYS:HE2  | 4:ZO:174:ASP:OD2  | 2.21                     | 0.41              |
| 4:ZR:183:THR:HG22 | 4:ZR:197:ASN:HD22 | 1.86                     | 0.41              |
| 4:ZU:97:ASN:ND2   | 4:ZU:99:GLN:HB2   | 2.36                     | 0.41              |
| 4:ZU:230:LEU:HD22 | 4:ZU:238:LEU:HD11 | 2.03                     | 0.41              |
| 4:ZV:269:GLN:HG3  | 4:Zb:286:PRO:CG   | 2.50                     | 0.41              |
| 4:ZV:379:GLN:OE1  | 4:Za:391:THR:HG23 | 2.21                     | 0.41              |
| 4:ZW:75:VAL:O     | 4:ZW:98:GLY:HA3   | 2.21                     | 0.41              |
| 4:ZW:181:LYS:O    | 4:Zh:131:GLY:HA3  | 2.20                     | 0.41              |
| 4:ZW:373:VAL:HG11 | 4:Zc:7:VAL:HG22   | 2.03                     | 0.41              |
| 4:ZX:56:GLY:HA2   | 4:Zc:47:LYS:HZ3   | 1.84                     | 0.41              |
| 4:ZY:24:ILE:HD13  | 4:ZY:24:ILE:HG21  | 1.85                     | 0.41              |
| 4:ZZ:74:ASP:HB3   | 4:ZZ:361:LEU:HG   | 2.03                     | 0.41              |
| 4:ZZ:188:ASP:OD1  | 4:ZZ:192:ASN:N    | 2.52                     | 0.41              |
| 5:AE:16:LEU:HD21  | 3:AJ:253:MET:HE3  | 1.97                     | 0.41              |
| 5:AE:243:ARG:HD3  | 12:BF:113:GLN:CD  | 2.46                     | 0.41              |
| 6:Ac:235:LEU:HB3  | 6:Ad:244:ARG:NH2  | 2.36                     | 0.41              |
| 6:Ae:235:LEU:HB3  | 6:Af:244:ARG:NH2  | 2.36                     | 0.41              |
| 6:Ai:235:LEU:HB3  | 6:Aj:244:ARG:NH2  | 2.36                     | 0.41              |
| 7:Aq:74:LEU:HD22  | 9:Aw:229:VAL:HG12 | 2.03                     | 0.41              |
| 7:Aq:89:GLY:C     | 6:WW:164:LEU:CD1  | 2.92                     | 0.41              |
| 7:As:39:GLN:CB    | 8:At:211:LEU:HD22 | 2.50                     | 0.41              |
| 7:As:39:GLN:HB3   | 8:At:211:LEU:HD22 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:Ay:241:GLN:NE2  | 6:WG:164:LEU:HD12 | 2.36                     | 0.41              |
| 10:A4:7:ILE:O     | 10:A4:11:ILE:HG23 | 2.21                     | 0.41              |
| 6:UN:54:LEU:HG    | 6:UN:55:PHE:CD2   | 2.56                     | 0.41              |
| 6:UO:165:PHE:HD1  | 6:UO:165:PHE:HA   | 1.77                     | 0.41              |
| 12:BA:22:ASN:HD21 | 12:BF:5:ASN:ND2   | 2.19                     | 0.41              |
| 6:WC:193:ALA:CB   | 6:WD:213:VAL:HG11 | 2.44                     | 0.41              |
| 6:WH:200:SER:O    | 6:WI:158:ALA:HB3  | 2.13                     | 0.41              |
| 6:WL:190:GLN:HG2  | 6:WM:216:SER:O    | 2.21                     | 0.41              |
| 6:WQ:121:PHE:O    | 6:WQ:122:GLY:C    | 2.64                     | 0.41              |
| 12:BD:8:ASP:C     | 12:BD:8:ASP:OD2   | 2.64                     | 0.41              |
| 6:BP:316:LEU:HD12 | 6:BP:316:LEU:HA   | 1.87                     | 0.41              |
| 6:BS:404:LEU:HD22 | 6:BS:409:MET:HE3  | 2.02                     | 0.41              |
| 6:BV:404:LEU:HD22 | 6:BV:409:MET:HE3  | 2.02                     | 0.41              |
| 1:A:169:ILE:HG22  | 1:A:171:ILE:HG12  | 2.02                     | 0.40              |
| 1:B:47:ALA:HB3    | 2:y:178:GLN:CD    | 2.45                     | 0.40              |
| 1:B:106:PHE:CD1   | 1:C:126:ALA:HB2   | 2.56                     | 0.40              |
| 1:D:47:ALA:HB3    | 2:a:178:GLN:CD    | 2.45                     | 0.40              |
| 1:E:169:ILE:HG22  | 1:E:171:ILE:HG12  | 2.02                     | 0.40              |
| 1:F:166:GLU:HB2   | 1:G:35:THR:CG2    | 2.30                     | 0.40              |
| 1:G:50:SER:HB3    | 2:d:32:ARG:HH11   | 1.81                     | 0.40              |
| 1:G:113:LEU:HD12  | 1:G:113:LEU:HA    | 1.90                     | 0.40              |
| 1:H:106:PHE:CD1   | 1:I:126:ALA:HB2   | 2.56                     | 0.40              |
| 1:K:169:ILE:HG22  | 1:K:171:ILE:HG12  | 2.02                     | 0.40              |
| 1:Q:93:SER:OG     | 1:R:139:ASN:OD1   | 2.39                     | 0.40              |
| 1:T:47:ALA:HB3    | 2:q:178:GLN:CD    | 2.45                     | 0.40              |
| 1:U:203:ALA:HB3   | 1:V:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:W:203:ALA:HB3   | 1:X:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:Y:93:SER:OG     | 1:Z:139:ASN:OD1   | 2.39                     | 0.40              |
| 1:Z:169:ILE:HG22  | 1:Z:171:ILE:HG12  | 2.02                     | 0.40              |
| 2:b:188:GLN:HE21  | 2:b:188:GLN:HB2   | 1.63                     | 0.40              |
| 2:b:258:ARG:HH12  | 2:d:140:ASN:HD21  | 1.64                     | 0.40              |
| 2:g:93:TYR:HA     | 2:g:94:PRO:HD3    | 1.95                     | 0.40              |
| 2:h:247:THR:O     | 2:h:248:PRO:C     | 2.64                     | 0.40              |
| 2:j:247:THR:O     | 2:j:248:PRO:C     | 2.64                     | 0.40              |
| 2:k:247:THR:O     | 2:k:248:PRO:C     | 2.64                     | 0.40              |
| 2:k:259:THR:HG22  | 2:l:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:l:259:THR:HG22  | 2:m:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:r:250:ASP:OD1   | 2:s:23:ARG:NE     | 2.51                     | 0.40              |
| 2:s:247:THR:O     | 2:s:248:PRO:C     | 2.64                     | 0.40              |
| 2:v:21:ARG:HH21   | 2:v:246:VAL:CG2   | 2.32                     | 0.40              |
| 3:1:95:VAL:O      | 3:1:118:GLY:HA3   | 2.20                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:1:178:PHE:CE1   | 3:1:201:PRO:HB3   | 2.50                     | 0.40              |
| 3:1:260:LEU:O     | 3:AJ:245:LYS:NZ   | 2.45                     | 0.40              |
| 3:4:127:GLN:NE2   | 3:4:141:THR:OG1   | 2.51                     | 0.40              |
| 3:5:260:LEU:HD23  | 3:5:260:LEU:HA    | 1.81                     | 0.40              |
| 3:7:241:GLU:CG    | 3:ZC:256:LYS:HG3  | 2.48                     | 0.40              |
| 3:ZA:45:LEU:CD1   | 3:AN:83:GLN:CG    | 2.98                     | 0.40              |
| 3:ZB:35:LYS:NZ    | 3:ZB:220:GLU:OE2  | 2.53                     | 0.40              |
| 3:ZC:10:THR:OG1   | 3:ZC:72:VAL:O     | 2.39                     | 0.40              |
| 3:ZD:208:LEU:HB3  | 3:ZD:209:ASN:H    | 1.63                     | 0.40              |
| 3:ZE:147:LEU:CD2  | 4:ZJ:352:ASN:HA   | 2.51                     | 0.40              |
| 4:ZF:319:ASN:OD1  | 4:ZF:320:PHE:N    | 2.54                     | 0.40              |
| 4:ZG:125:PRO:HA   | 4:ZG:126:PRO:HD3  | 1.95                     | 0.40              |
| 4:ZG:380:ARG:NH1  | 4:ZG:383:GLN:OE1  | 2.54                     | 0.40              |
| 4:ZJ:387:GLN:CG   | 4:ZP:400:VAL:HG13 | 2.50                     | 0.40              |
| 4:ZL:34:SER:HB3   | 4:ZL:366:VAL:HG22 | 2.02                     | 0.40              |
| 4:ZM:180:LYS:HG3  | 4:ZM:181:LYS:N    | 2.37                     | 0.40              |
| 4:ZN:109:VAL:HG12 | 4:ZN:115:GLN:HA   | 2.02                     | 0.40              |
| 4:ZQ:379:GLN:CG   | 4:ZV:394:GLN:NE2  | 2.84                     | 0.40              |
| 4:ZQ:389:ILE:HG22 | 4:ZV:402:LEU:HD13 | 2.03                     | 0.40              |
| 4:ZS:146:ALA:HB2  | 4:ZS:286:PRO:HD3  | 2.02                     | 0.40              |
| 4:ZS:181:LYS:HD3  | 4:Zd:129:GLN:HE22 | 1.85                     | 0.40              |
| 4:ZV:46:SER:HB3   | 4:ZV:48:VAL:HG22  | 2.03                     | 0.40              |
| 4:ZV:368:LEU:HD23 | 4:ZV:368:LEU:HA   | 1.84                     | 0.40              |
| 4:ZW:17:LEU:HD23  | 4:ZW:17:LEU:HA    | 1.93                     | 0.40              |
| 4:ZX:159:ASN:HD21 | 4:ZX:161:THR:HG1  | 1.63                     | 0.40              |
| 4:ZY:144:MET:HG2  | 4:ZY:145:ALA:O    | 2.21                     | 0.40              |
| 4:ZZ:104:GLU:HB3  | 4:Ze:339:ALA:O    | 2.21                     | 0.40              |
| 4:Zb:308:GLN:NE2  | 4:Zb:309:GLU:OE1  | 2.54                     | 0.40              |
| 4:Ze:30:TYR:HD1   | 4:Ze:363:ALA:HA   | 1.85                     | 0.40              |
| 4:Ze:78:SER:O     | 4:Ze:354:GLY:HA3  | 2.20                     | 0.40              |
| 4:Ze:128:ILE:HD11 | 4:Ze:311:VAL:HG21 | 2.03                     | 0.40              |
| 4:Zf:228:THR:HB   | 4:Zf:244:VAL:HG21 | 2.02                     | 0.40              |
| 4:Zg:75:VAL:HG21  | 4:Zg:294:ILE:HG21 | 2.02                     | 0.40              |
| 4:Zh:71:ARG:HD3   | 4:Zh:73:LEU:HB2   | 2.03                     | 0.40              |
| 5:AA:79:ASP:HB3   | 5:AA:206:LEU:CD1  | 2.51                     | 0.40              |
| 5:AA:82:LEU:HD21  | 5:AA:88:LEU:HD12  | 2.03                     | 0.40              |
| 5:AA:202:MET:HE2  | 3:AL:73:ARG:NE    | 2.35                     | 0.40              |
| 5:AC:50:SER:HB2   | 11:A8:90:PRO:O    | 2.20                     | 0.40              |
| 5:AC:72:ASP:OD2   | 5:AC:72:ASP:C     | 2.64                     | 0.40              |
| 5:AD:2:ASP:OD2    | 5:AD:2:ASP:C      | 2.64                     | 0.40              |
| 5:AD:89:VAL:HG22  | 5:AD:99:TYR:HD1   | 1.86                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AG:74:PRO:HB2   | 3:AL:66:LEU:HD22   | 2.03                     | 0.40              |
| 3:AH:35:LYS:HA    | 3:AH:35:LYS:HD3    | 1.91                     | 0.40              |
| 3:AL:125:ASN:O    | 3:AL:126:GLY:C     | 2.64                     | 0.40              |
| 3:AM:49:ILE:O     | 3:AM:65:GLY:HA3    | 2.21                     | 0.40              |
| 3:AN:140:ILE:HD13 | 3:AN:157:VAL:HG21  | 2.03                     | 0.40              |
| 6:AR:235:LEU:HB3  | 6:Ac:244:ARG:NH2   | 2.36                     | 0.40              |
| 6:AR:404:LEU:HD22 | 6:AR:409:MET:HE3   | 2.02                     | 0.40              |
| 6:Ad:360:ARG:NH1  | 6:Ad:362:GLU:OE1   | 2.55                     | 0.40              |
| 6:Ah:235:LEU:HB3  | 6:Ai:244:ARG:NH2   | 2.36                     | 0.40              |
| 6:AO:360:ARG:NH1  | 6:AO:362:GLU:OE1   | 2.55                     | 0.40              |
| 7:As:23:PRO:HG2   | 7:As:69:MET:HE2    | 2.03                     | 0.40              |
| 8:At:231:ALA:O    | 8:At:234:PRO:HD2   | 2.21                     | 0.40              |
| 8:At:252:ALA:HB2  | 6:WK:163:SER:O     | 2.21                     | 0.40              |
| 9:Aw:189:ILE:O    | 9:Aw:192:PRO:HD2   | 2.21                     | 0.40              |
| 9:Aw:189:ILE:HD13 | 9:Aw:235:LEU:HD11  | 2.03                     | 0.40              |
| 6:UI:51:TYR:HB2   | 6:UI:78:ARG:CZ     | 2.51                     | 0.40              |
| 6:UO:212:LEU:HG   | 6:UO:220:LEU:HD12  | 2.03                     | 0.40              |
| 6:UP:54:LEU:HG    | 6:UP:55:PHE:CD2    | 2.56                     | 0.40              |
| 12:BA:47:VAL:O    | 6:BH:313:PRO:HD2   | 2.21                     | 0.40              |
| 12:BB:10:ALA:HB3  | 12:BB:119:LEU:HD13 | 2.02                     | 0.40              |
| 6:WD:190:GLN:O    | 6:WD:191:ILE:C     | 2.64                     | 0.40              |
| 6:WV:128:GLU:CG   | 6:WW:126:PHE:CE2   | 3.02                     | 0.40              |
| 12:BF:55:PRO:HG2  | 6:BG:320:PRO:CB    | 2.51                     | 0.40              |
| 6:BT:404:LEU:HD22 | 6:BT:409:MET:HE3   | 2.02                     | 0.40              |
| 1:B:144:PHE:CE2   | 1:C:171:ILE:CD1    | 3.01                     | 0.40              |
| 1:I:93:SER:OG     | 1:J:139:ASN:OD1    | 2.39                     | 0.40              |
| 1:N:28:LYS:HD3    | 1:N:28:LYS:HA      | 1.89                     | 0.40              |
| 1:N:106:PHE:CD1   | 1:O:126:ALA:HB2    | 2.56                     | 0.40              |
| 1:R:47:ALA:HB3    | 2:o:178:GLN:CD     | 2.45                     | 0.40              |
| 1:R:136:GLY:CA    | 1:T:213:ILE:HG23   | 2.42                     | 0.40              |
| 1:S:93:SER:OG     | 1:T:139:ASN:OD1    | 2.39                     | 0.40              |
| 1:T:203:ALA:HB3   | 1:U:167:LYS:HG3    | 2.04                     | 0.40              |
| 1:Y:203:ALA:HB3   | 1:Z:167:LYS:HG3    | 2.04                     | 0.40              |
| 2:a:259:THR:HG22  | 2:b:144:GLY:HA3    | 2.03                     | 0.40              |
| 2:c:194:PHE:CZ    | 2:c:218:ALA:HB2    | 2.57                     | 0.40              |
| 2:e:188:GLN:HE21  | 2:e:188:GLN:HB2    | 1.63                     | 0.40              |
| 2:f:247:THR:O     | 2:f:248:PRO:C      | 2.64                     | 0.40              |
| 2:i:362:LEU:HD23  | 2:k:166:THR:HG21   | 2.03                     | 0.40              |
| 2:j:51:GLN:HE21   | 3:6:58:GLU:CD      | 2.29                     | 0.40              |
| 2:m:194:PHE:CZ    | 2:m:218:ALA:HB2    | 2.57                     | 0.40              |
| 2:m:247:THR:O     | 2:m:248:PRO:C      | 2.64                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:n:194:PHE:CZ    | 2:n:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:n:359:ARG:HE    | 2:o:21:ARG:HH22   | 1.69                     | 0.40              |
| 2:n:362:LEU:HD23  | 2:p:166:THR:HG21  | 2.03                     | 0.40              |
| 2:o:194:PHE:CZ    | 2:o:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:o:247:THR:O     | 2:o:248:PRO:C     | 2.64                     | 0.40              |
| 2:p:362:LEU:HD23  | 2:r:166:THR:HG21  | 2.03                     | 0.40              |
| 2:s:258:ARG:HH12  | 2:u:140:ASN:HD21  | 1.64                     | 0.40              |
| 2:u:21:ARG:HH21   | 2:u:246:VAL:CG2   | 2.32                     | 0.40              |
| 2:u:259:THR:HG22  | 2:v:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:w:359:ARG:HE    | 2:x:21:ARG:HH22   | 1.69                     | 0.40              |
| 2:y:188:GLN:HE21  | 2:y:188:GLN:HB2   | 1.63                     | 0.40              |
| 2:y:192:GLU:H     | 2:y:192:GLU:HG3   | 1.53                     | 0.40              |
| 3:2:100:GLN:NE2   | 3:2:210:GLY:O     | 2.43                     | 0.40              |
| 3:7:119:SER:OG    | 3:ZC:38:ARG:NH2   | 2.54                     | 0.40              |
| 3:7:175:LEU:HG    | 3:7:206:PRO:HG3   | 2.02                     | 0.40              |
| 3:7:184:LEU:HB3   | 3:7:192:TYR:HB3   | 2.04                     | 0.40              |
| 3:8:35:LYS:HA     | 3:8:35:LYS:HD3    | 1.96                     | 0.40              |
| 3:ZA:240:TYR:OH   | 4:ZF:399:LEU:CD2  | 2.69                     | 0.40              |
| 3:ZB:116:ARG:HH21 | 3:ZB:220:GLU:CD   | 2.28                     | 0.40              |
| 4:ZF:174:ASP:HB3  | 4:ZF:176:ASP:OD1  | 2.21                     | 0.40              |
| 4:ZI:159:ASN:HB3  | 4:ZI:162:ASP:OD1  | 2.22                     | 0.40              |
| 4:ZL:145:ALA:O    | 4:ZL:284:TYR:HE1  | 2.05                     | 0.40              |
| 4:ZP:75:VAL:O     | 4:ZP:98:GLY:HA3   | 2.21                     | 0.40              |
| 4:ZP:85:LEU:HD23  | 4:ZP:116:LEU:HA   | 2.03                     | 0.40              |
| 4:ZQ:97:ASN:HD22  | 4:ZQ:332:ASN:HD21 | 1.70                     | 0.40              |
| 4:ZQ:234:GLU:HB3  | 4:ZW:255:THR:OG1  | 2.22                     | 0.40              |
| 4:ZS:180:LYS:HB2  | 4:ZS:274:ASN:ND2  | 2.36                     | 0.40              |
| 4:ZT:22:ASN:HB2   | 4:ZY:5:GLN:OE1    | 2.21                     | 0.40              |
| 4:ZT:269:GLN:HG2  | 4:ZZ:190:GLN:HA   | 2.02                     | 0.40              |
| 4:ZT:270:ASN:N    | 4:ZZ:190:GLN:O    | 2.50                     | 0.40              |
| 4:ZT:328:SER:OG   | 4:ZY:43:PHE:CD2   | 2.65                     | 0.40              |
| 4:ZV:331:ASP:HA   | 4:Za:40:ALA:HB1   | 2.03                     | 0.40              |
| 4:ZW:230:LEU:HD23 | 4:ZW:230:LEU:HA   | 1.85                     | 0.40              |
| 4:ZW:330:GLY:N    | 4:Zb:43:PHE:HB2   | 2.36                     | 0.40              |
| 4:Zc:269:GLN:HG2  | 4:Zc:270:ASN:H    | 1.87                     | 0.40              |
| 4:Zd:88:SER:C     | 4:Zd:90:GLY:H     | 2.29                     | 0.40              |
| 5:AA:215:GLU:HG3  | 3:AG:9:LYS:NZ     | 2.37                     | 0.40              |
| 5:AD:80:VAL:HB    | 5:AD:201:ILE:HD11 | 2.04                     | 0.40              |
| 3:AH:3:SER:HB2    | 12:BC:75:LYS:HD3  | 2.04                     | 0.40              |
| 3:AH:44:LEU:HD21  | 12:BC:78:TYR:CG   | 2.57                     | 0.40              |
| 3:AI:164:GLN:C    | 3:AI:166:ALA:N    | 2.77                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AJ:104:GLN:HB3  | 3:AJ:137:GLN:O    | 2.21                     | 0.40              |
| 3:AJ:260:LEU:HD12 | 12:BE:106:MET:SD  | 2.57                     | 0.40              |
| 3:AL:107:LEU:HD23 | 3:AL:107:LEU:HA   | 1.96                     | 0.40              |
| 3:AM:209:ASN:HD22 | 3:AM:209:ASN:HA   | 1.61                     | 0.40              |
| 6:AW:278:THR:HG22 | 10:A3:14:LEU:HD23 | 2.04                     | 0.40              |
| 6:AZ:404:LEU:HD22 | 6:AZ:409:MET:HE3  | 2.02                     | 0.40              |
| 6:Aa:360:ARG:NH1  | 6:Aa:362:GLU:OE1  | 2.55                     | 0.40              |
| 7:Ab:69:MET:HE3   | 7:Ab:69:MET:HB3   | 1.72                     | 0.40              |
| 6:Ag:360:ARG:NH1  | 6:Ag:362:GLU:OE1  | 2.55                     | 0.40              |
| 6:An:360:ARG:NH1  | 6:An:362:GLU:OE1  | 2.55                     | 0.40              |
| 8:At:13:LEU:O     | 8:At:17:PHE:HB2   | 2.22                     | 0.40              |
| 8:At:102:ILE:O    | 8:At:106:MET:HG2  | 2.21                     | 0.40              |
| 8:At:144:LEU:HB3  | 6:WJ:164:LEU:CD2  | 2.51                     | 0.40              |
| 9:Aw:152:ARG:NH2  | 6:WC:165:PHE:HD2  | 2.05                     | 0.40              |
| 11:A0:63:VAL:H    | 6:BX:297:GLN:HE22 | 1.69                     | 0.40              |
| 6:UI:212:LEU:HG   | 6:UI:220:LEU:HD12 | 2.04                     | 0.40              |
| 6:UK:54:LEU:HG    | 6:UK:55:PHE:CD2   | 2.57                     | 0.40              |
| 6:UM:51:TYR:HB2   | 6:UM:78:ARG:CZ    | 2.52                     | 0.40              |
| 6:UO:51:TYR:HB2   | 6:UO:78:ARG:CZ    | 2.51                     | 0.40              |
| 6:WG:200:SER:HG   | 6:WH:175:SER:HB2  | 1.77                     | 0.40              |
| 6:WH:186:LEU:HD22 | 6:WH:190:GLN:CG   | 2.52                     | 0.40              |
| 12:BF:50:GLN:OE1  | 12:BF:63:LYS:NZ   | 2.46                     | 0.40              |
| 6:BS:360:ARG:NH1  | 6:BS:362:GLU:OE1  | 2.55                     | 0.40              |
| 6:BT:421:GLY:O    | 6:BT:426:ARG:NH2  | 2.51                     | 0.40              |
| 1:A:203:ALA:HB3   | 1:B:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:B:203:ALA:HB3   | 1:C:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:C:47:ALA:HB3    | 2:z:178:GLN:CD    | 2.45                     | 0.40              |
| 1:C:203:ALA:HB3   | 1:D:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:D:232:MET:HE3   | 1:D:232:MET:HB2   | 1.90                     | 0.40              |
| 1:E:106:PHE:CD1   | 1:F:126:ALA:HB2   | 2.56                     | 0.40              |
| 1:H:93:SER:OG     | 1:I:139:ASN:OD1   | 2.39                     | 0.40              |
| 1:K:106:PHE:CD1   | 1:L:126:ALA:HB2   | 2.56                     | 0.40              |
| 1:M:93:SER:OG     | 1:N:139:ASN:OD1   | 2.39                     | 0.40              |
| 1:O:47:ALA:HB3    | 2:l:178:GLN:CD    | 2.45                     | 0.40              |
| 1:P:47:ALA:HB3    | 2:m:178:GLN:CD    | 2.45                     | 0.40              |
| 1:P:93:SER:OG     | 1:Q:139:ASN:OD1   | 2.39                     | 0.40              |
| 1:P:106:PHE:CD1   | 1:Q:126:ALA:HB2   | 2.56                     | 0.40              |
| 1:R:203:ALA:HB3   | 1:S:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:X:203:ALA:HB3   | 1:Y:167:LYS:HG3   | 2.04                     | 0.40              |
| 2:a:194:PHE:CZ    | 2:a:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:c:39:TYR:CE2    | 2:c:61:THR:HG21   | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:d:259:THR:HG22  | 2:e:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:e:259:THR:HG22  | 2:f:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:g:259:THR:HG22  | 2:h:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:h:362:LEU:HD23  | 2:j:166:THR:HG21  | 2.03                     | 0.40              |
| 2:j:362:LEU:HD23  | 2:l:166:THR:HG21  | 2.03                     | 0.40              |
| 2:m:259:THR:HG22  | 2:n:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:n:93:TYR:HA     | 2:n:94:PRO:HD3    | 1.95                     | 0.40              |
| 2:o:362:LEU:HD23  | 2:q:166:THR:HG21  | 2.03                     | 0.40              |
| 2:p:194:PHE:CZ    | 2:p:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:q:250:ASP:OD1   | 2:r:23:ARG:NE     | 2.51                     | 0.40              |
| 2:s:21:ARG:HH21   | 2:s:246:VAL:CG2   | 2.32                     | 0.40              |
| 2:s:273:CYS:CA    | 2:t:328:LEU:HD21  | 2.40                     | 0.40              |
| 2:t:259:THR:HG22  | 2:u:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:u:250:ASP:OD1   | 2:v:23:ARG:NE     | 2.51                     | 0.40              |
| 2:v:251:ALA:HB2   | 2:v:267:GLU:O     | 2.20                     | 0.40              |
| 2:w:259:THR:HG22  | 2:x:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:y:247:THR:O     | 2:y:248:PRO:C     | 2.64                     | 0.40              |
| 3:1:179:MET:HE2   | 3:AK:126:GLY:CA   | 2.51                     | 0.40              |
| 3:2:58:GLU:CD     | 5:AA:140:ASP:OD2  | 2.64                     | 0.40              |
| 3:3:74:PRO:HB2    | 3:8:66:LEU:CD1    | 2.52                     | 0.40              |
| 3:5:26:LEU:HB3    | 3:ZA:243:ASN:OD1  | 2.20                     | 0.40              |
| 3:6:22:ILE:HD11   | 3:6:232:ASN:HB3   | 2.03                     | 0.40              |
| 3:7:173:LEU:HD23  | 3:7:214:LEU:HD13  | 2.03                     | 0.40              |
| 3:8:73:ARG:HG3    | 3:AL:218:TYR:OH   | 2.21                     | 0.40              |
| 3:8:86:LEU:HD22   | 3:8:96:ALA:HB1    | 2.03                     | 0.40              |
| 3:ZD:1:MET:HE3    | 3:ZD:1:MET:HB2    | 1.68                     | 0.40              |
| 3:ZD:173:LEU:HD23 | 3:ZD:214:LEU:HD13 | 2.04                     | 0.40              |
| 4:ZF:205:ASP:OD1  | 4:ZL:252:ASN:HA   | 2.22                     | 0.40              |
| 4:ZI:233:ASN:OD1  | 4:ZI:237:ILE:N    | 2.47                     | 0.40              |
| 4:ZM:380:ARG:CZ   | 4:ZS:393:ASP:OD1  | 2.70                     | 0.40              |
| 4:ZP:150:THR:HG22 | 4:ZP:282:ASN:HD21 | 1.87                     | 0.40              |
| 4:ZT:233:ASN:ND2  | 4:ZT:237:ILE:HB   | 2.37                     | 0.40              |
| 4:ZU:24:ILE:HG23  | 4:ZZ:384:SER:OG   | 2.22                     | 0.40              |
| 4:ZU:281:GLN:NE2  | 4:ZU:283:GLY:O    | 2.53                     | 0.40              |
| 4:ZU:299:THR:HG22 | 4:ZU:314:GLN:OE1  | 2.21                     | 0.40              |
| 4:ZU:330:GLY:N    | 4:ZZ:43:PHE:HB2   | 2.36                     | 0.40              |
| 4:Zb:380:ARG:HD3  | 4:Zb:380:ARG:HA   | 1.90                     | 0.40              |
| 4:Ze:38:SER:O     | 4:Ze:55:ALA:N     | 2.52                     | 0.40              |
| 4:Ze:71:ARG:NH2   | 4:Ze:74:ASP:OD1   | 2.54                     | 0.40              |
| 4:Zf:58:THR:HG23  | 4:Zf:324:GLU:HG2  | 2.02                     | 0.40              |
| 4:Zf:284:TYR:CD2  | 4:Zf:308:GLN:HG3  | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Zh:99:GLN:HE21  | 4:Zh:361:LEU:HD22 | 1.86                     | 0.40              |
| 5:AA:229:MET:CG   | 3:AG:258:THR:CG2  | 2.93                     | 0.40              |
| 5:AB:132:GLY:N    | 3:AG:179:MET:SD   | 2.95                     | 0.40              |
| 5:AB:234:ILE:HG21 | 3:AG:260:LEU:HD21 | 2.03                     | 0.40              |
| 5:AC:152:PRO:HD2  | 3:AN:193:ILE:HD12 | 2.00                     | 0.40              |
| 5:AD:214:VAL:CG1  | 3:AJ:12:LEU:HD12  | 2.51                     | 0.40              |
| 3:AH:66:LEU:HD22  | 3:AH:66:LEU:HA    | 1.93                     | 0.40              |
| 3:AH:112:SER:HB3  | 3:AH:137:GLN:NE2  | 2.36                     | 0.40              |
| 3:AN:178:PHE:CE1  | 3:AN:201:PRO:HB3  | 2.56                     | 0.40              |
| 6:AS:366:TYR:O    | 11:A0:72:HIS:CE1  | 2.74                     | 0.40              |
| 6:AT:425:LYS:HE3  | 6:AT:425:LYS:HB3  | 1.96                     | 0.40              |
| 6:AW:404:LEU:HD22 | 6:AW:409:MET:HE3  | 2.02                     | 0.40              |
| 7:Ab:4:GLU:O      | 7:Ab:5:SER:C      | 2.65                     | 0.40              |
| 7:Ab:20:LEU:HD11  | 7:Ab:73:LEU:HD21  | 2.03                     | 0.40              |
| 6:Ak:235:LEU:HB3  | 6:Al:244:ARG:NH2  | 2.36                     | 0.40              |
| 6:AP:360:ARG:NH1  | 6:AP:362:GLU:OE1  | 2.55                     | 0.40              |
| 7:As:24:LEU:HD13  | 9:Ay:203:VAL:CG2  | 2.52                     | 0.40              |
| 8:At:176:GLY:HA2  | 8:At:179:ILE:CD1  | 2.49                     | 0.40              |
| 9:Aw:162:PRO:HD2  | 6:WA:167:ARG:HH21 | 1.84                     | 0.40              |
| 10:A3:7:ILE:O     | 10:A3:11:ILE:HG23 | 2.21                     | 0.40              |
| 11:A6:19:ARG:HD3  | 11:A6:19:ARG:HA   | 1.89                     | 0.40              |
| 6:UI:54:LEU:HG    | 6:UI:55:PHE:CD2   | 2.57                     | 0.40              |
| 6:UK:212:LEU:HG   | 6:UK:220:LEU:HD12 | 2.04                     | 0.40              |
| 6:UM:129:GLN:O    | 6:UM:133:GLN:N    | 2.29                     | 0.40              |
| 6:WA:168:GLU:OE1  | 6:WW:169:GLN:HB2  | 2.21                     | 0.40              |
| 6:WG:187:ASP:HB3  | 6:WG:190:GLN:H    | 1.87                     | 0.40              |
| 6:WR:193:ALA:HB1  | 6:WS:213:VAL:HG21 | 2.03                     | 0.40              |
| 6:WU:145:GLU:O    | 6:WU:147:LEU:N    | 2.54                     | 0.40              |
| 12:BF:55:PRO:HG2  | 6:BG:320:PRO:HB3  | 2.03                     | 0.40              |
| 12:BF:97:ASP:OD1  | 12:BF:97:ASP:N    | 2.45                     | 0.40              |
| 6:BR:360:ARG:NH1  | 6:BR:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:A:126:ALA:HB2   | 1:Z:106:PHE:CD1   | 2.56                     | 0.40              |
| 1:C:113:LEU:HD12  | 1:C:113:LEU:HA    | 1.90                     | 0.40              |
| 1:D:144:PHE:CE2   | 1:E:171:ILE:CD1   | 3.01                     | 0.40              |
| 1:H:28:LYS:HA     | 1:H:28:LYS:HD3    | 1.89                     | 0.40              |
| 1:H:166:GLU:HB2   | 1:I:35:THR:CG2    | 2.30                     | 0.40              |
| 1:L:169:ILE:HG22  | 1:L:171:ILE:HG12  | 2.02                     | 0.40              |
| 1:P:28:LYS:HD3    | 1:P:28:LYS:HA     | 1.89                     | 0.40              |
| 1:Q:203:ALA:HB3   | 1:R:167:LYS:HG3   | 2.04                     | 0.40              |
| 1:S:165:GLY:C     | 1:T:35:THR:HG21   | 2.40                     | 0.40              |
| 1:U:47:ALA:HB3    | 2:r:178:GLN:CD    | 2.45                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:V:93:SER:OG     | 1:W:139:ASN:OD1   | 2.39                     | 0.40              |
| 1:W:47:ALA:HB3    | 2:t:178:GLN:CD    | 2.45                     | 0.40              |
| 2:c:259:THR:HG22  | 2:d:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:e:192:GLU:H     | 2:e:192:GLU:HG3   | 1.53                     | 0.40              |
| 2:h:39:TYR:CE2    | 2:h:61:THR:HG21   | 2.56                     | 0.40              |
| 2:j:259:THR:HG22  | 2:k:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:l:39:TYR:CE2    | 2:l:61:THR:HG21   | 2.56                     | 0.40              |
| 2:l:194:PHE:CZ    | 2:l:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:l:258:ARG:HH12  | 2:n:140:ASN:HD21  | 1.64                     | 0.40              |
| 2:m:362:LEU:HD23  | 2:o:166:THR:HG21  | 2.03                     | 0.40              |
| 2:n:259:THR:HG22  | 2:o:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:p:250:ASP:OD1   | 2:q:23:ARG:NE     | 2.51                     | 0.40              |
| 2:q:259:THR:HG22  | 2:r:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:t:21:ARG:HH21   | 2:t:246:VAL:CG2   | 2.32                     | 0.40              |
| 2:v:247:THR:O     | 2:v:248:PRO:C     | 2.64                     | 0.40              |
| 2:x:93:TYR:HA     | 2:x:94:PRO:HD3    | 1.95                     | 0.40              |
| 2:x:194:PHE:CZ    | 2:x:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:y:39:TYR:CE2    | 2:y:61:THR:HG21   | 2.56                     | 0.40              |
| 3:2:257:LEU:CG    | 3:AF:230:LEU:HD12 | 2.46                     | 0.40              |
| 3:5:257:LEU:HG    | 3:AI:230:LEU:HD13 | 1.96                     | 0.40              |
| 3:6:208:LEU:O     | 3:6:209:ASN:HB2   | 2.21                     | 0.40              |
| 3:8:38:ARG:NH1    | 3:8:228:GLU:OE2   | 2.55                     | 0.40              |
| 3:ZD:3:SER:O      | 3:ZD:4:SER:C      | 2.64                     | 0.40              |
| 4:ZP:292:TYR:CD1  | 4:ZP:292:TYR:C    | 3.00                     | 0.40              |
| 4:ZT:200:PHE:HZ   | 4:ZT:263:PHE:HE2  | 1.69                     | 0.40              |
| 4:ZU:65:THR:HA    | 4:Zf:50:LEU:HD13  | 2.04                     | 0.40              |
| 4:ZU:172:VAL:HG11 | 4:ZU:223:PRO:HD2  | 2.03                     | 0.40              |
| 4:ZU:206:ASN:OD1  | 4:Za:252:ASN:O    | 2.40                     | 0.40              |
| 4:ZW:78:SER:O     | 4:ZW:354:GLY:HA3  | 2.22                     | 0.40              |
| 4:ZX:109:VAL:HG12 | 4:ZX:115:GLN:HA   | 2.04                     | 0.40              |
| 4:ZX:230:LEU:HD11 | 4:ZX:263:PHE:HD2  | 1.87                     | 0.40              |
| 4:Zc:299:THR:HA   | 4:Zc:314:GLN:HA   | 2.02                     | 0.40              |
| 4:Zd:322:ASN:HB3  | 4:Zd:340:SER:HA   | 2.04                     | 0.40              |
| 4:Ze:84:ARG:C     | 4:Ze:85:LEU:HD12  | 2.46                     | 0.40              |
| 4:Zg:5:GLN:H      | 4:Zg:5:GLN:HG3    | 1.59                     | 0.40              |
| 4:Zh:33:LYS:O     | 4:Zh:59:GLN:NE2   | 2.54                     | 0.40              |
| 4:Zh:324:GLU:OE2  | 4:Zh:324:GLU:N    | 2.45                     | 0.40              |
| 5:AA:70:GLN:HB3   | 3:AL:6:TRP:CB     | 2.38                     | 0.40              |
| 5:AD:35:ARG:HA    | 5:AD:210:ASN:ND2  | 2.37                     | 0.40              |
| 5:AE:248:LEU:HD21 | 11:A0:106:ARG:HG2 | 2.02                     | 0.40              |
| 3:AF:44:LEU:HD12  | 3:AF:44:LEU:H     | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AF:44:LEU:HD13  | 3:AF:70:THR:HG22  | 2.02                     | 0.40              |
| 3:AI:102:PHE:HB3  | 3:AI:114:TYR:HB3  | 2.04                     | 0.40              |
| 3:AK:85:ASN:O     | 3:AK:221:THR:OG1  | 2.32                     | 0.40              |
| 3:AL:130:THR:OG1  | 3:AL:131:ALA:N    | 2.54                     | 0.40              |
| 3:AL:136:VAL:O    | 3:AL:137:GLN:C    | 2.64                     | 0.40              |
| 3:AM:194:GLU:OE2  | 3:AM:201:PRO:HD3  | 2.21                     | 0.40              |
| 3:AN:73:ARG:HG3   | 3:AN:73:ARG:O     | 2.21                     | 0.40              |
| 6:Aj:360:ARG:NH1  | 6:Aj:362:GLU:OE1  | 2.55                     | 0.40              |
| 6:Am:290:LYS:HE3  | 6:Am:290:LYS:HB2  | 1.93                     | 0.40              |
| 7:Aq:39:GLN:NE2   | 7:Aq:49:LEU:HD12  | 2.30                     | 0.40              |
| 7:Aq:51:PHE:CE2   | 7:Aq:55:ILE:HD11  | 2.56                     | 0.40              |
| 8:At:144:LEU:HB3  | 6:WJ:164:LEU:HD21 | 2.04                     | 0.40              |
| 9:Av:69:ILE:HG12  | 9:Aw:83:ALA:O     | 2.22                     | 0.40              |
| 9:Aw:71:PHE:HD1   | 9:Aw:71:PHE:HA    | 1.80                     | 0.40              |
| 10:A2:92:LEU:HD23 | 10:A2:92:LEU:HA   | 1.82                     | 0.40              |
| 11:A7:31:ALA:HB1  | 12:BB:13:ALA:HB2  | 2.04                     | 0.40              |
| 11:A8:67:LEU:CA   | 11:A8:72:HIS:HE2  | 2.34                     | 0.40              |
| 6:UM:165:PHE:HD1  | 6:UM:165:PHE:HA   | 1.77                     | 0.40              |
| 6:WJ:144:ILE:O    | 6:WJ:147:LEU:HB2  | 2.21                     | 0.40              |
| 12:BE:45:LYS:C    | 12:BE:46:GLN:HG2  | 2.46                     | 0.40              |
| 6:BU:360:ARG:NH1  | 6:BU:362:GLU:OE1  | 2.55                     | 0.40              |
| 1:E:28:LYS:HD3    | 1:E:28:LYS:HA     | 1.89                     | 0.40              |
| 1:E:203:ALA:HB3   | 1:F:167:LYS:HG3   | 2.03                     | 0.40              |
| 1:G:169:ILE:HG22  | 1:G:171:ILE:HG12  | 2.02                     | 0.40              |
| 1:U:106:PHE:CD1   | 1:V:126:ALA:HB2   | 2.56                     | 0.40              |
| 1:V:203:ALA:HB3   | 1:W:167:LYS:HG3   | 2.04                     | 0.40              |
| 2:b:259:THR:HG22  | 2:c:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:b:273:CYS:CB    | 2:c:265:ASN:HA    | 2.52                     | 0.40              |
| 2:c:192:GLU:H     | 2:c:192:GLU:HG3   | 1.53                     | 0.40              |
| 2:f:194:PHE:CZ    | 2:f:218:ALA:HB2   | 2.57                     | 0.40              |
| 2:k:39:TYR:CE2    | 2:k:61:THR:HG21   | 2.56                     | 0.40              |
| 2:p:259:THR:HG22  | 2:q:144:GLY:HA3   | 2.03                     | 0.40              |
| 2:r:21:ARG:HH21   | 2:r:246:VAL:CG2   | 2.32                     | 0.40              |
| 2:r:259:THR:HG22  | 2:s:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:x:39:TYR:CE2    | 2:x:61:THR:HG21   | 2.56                     | 0.40              |
| 2:x:259:THR:HG22  | 2:y:144:GLY:HA3   | 2.04                     | 0.40              |
| 2:z:39:TYR:CE2    | 2:z:61:THR:HG21   | 2.56                     | 0.40              |
| 3:1:242:ILE:HG21  | 3:AK:26:LEU:HD22  | 2.04                     | 0.40              |
| 3:1:260:LEU:CG    | 5:AE:221:ILE:HD11 | 2.51                     | 0.40              |
| 3:3:155:GLY:HA2   | 3:3:214:LEU:HD12  | 2.04                     | 0.40              |
| 3:4:1:MET:HB2     | 3:AM:235:GLN:HG3  | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:19:MET:HB2    | 3:8:236:VAL:HG11  | 2.03                     | 0.40              |
| 3:8:19:MET:O      | 3:8:20:ASP:C      | 2.65                     | 0.40              |
| 3:8:238:ARG:CZ    | 3:ZE:255:GLN:HB2  | 2.51                     | 0.40              |
| 3:9:56:SER:CA     | 3:AH:153:ARG:H    | 2.35                     | 0.40              |
| 3:ZA:45:LEU:HD11  | 3:AN:83:GLN:NE2   | 2.36                     | 0.40              |
| 3:ZC:50:ARG:CZ    | 3:ZC:62:LEU:HD11  | 2.52                     | 0.40              |
| 3:ZC:77:THR:HG23  | 4:ZH:47:LYS:HG2   | 2.04                     | 0.40              |
| 3:ZC:257:LEU:HA   | 3:ZC:260:LEU:HG   | 2.03                     | 0.40              |
| 3:ZD:237:GLN:HA   | 4:ZI:395:ILE:HD11 | 2.02                     | 0.40              |
| 3:ZE:95:VAL:O     | 3:ZE:118:GLY:HA3  | 2.22                     | 0.40              |
| 4:ZH:144:MET:SD   | 4:ZH:310:GLN:NE2  | 2.95                     | 0.40              |
| 4:ZI:73:LEU:HD23  | 4:ZI:73:LEU:HA    | 1.85                     | 0.40              |
| 4:ZP:185:THR:HG22 | 4:ZP:187:TYR:HE1  | 1.87                     | 0.40              |
| 4:ZQ:175:ALA:HA   | 4:ZQ:178:TYR:CZ   | 2.57                     | 0.40              |
| 4:ZS:380:ARG:NH2  | 4:ZY:397:ASN:OD1  | 2.55                     | 0.40              |
| 4:ZU:208:TRP:HE1  | 4:ZU:268:GLN:HG3  | 1.86                     | 0.40              |
| 4:ZX:17:LEU:CD1   | 4:Zc:395:ILE:HD11 | 2.49                     | 0.40              |
| 4:ZX:104:GLU:H    | 4:ZX:104:GLU:CD   | 2.29                     | 0.40              |
| 4:Za:190:GLN:HG3  | 4:Za:254:ALA:HB2  | 2.03                     | 0.40              |
| 4:Za:204:LYS:HG2  | 4:Za:205:ASP:H    | 1.86                     | 0.40              |
| 4:Za:368:LEU:O    | 4:Za:372:LEU:N    | 2.47                     | 0.40              |
| 4:Za:395:ILE:HD13 | 4:Za:395:ILE:HA   | 1.88                     | 0.40              |
| 4:Zd:183:THR:HG23 | 4:Zd:195:ASP:OD2  | 2.21                     | 0.40              |
| 4:Zg:17:LEU:HD23  | 4:Zg:17:LEU:HA    | 1.97                     | 0.40              |
| 4:Zg:396:LEU:HD23 | 4:Zg:396:LEU:HA   | 1.78                     | 0.40              |
| 5:AC:35:ARG:HE    | 5:AC:101:ARG:HG3  | 1.87                     | 0.40              |
| 5:AC:137:ILE:HG22 | 5:AC:201:ILE:HD11 | 2.03                     | 0.40              |
| 5:AD:217:MET:CE   | 3:AI:242:ILE:CD1  | 2.95                     | 0.40              |
| 5:AE:49:LEU:O     | 5:AE:50:SER:HB3   | 2.21                     | 0.40              |
| 5:AE:175:ASP:CG   | 3:AJ:46:TYR:O     | 2.65                     | 0.40              |
| 3:AF:75:VAL:HG23  | 3:AF:76:ALA:H     | 1.87                     | 0.40              |
| 3:AF:151:ILE:HB   | 3:AF:216:GLN:HG3  | 2.02                     | 0.40              |
| 3:AL:179:MET:HE2  | 3:AL:200:ALA:HB3  | 2.03                     | 0.40              |
| 3:AN:129:VAL:HG12 | 3:AN:135:GLN:HA   | 2.02                     | 0.40              |
| 6:AX:235:LEU:HB3  | 6:AY:244:ARG:NH2  | 2.36                     | 0.40              |
| 6:Ah:290:LYS:HE3  | 6:Ah:290:LYS:HB2  | 1.93                     | 0.40              |
| 6:AQ:290:LYS:HE3  | 6:AQ:290:LYS:HB2  | 1.93                     | 0.40              |
| 9:Aw:143:ARG:NH1  | 6:WW:165:PHE:CZ   | 2.90                     | 0.40              |
| 10:A2:61:LEU:HD22 | 11:A7:50:LYS:CE   | 2.50                     | 0.40              |
| 10:A5:7:ILE:O     | 10:A5:11:ILE:HG23 | 2.21                     | 0.40              |
| 11:A8:32:ASN:HA   | 12:BC:62:VAL:CG2  | 2.52                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A8:92:GLN:NE2  | 12:BD:19:LYS:HA   | 2.37                     | 0.40              |
| 6:UJ:54:LEU:HG    | 6:UJ:55:PHE:CD2   | 2.57                     | 0.40              |
| 6:UJ:263:ASP:OD2  | 6:UJ:267:HIS:HB2  | 2.20                     | 0.40              |
| 6:UN:212:LEU:HG   | 6:UN:220:LEU:HD12 | 2.04                     | 0.40              |
| 6:WC:193:ALA:CB   | 6:WD:213:VAL:CG1  | 3.00                     | 0.40              |
| 6:WR:193:ALA:HB1  | 6:WS:213:VAL:CG2  | 2.52                     | 0.40              |
| 6:WS:115:LEU:HA   | 6:WS:118:GLN:OE1  | 2.21                     | 0.40              |
| 6:WV:145:GLU:O    | 6:WV:147:LEU:N    | 2.54                     | 0.40              |
| 12:BF:35:THR:OG1  | 12:BF:39:GLY:HA2  | 2.22                     | 0.40              |
| 6:BU:404:LEU:HD22 | 6:BU:409:MET:HE3  | 2.02                     | 0.40              |
| 6:BX:404:LEU:HD22 | 6:BX:409:MET:HE3  | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | K     | 51/232 (22%)  | 50 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | M     | 117/232 (50%) | 114 (97%) | 2 (2%)  | 1 (1%)   | 14          | 49  |
| 1   | N     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | O     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | P     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | Q     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | R     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | S     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | T     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | U     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | V     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | W     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | X     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | Y     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 1   | Z     | 209/232 (90%) | 204 (98%) | 4 (2%)  | 1 (0%)   | 24          | 61  |
| 2   | a     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | b     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | c     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | d     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | e     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | f     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | g     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | h     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | i     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | j     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | k     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | l     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | m     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | n     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | o     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | p     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | q     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | r     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | s     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | t     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | u     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | v     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | w     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | x     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | y     | 297/365 (81%) | 289 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | z     | 297/365 (81%) | 288 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 3   | 0     | 244/260 (94%) | 236 (97%) | 5 (2%)  | 3 (1%)   | 10          | 42  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | 1     | 248/260 (95%) | 238 (96%) | 9 (4%)  | 1 (0%)   | 30          | 65  |
| 3   | 2     | 258/260 (99%) | 242 (94%) | 14 (5%) | 2 (1%)   | 16          | 52  |
| 3   | 3     | 258/260 (99%) | 247 (96%) | 9 (4%)  | 2 (1%)   | 16          | 52  |
| 3   | 4     | 258/260 (99%) | 245 (95%) | 11 (4%) | 2 (1%)   | 16          | 52  |
| 3   | 5     | 258/260 (99%) | 240 (93%) | 15 (6%) | 3 (1%)   | 10          | 42  |
| 3   | 6     | 258/260 (99%) | 244 (95%) | 10 (4%) | 4 (2%)   | 7           | 37  |
| 3   | 7     | 258/260 (99%) | 244 (95%) | 11 (4%) | 3 (1%)   | 10          | 42  |
| 3   | 8     | 258/260 (99%) | 243 (94%) | 12 (5%) | 3 (1%)   | 10          | 42  |
| 3   | 9     | 258/260 (99%) | 244 (95%) | 13 (5%) | 1 (0%)   | 30          | 65  |
| 3   | AF    | 250/260 (96%) | 238 (95%) | 11 (4%) | 1 (0%)   | 30          | 65  |
| 3   | AG    | 251/260 (96%) | 234 (93%) | 14 (6%) | 3 (1%)   | 10          | 42  |
| 3   | AH    | 252/260 (97%) | 234 (93%) | 16 (6%) | 2 (1%)   | 16          | 52  |
| 3   | AI    | 250/260 (96%) | 239 (96%) | 9 (4%)  | 2 (1%)   | 16          | 52  |
| 3   | AJ    | 251/260 (96%) | 235 (94%) | 10 (4%) | 6 (2%)   | 4           | 30  |
| 3   | AK    | 239/260 (92%) | 231 (97%) | 7 (3%)  | 1 (0%)   | 30          | 65  |
| 3   | AL    | 244/260 (94%) | 229 (94%) | 10 (4%) | 5 (2%)   | 6           | 33  |
| 3   | AM    | 244/260 (94%) | 234 (96%) | 9 (4%)  | 1 (0%)   | 30          | 65  |
| 3   | AN    | 244/260 (94%) | 239 (98%) | 4 (2%)  | 1 (0%)   | 30          | 65  |
| 3   | ZA    | 258/260 (99%) | 243 (94%) | 12 (5%) | 3 (1%)   | 10          | 42  |
| 3   | ZB    | 258/260 (99%) | 242 (94%) | 13 (5%) | 3 (1%)   | 10          | 42  |
| 3   | ZC    | 258/260 (99%) | 242 (94%) | 14 (5%) | 2 (1%)   | 16          | 52  |
| 3   | ZD    | 258/260 (99%) | 237 (92%) | 18 (7%) | 3 (1%)   | 10          | 42  |
| 3   | ZE    | 258/260 (99%) | 243 (94%) | 14 (5%) | 1 (0%)   | 30          | 65  |
| 4   | ZF    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |
| 4   | ZG    | 399/403 (99%) | 388 (97%) | 10 (2%) | 1 (0%)   | 36          | 70  |
| 4   | ZH    | 399/403 (99%) | 385 (96%) | 14 (4%) | 0        | 100         | 100 |
| 4   | ZI    | 399/403 (99%) | 387 (97%) | 10 (2%) | 2 (0%)   | 24          | 61  |
| 4   | ZJ    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |
| 4   | ZK    | 399/403 (99%) | 387 (97%) | 11 (3%) | 1 (0%)   | 36          | 70  |
| 4   | ZL    | 399/403 (99%) | 389 (98%) | 9 (2%)  | 1 (0%)   | 36          | 70  |
| 4   | ZM    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | ZN    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 4   | ZO    | 399/403 (99%) | 381 (96%) | 15 (4%) | 3 (1%)   | 16          | 52  |
| 4   | ZP    | 399/403 (99%) | 386 (97%) | 12 (3%) | 1 (0%)   | 36          | 70  |
| 4   | ZQ    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 4   | ZR    | 399/403 (99%) | 391 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 4   | ZS    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 4   | ZT    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 4   | ZU    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |
| 4   | ZV    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 4   | ZW    | 399/403 (99%) | 380 (95%) | 18 (4%) | 1 (0%)   | 36          | 70  |
| 4   | ZX    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 4   | ZY    | 399/403 (99%) | 385 (96%) | 14 (4%) | 0        | 100         | 100 |
| 4   | ZZ    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 4   | Za    | 399/403 (99%) | 386 (97%) | 12 (3%) | 1 (0%)   | 36          | 70  |
| 4   | Zb    | 399/403 (99%) | 392 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 4   | Zc    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 4   | Zd    | 399/403 (99%) | 384 (96%) | 15 (4%) | 0        | 100         | 100 |
| 4   | Ze    | 399/403 (99%) | 385 (96%) | 13 (3%) | 1 (0%)   | 36          | 70  |
| 4   | Zf    | 399/403 (99%) | 386 (97%) | 13 (3%) | 0        | 100         | 100 |
| 4   | Zg    | 399/403 (99%) | 383 (96%) | 16 (4%) | 0        | 100         | 100 |
| 4   | Zh    | 399/403 (99%) | 391 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 5   | AA    | 246/251 (98%) | 238 (97%) | 7 (3%)  | 1 (0%)   | 30          | 65  |
| 5   | AB    | 247/251 (98%) | 242 (98%) | 4 (2%)  | 1 (0%)   | 30          | 65  |
| 5   | AC    | 248/251 (99%) | 233 (94%) | 13 (5%) | 2 (1%)   | 16          | 52  |
| 5   | AD    | 248/251 (99%) | 235 (95%) | 13 (5%) | 0        | 100         | 100 |
| 5   | AE    | 247/251 (98%) | 236 (96%) | 9 (4%)  | 2 (1%)   | 16          | 52  |
| 6   | AO    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AP    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AQ    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AR    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AS    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 6   | AT    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AU    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AV    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AW    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AX    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AY    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | AZ    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Aa    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ac    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ad    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ae    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Af    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ag    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ah    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ai    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Aj    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ak    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Al    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Am    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | An    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ao    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | Ap    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BG    | 11/560 (2%)   | 9 (82%)   | 2 (18%) | 0        | 100         | 100 |
| 6   | BH    | 14/560 (2%)   | 12 (86%)  | 2 (14%) | 0        | 100         | 100 |
| 6   | BI    | 18/560 (3%)   | 18 (100%) | 0       | 0        | 100         | 100 |
| 6   | BJ    | 14/560 (2%)   | 14 (100%) | 0       | 0        | 100         | 100 |
| 6   | BK    | 19/560 (3%)   | 17 (90%)  | 2 (10%) | 0        | 100         | 100 |
| 6   | BL    | 14/560 (2%)   | 13 (93%)  | 1 (7%)  | 0        | 100         | 100 |
| 6   | BM    | 19/560 (3%)   | 19 (100%) | 0       | 0        | 100         | 100 |
| 6   | BN    | 14/560 (2%)   | 14 (100%) | 0       | 0        | 100         | 100 |
| 6   | BO    | 18/560 (3%)   | 18 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 6   | BP    | 14/560 (2%)   | 14 (100%) | 0       | 0        | 100         | 100 |
| 6   | BQ    | 19/560 (3%)   | 19 (100%) | 0       | 0        | 100         | 100 |
| 6   | BR    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BS    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BT    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BU    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BV    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BW    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | BX    | 160/560 (29%) | 158 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | UI    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | UJ    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | UK    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | UL    | 151/560 (27%) | 142 (94%) | 7 (5%)  | 2 (1%)   | 9           | 41  |
| 6   | UM    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | UN    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | UO    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | UP    | 151/560 (27%) | 146 (97%) | 3 (2%)  | 2 (1%)   | 9           | 41  |
| 6   | WA    | 111/560 (20%) | 99 (89%)  | 9 (8%)  | 3 (3%)   | 4           | 28  |
| 6   | WB    | 109/560 (20%) | 94 (86%)  | 10 (9%) | 5 (5%)   | 2           | 19  |
| 6   | WC    | 106/560 (19%) | 96 (91%)  | 9 (8%)  | 1 (1%)   | 14          | 49  |
| 6   | WD    | 108/560 (19%) | 99 (92%)  | 4 (4%)  | 5 (5%)   | 2           | 19  |
| 6   | WE    | 110/560 (20%) | 98 (89%)  | 8 (7%)  | 4 (4%)   | 2           | 22  |
| 6   | WF    | 109/560 (20%) | 98 (90%)  | 8 (7%)  | 3 (3%)   | 4           | 27  |
| 6   | WG    | 110/560 (20%) | 98 (89%)  | 10 (9%) | 2 (2%)   | 6           | 35  |
| 6   | WH    | 93/560 (17%)  | 86 (92%)  | 5 (5%)  | 2 (2%)   | 5           | 31  |
| 6   | WI    | 93/560 (17%)  | 82 (88%)  | 5 (5%)  | 6 (6%)   | 1           | 15  |
| 6   | WJ    | 97/560 (17%)  | 89 (92%)  | 7 (7%)  | 1 (1%)   | 12          | 46  |
| 6   | WK    | 96/560 (17%)  | 84 (88%)  | 9 (9%)  | 3 (3%)   | 3           | 25  |
| 6   | WL    | 81/560 (14%)  | 75 (93%)  | 4 (5%)  | 2 (2%)   | 4           | 29  |
| 6   | WM    | 78/560 (14%)  | 72 (92%)  | 4 (5%)  | 2 (3%)   | 4           | 28  |
| 6   | WN    | 80/560 (14%)  | 75 (94%)  | 2 (2%)  | 3 (4%)   | 2           | 21  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 6   | WO    | 94/560 (17%)  | 85 (90%)  | 7 (7%)  | 2 (2%)   | 5           | 32  |
| 6   | WP    | 98/560 (18%)  | 87 (89%)  | 6 (6%)  | 5 (5%)   | 1           | 17  |
| 6   | WQ    | 109/560 (20%) | 100 (92%) | 5 (5%)  | 4 (4%)   | 2           | 22  |
| 6   | WR    | 109/560 (20%) | 94 (86%)  | 8 (7%)  | 7 (6%)   | 1           | 15  |
| 6   | WS    | 109/560 (20%) | 96 (88%)  | 7 (6%)  | 6 (6%)   | 1           | 17  |
| 6   | WT    | 109/560 (20%) | 97 (89%)  | 5 (5%)  | 7 (6%)   | 1           | 15  |
| 6   | WU    | 110/560 (20%) | 101 (92%) | 8 (7%)  | 1 (1%)   | 14          | 49  |
| 6   | WV    | 108/560 (19%) | 97 (90%)  | 9 (8%)  | 2 (2%)   | 6           | 34  |
| 6   | WW    | 109/560 (20%) | 95 (87%)  | 9 (8%)  | 5 (5%)   | 2           | 19  |
| 7   | Ab    | 87/89 (98%)   | 81 (93%)  | 4 (5%)  | 2 (2%)   | 5           | 31  |
| 7   | Aq    | 87/89 (98%)   | 86 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 7   | Ar    | 87/89 (98%)   | 86 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 7   | As    | 87/89 (98%)   | 85 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 8   | At    | 251/264 (95%) | 233 (93%) | 16 (6%) | 2 (1%)   | 16          | 52  |
| 9   | Au    | 205/245 (84%) | 197 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 9   | Av    | 207/245 (84%) | 199 (96%) | 6 (3%)  | 2 (1%)   | 12          | 46  |
| 9   | Aw    | 206/245 (84%) | 201 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 9   | Ax    | 206/245 (84%) | 199 (97%) | 6 (3%)  | 1 (0%)   | 24          | 61  |
| 9   | Ay    | 207/245 (84%) | 192 (93%) | 10 (5%) | 5 (2%)   | 4           | 30  |
| 10  | A1    | 87/104 (84%)  | 87 (100%) | 0       | 0        | 100         | 100 |
| 10  | A2    | 89/104 (86%)  | 87 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 10  | A3    | 89/104 (86%)  | 89 (100%) | 0       | 0        | 100         | 100 |
| 10  | A4    | 89/104 (86%)  | 89 (100%) | 0       | 0        | 100         | 100 |
| 10  | A5    | 88/104 (85%)  | 88 (100%) | 0       | 0        | 100         | 100 |
| 10  | Az    | 55/104 (53%)  | 52 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 11  | A0    | 117/138 (85%) | 115 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 11  | A6    | 132/138 (96%) | 127 (96%) | 4 (3%)  | 1 (1%)   | 16          | 52  |
| 11  | A7    | 115/138 (83%) | 114 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 11  | A8    | 119/138 (86%) | 116 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 11  | A9    | 121/138 (88%) | 119 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 12  | BA    | 131/134 (98%) | 122 (93%) | 9 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 12  | BB    | 130/134 (97%)     | 123 (95%)   | 7 (5%)    | 0        | 100         | 100 |
| 12  | BC    | 131/134 (98%)     | 124 (95%)   | 7 (5%)    | 0        | 100         | 100 |
| 12  | BD    | 131/134 (98%)     | 121 (92%)   | 7 (5%)    | 3 (2%)   | 5           | 31  |
| 12  | BE    | 129/134 (96%)     | 123 (95%)   | 5 (4%)    | 1 (1%)   | 16          | 52  |
| 12  | BF    | 131/134 (98%)     | 124 (95%)   | 7 (5%)    | 0        | 100         | 100 |
| All | All   | 42157/78675 (54%) | 40652 (96%) | 1301 (3%) | 204 (0%) | 26          | 61  |

All (204) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 209 | ASN  |
| 3   | 4     | 140 | ILE  |
| 3   | 5     | 209 | ASN  |
| 3   | 6     | 139 | ALA  |
| 3   | 8     | 209 | ASN  |
| 3   | ZA    | 92  | SER  |
| 3   | ZA    | 209 | ASN  |
| 3   | ZB    | 164 | GLN  |
| 4   | ZG    | 46  | SER  |
| 5   | AE    | 155 | VAL  |
| 3   | AL    | 90  | ASN  |
| 7   | Ab    | 84  | LEU  |
| 9   | Ay    | 83  | ALA  |
| 9   | Ay    | 87  | GLN  |
| 6   | WB    | 163 | SER  |
| 6   | WO    | 168 | GLU  |
| 6   | WR    | 123 | ILE  |
| 6   | WR    | 165 | PHE  |
| 6   | WR    | 166 | VAL  |
| 6   | WS    | 187 | ASP  |
| 3   | 0     | 90  | ASN  |
| 3   | 8     | 165 | ALA  |
| 3   | ZB    | 165 | ALA  |
| 3   | ZB    | 209 | ASN  |
| 3   | ZC    | 209 | ASN  |
| 3   | ZD    | 209 | ASN  |
| 3   | ZE    | 209 | ASN  |
| 4   | ZI    | 375 | MET  |
| 4   | ZO    | 237 | ILE  |
| 5   | AC    | 50  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AE    | 53  | THR  |
| 3   | AI    | 127 | GLN  |
| 3   | AI    | 165 | ALA  |
| 3   | AJ    | 204 | SER  |
| 3   | AL    | 4   | SER  |
| 3   | AN    | 127 | GLN  |
| 8   | At    | 167 | ASN  |
| 8   | At    | 213 | ILE  |
| 9   | Av    | 83  | ALA  |
| 9   | Ax    | 160 | GLN  |
| 9   | Ay    | 86  | ASN  |
| 6   | WB    | 148 | GLY  |
| 6   | WD    | 146 | THR  |
| 6   | WD    | 148 | GLY  |
| 6   | WF    | 118 | GLN  |
| 6   | WI    | 146 | THR  |
| 6   | WI    | 160 | PRO  |
| 6   | WI    | 170 | LYS  |
| 6   | WK    | 166 | VAL  |
| 6   | WM    | 148 | GLY  |
| 6   | WN    | 146 | THR  |
| 6   | WN    | 148 | GLY  |
| 6   | WP    | 146 | THR  |
| 6   | WQ    | 146 | THR  |
| 6   | WQ    | 148 | GLY  |
| 6   | WQ    | 169 | GLN  |
| 6   | WS    | 146 | THR  |
| 6   | WT    | 146 | THR  |
| 6   | WT    | 162 | PRO  |
| 6   | WW    | 146 | THR  |
| 6   | WW    | 148 | GLY  |
| 12  | BD    | 54  | ALA  |
| 3   | 0     | 3   | SER  |
| 3   | 0     | 127 | GLN  |
| 3   | 2     | 49  | ILE  |
| 3   | 3     | 49  | ILE  |
| 3   | 3     | 181 | ASP  |
| 3   | 4     | 49  | ILE  |
| 3   | 5     | 49  | ILE  |
| 3   | 6     | 138 | PRO  |
| 3   | 7     | 55  | GLN  |
| 4   | ZK    | 375 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZL    | 374 | ASN  |
| 3   | AF    | 127 | GLN  |
| 3   | AH    | 198 | SER  |
| 3   | AJ    | 164 | GLN  |
| 3   | AJ    | 206 | PRO  |
| 3   | AL    | 3   | SER  |
| 3   | AL    | 127 | GLN  |
| 3   | AM    | 127 | GLN  |
| 9   | Ay    | 140 | ARG  |
| 11  | A6    | 77  | ALA  |
| 6   | UI    | 162 | PRO  |
| 6   | UJ    | 162 | PRO  |
| 6   | UK    | 162 | PRO  |
| 6   | UL    | 162 | PRO  |
| 6   | UM    | 162 | PRO  |
| 6   | UN    | 162 | PRO  |
| 6   | UO    | 162 | PRO  |
| 6   | UP    | 162 | PRO  |
| 6   | WB    | 146 | THR  |
| 6   | WB    | 164 | LEU  |
| 6   | WD    | 118 | GLN  |
| 6   | WE    | 160 | PRO  |
| 6   | WE    | 162 | PRO  |
| 6   | WI    | 148 | GLY  |
| 6   | WP    | 148 | GLY  |
| 6   | WS    | 118 | GLN  |
| 6   | WS    | 169 | GLN  |
| 6   | WT    | 165 | PHE  |
| 6   | WW    | 118 | GLN  |
| 6   | WW    | 168 | GLU  |
| 12  | BD    | 58  | ALA  |
| 1   | M     | 172 | ASN  |
| 1   | N     | 172 | ASN  |
| 1   | O     | 172 | ASN  |
| 1   | P     | 172 | ASN  |
| 1   | Q     | 172 | ASN  |
| 1   | R     | 172 | ASN  |
| 1   | S     | 172 | ASN  |
| 1   | T     | 172 | ASN  |
| 1   | U     | 172 | ASN  |
| 1   | V     | 172 | ASN  |
| 1   | W     | 172 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 172 | ASN  |
| 1   | Y     | 172 | ASN  |
| 1   | Z     | 172 | ASN  |
| 3   | 6     | 49  | ILE  |
| 3   | 6     | 58  | GLU  |
| 3   | 7     | 49  | ILE  |
| 3   | 8     | 49  | ILE  |
| 3   | 9     | 49  | ILE  |
| 3   | ZA    | 138 | PRO  |
| 4   | ZO    | 142 | THR  |
| 4   | ZP    | 374 | ASN  |
| 3   | AG    | 81  | HIS  |
| 3   | AG    | 127 | GLN  |
| 3   | AJ    | 203 | GLU  |
| 3   | AK    | 127 | GLN  |
| 6   | UI    | 163 | SER  |
| 6   | UJ    | 163 | SER  |
| 6   | UK    | 163 | SER  |
| 6   | UL    | 163 | SER  |
| 6   | UM    | 163 | SER  |
| 6   | UN    | 163 | SER  |
| 6   | UO    | 163 | SER  |
| 6   | UP    | 163 | SER  |
| 6   | WA    | 182 | PRO  |
| 6   | WB    | 182 | PRO  |
| 6   | WD    | 165 | PHE  |
| 6   | WD    | 182 | PRO  |
| 6   | WE    | 182 | PRO  |
| 6   | WF    | 182 | PRO  |
| 6   | WG    | 182 | PRO  |
| 6   | WH    | 165 | PHE  |
| 6   | WH    | 182 | PRO  |
| 6   | WI    | 169 | GLN  |
| 6   | WI    | 182 | PRO  |
| 6   | WJ    | 182 | PRO  |
| 6   | WK    | 182 | PRO  |
| 6   | WL    | 182 | PRO  |
| 6   | WM    | 182 | PRO  |
| 6   | WN    | 182 | PRO  |
| 6   | WO    | 182 | PRO  |
| 6   | WP    | 182 | PRO  |
| 6   | WQ    | 182 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | WR    | 112 | GLY  |
| 6   | WR    | 182 | PRO  |
| 6   | WS    | 182 | PRO  |
| 6   | WT    | 182 | PRO  |
| 6   | WU    | 182 | PRO  |
| 6   | WV    | 148 | GLY  |
| 6   | WV    | 182 | PRO  |
| 6   | WW    | 182 | PRO  |
| 12  | BD    | 55  | PRO  |
| 3   | 1     | 127 | GLN  |
| 3   | 7     | 210 | GLY  |
| 3   | ZC    | 139 | ALA  |
| 3   | ZD    | 139 | ALA  |
| 5   | AB    | 52  | ALA  |
| 5   | AC    | 52  | ALA  |
| 3   | AG    | 139 | ALA  |
| 3   | AH    | 127 | GLN  |
| 3   | AJ    | 127 | GLN  |
| 7   | Ab    | 85  | PRO  |
| 9   | Av    | 162 | PRO  |
| 6   | WK    | 168 | GLU  |
| 6   | WR    | 121 | PHE  |
| 6   | WT    | 163 | SER  |
| 4   | ZO    | 375 | MET  |
| 4   | Za    | 97  | ASN  |
| 4   | Ze    | 134 | PRO  |
| 5   | AA    | 52  | ALA  |
| 3   | AJ    | 200 | ALA  |
| 6   | WC    | 182 | PRO  |
| 6   | WE    | 221 | THR  |
| 6   | WF    | 162 | PRO  |
| 6   | WG    | 163 | SER  |
| 12  | BE    | 58  | ALA  |
| 4   | ZI    | 325 | GLY  |
| 6   | WA    | 160 | PRO  |
| 6   | WL    | 148 | GLY  |
| 6   | WS    | 148 | GLY  |
| 6   | WT    | 148 | GLY  |
| 4   | ZW    | 75  | VAL  |
| 6   | WA    | 148 | GLY  |
| 6   | WP    | 123 | ILE  |
| 6   | WR    | 148 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 5     | 138 | PRO  |
| 3   | AL    | 136 | VAL  |
| 9   | Ay    | 229 | VAL  |
| 6   | WP    | 160 | PRO  |
| 6   | WT    | 161 | LYS  |
| 3   | ZD    | 138 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | B     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | C     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | D     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | E     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | F     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | G     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | H     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | I     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | J     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | K     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | L     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | M     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | N     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | O     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | P     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | Q     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | R     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | S     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | T     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | U     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | V     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | W     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | X     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | Y     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 1   | Z     | 170/186 (91%) | 161 (95%) | 9 (5%)   | 20          | 44 |
| 2   | a     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | b     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | c     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | d     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | e     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | f     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | g     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | h     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | i     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | j     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | k     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | l     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | m     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | n     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | o     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | p     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | q     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | r     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | s     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | t     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | u     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | v     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | w     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |
| 2   | x     | 248/294 (84%) | 241 (97%) | 7 (3%)   | 38          | 59 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |    |
|-----|-------|----------------|------------|----------|-------------|----|
| 2   | y     | 248/294 (84%)  | 241 (97%)  | 7 (3%)   | 38          | 59 |
| 2   | z     | 248/294 (84%)  | 241 (97%)  | 7 (3%)   | 38          | 59 |
| 3   | 0     | 205/215 (95%)  | 199 (97%)  | 6 (3%)   | 37          | 58 |
| 3   | 1     | 209/215 (97%)  | 206 (99%)  | 3 (1%)   | 59          | 71 |
| 3   | 2     | 215/215 (100%) | 214 (100%) | 1 (0%)   | 81          | 82 |
| 3   | 3     | 215/215 (100%) | 214 (100%) | 1 (0%)   | 81          | 82 |
| 3   | 4     | 215/215 (100%) | 212 (99%)  | 3 (1%)   | 59          | 71 |
| 3   | 5     | 215/215 (100%) | 211 (98%)  | 4 (2%)   | 50          | 67 |
| 3   | 6     | 215/215 (100%) | 212 (99%)  | 3 (1%)   | 59          | 71 |
| 3   | 7     | 215/215 (100%) | 214 (100%) | 1 (0%)   | 81          | 82 |
| 3   | 8     | 215/215 (100%) | 209 (97%)  | 6 (3%)   | 38          | 59 |
| 3   | 9     | 215/215 (100%) | 213 (99%)  | 2 (1%)   | 70          | 76 |
| 3   | AF    | 209/215 (97%)  | 207 (99%)  | 2 (1%)   | 68          | 76 |
| 3   | AG    | 210/215 (98%)  | 202 (96%)  | 8 (4%)   | 29          | 51 |
| 3   | AH    | 211/215 (98%)  | 204 (97%)  | 7 (3%)   | 33          | 55 |
| 3   | AI    | 209/215 (97%)  | 203 (97%)  | 6 (3%)   | 37          | 58 |
| 3   | AJ    | 210/215 (98%)  | 204 (97%)  | 6 (3%)   | 37          | 58 |
| 3   | AK    | 200/215 (93%)  | 196 (98%)  | 4 (2%)   | 48          | 66 |
| 3   | AL    | 205/215 (95%)  | 202 (98%)  | 3 (2%)   | 57          | 70 |
| 3   | AM    | 205/215 (95%)  | 200 (98%)  | 5 (2%)   | 43          | 63 |
| 3   | AN    | 205/215 (95%)  | 201 (98%)  | 4 (2%)   | 48          | 66 |
| 3   | ZA    | 215/215 (100%) | 214 (100%) | 1 (0%)   | 81          | 82 |
| 3   | ZB    | 215/215 (100%) | 213 (99%)  | 2 (1%)   | 70          | 76 |
| 3   | ZC    | 215/215 (100%) | 212 (99%)  | 3 (1%)   | 59          | 71 |
| 3   | ZD    | 215/215 (100%) | 208 (97%)  | 7 (3%)   | 33          | 55 |
| 3   | ZE    | 215/215 (100%) | 210 (98%)  | 5 (2%)   | 44          | 64 |
| 4   | ZF    | 321/323 (99%)  | 315 (98%)  | 6 (2%)   | 50          | 67 |
| 4   | ZG    | 321/323 (99%)  | 315 (98%)  | 6 (2%)   | 50          | 67 |
| 4   | ZH    | 321/323 (99%)  | 316 (98%)  | 5 (2%)   | 55          | 69 |
| 4   | ZI    | 321/323 (99%)  | 316 (98%)  | 5 (2%)   | 55          | 69 |
| 4   | ZJ    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | ZK    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | ZL    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | ZM    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | ZN    | 321/323 (99%)  | 317 (99%)  | 4 (1%)   | 63          | 73  |
| 4   | ZO    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | ZP    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | ZQ    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | ZR    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 85  |
| 4   | ZS    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 85  |
| 4   | ZT    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | ZU    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | ZV    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | ZW    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 85  |
| 4   | ZX    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | ZY    | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 4   | ZZ    | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 4   | Za    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 85  |
| 4   | Zb    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | Zc    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 76  |
| 4   | Zd    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 85  |
| 4   | Ze    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | Zf    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | Zg    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 85  |
| 4   | Zh    | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 5   | AA    | 190/193 (98%)  | 186 (98%)  | 4 (2%)   | 47          | 65  |
| 5   | AB    | 191/193 (99%)  | 186 (97%)  | 5 (3%)   | 40          | 61  |
| 5   | AC    | 192/193 (100%) | 191 (100%) | 1 (0%)   | 81          | 82  |
| 5   | AD    | 192/193 (100%) | 188 (98%)  | 4 (2%)   | 47          | 65  |
| 5   | AE    | 191/193 (99%)  | 186 (97%)  | 5 (3%)   | 40          | 61  |
| 6   | AO    | 141/467 (30%)  | 140 (99%)  | 1 (1%)   | 76          | 79  |
| 6   | AP    | 141/467 (30%)  | 140 (99%)  | 1 (1%)   | 76          | 79  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 6   | AQ    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AR    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AS    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AT    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AU    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AV    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AW    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AX    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AY    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | AZ    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Aa    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ac    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ad    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ae    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Af    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ag    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ah    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ai    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Aj    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ak    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Al    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Am    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | An    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ao    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | Ap    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BG    | 8/467 (2%)    | 7 (88%)   | 1 (12%)  | 4           | 19  |
| 6   | BH    | 11/467 (2%)   | 11 (100%) | 0        | 100         | 100 |
| 6   | BI    | 14/467 (3%)   | 12 (86%)  | 2 (14%)  | 3           | 16  |
| 6   | BJ    | 11/467 (2%)   | 11 (100%) | 0        | 100         | 100 |
| 6   | BK    | 15/467 (3%)   | 15 (100%) | 0        | 100         | 100 |
| 6   | BL    | 11/467 (2%)   | 11 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 6   | BM    | 15/467 (3%)   | 15 (100%) | 0        | 100         | 100 |
| 6   | BN    | 11/467 (2%)   | 11 (100%) | 0        | 100         | 100 |
| 6   | BO    | 14/467 (3%)   | 13 (93%)  | 1 (7%)   | 13          | 37  |
| 6   | BP    | 11/467 (2%)   | 11 (100%) | 0        | 100         | 100 |
| 6   | BQ    | 15/467 (3%)   | 14 (93%)  | 1 (7%)   | 15          | 39  |
| 6   | BR    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BS    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BT    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BU    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BV    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BW    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | BX    | 141/467 (30%) | 140 (99%) | 1 (1%)   | 76          | 79  |
| 6   | UI    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 47  |
| 6   | UJ    | 128/467 (27%) | 121 (94%) | 7 (6%)   | 19          | 44  |
| 6   | UK    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 47  |
| 6   | UL    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 47  |
| 6   | UM    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 47  |
| 6   | UN    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 47  |
| 6   | UO    | 128/467 (27%) | 122 (95%) | 6 (5%)   | 23          | 47  |
| 6   | UP    | 128/467 (27%) | 121 (94%) | 7 (6%)   | 19          | 44  |
| 6   | WA    | 95/467 (20%)  | 91 (96%)  | 4 (4%)   | 26          | 49  |
| 6   | WB    | 93/467 (20%)  | 86 (92%)  | 7 (8%)   | 12          | 35  |
| 6   | WC    | 91/467 (20%)  | 83 (91%)  | 8 (9%)   | 9           | 31  |
| 6   | WD    | 92/467 (20%)  | 88 (96%)  | 4 (4%)   | 26          | 49  |
| 6   | WE    | 94/467 (20%)  | 87 (93%)  | 7 (7%)   | 13          | 35  |
| 6   | WF    | 93/467 (20%)  | 84 (90%)  | 9 (10%)  | 8           | 27  |
| 6   | WG    | 94/467 (20%)  | 85 (90%)  | 9 (10%)  | 8           | 27  |
| 6   | WH    | 79/467 (17%)  | 75 (95%)  | 4 (5%)   | 21          | 45  |
| 6   | WI    | 79/467 (17%)  | 75 (95%)  | 4 (5%)   | 21          | 45  |
| 6   | WJ    | 83/467 (18%)  | 80 (96%)  | 3 (4%)   | 31          | 53  |
| 6   | WK    | 82/467 (18%)  | 76 (93%)  | 6 (7%)   | 13          | 36  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 6   | WL    | 69/467 (15%)  | 67 (97%)   | 2 (3%)   | 37          | 58  |
| 6   | WM    | 66/467 (14%)  | 64 (97%)   | 2 (3%)   | 36          | 57  |
| 6   | WN    | 68/467 (15%)  | 66 (97%)   | 2 (3%)   | 37          | 58  |
| 6   | WO    | 80/467 (17%)  | 76 (95%)   | 4 (5%)   | 22          | 45  |
| 6   | WP    | 83/467 (18%)  | 80 (96%)   | 3 (4%)   | 31          | 53  |
| 6   | WQ    | 93/467 (20%)  | 90 (97%)   | 3 (3%)   | 34          | 56  |
| 6   | WR    | 93/467 (20%)  | 85 (91%)   | 8 (9%)   | 10          | 32  |
| 6   | WS    | 93/467 (20%)  | 89 (96%)   | 4 (4%)   | 26          | 49  |
| 6   | WT    | 93/467 (20%)  | 86 (92%)   | 7 (8%)   | 12          | 35  |
| 6   | WU    | 94/467 (20%)  | 88 (94%)   | 6 (6%)   | 16          | 40  |
| 6   | WV    | 92/467 (20%)  | 82 (89%)   | 10 (11%) | 6           | 23  |
| 6   | WW    | 93/467 (20%)  | 85 (91%)   | 8 (9%)   | 10          | 32  |
| 7   | Ab    | 74/74 (100%)  | 67 (90%)   | 7 (10%)  | 8           | 27  |
| 7   | Aq    | 74/74 (100%)  | 72 (97%)   | 2 (3%)   | 39          | 60  |
| 7   | Ar    | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 7   | As    | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 8   | At    | 210/221 (95%) | 209 (100%) | 1 (0%)   | 81          | 82  |
| 9   | Au    | 177/204 (87%) | 174 (98%)  | 3 (2%)   | 53          | 68  |
| 9   | Av    | 179/204 (88%) | 175 (98%)  | 4 (2%)   | 45          | 64  |
| 9   | Aw    | 178/204 (87%) | 176 (99%)  | 2 (1%)   | 65          | 74  |
| 9   | Ax    | 178/204 (87%) | 174 (98%)  | 4 (2%)   | 45          | 64  |
| 9   | Ay    | 179/204 (88%) | 174 (97%)  | 5 (3%)   | 38          | 59  |
| 10  | A1    | 68/79 (86%)   | 65 (96%)   | 3 (4%)   | 25          | 48  |
| 10  | A2    | 70/79 (89%)   | 68 (97%)   | 2 (3%)   | 37          | 58  |
| 10  | A3    | 70/79 (89%)   | 66 (94%)   | 4 (6%)   | 18          | 43  |
| 10  | A4    | 70/79 (89%)   | 68 (97%)   | 2 (3%)   | 37          | 58  |
| 10  | A5    | 69/79 (87%)   | 63 (91%)   | 6 (9%)   | 9           | 31  |
| 10  | Az    | 45/79 (57%)   | 43 (96%)   | 2 (4%)   | 25          | 48  |
| 11  | A0    | 102/113 (90%) | 100 (98%)  | 2 (2%)   | 48          | 66  |
| 11  | A6    | 110/113 (97%) | 106 (96%)  | 4 (4%)   | 31          | 53  |
| 11  | A7    | 101/113 (89%) | 101 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 11  | A8    | 103/113 (91%)     | 98 (95%)    | 5 (5%)   | 22          | 46  |
| 11  | A9    | 104/113 (92%)     | 103 (99%)   | 1 (1%)   | 68          | 76  |
| 12  | BA    | 104/105 (99%)     | 104 (100%)  | 0        | 100         | 100 |
| 12  | BB    | 104/105 (99%)     | 100 (96%)   | 4 (4%)   | 29          | 51  |
| 12  | BC    | 104/105 (99%)     | 102 (98%)   | 2 (2%)   | 50          | 67  |
| 12  | BD    | 104/105 (99%)     | 100 (96%)   | 4 (4%)   | 29          | 51  |
| 12  | BE    | 103/105 (98%)     | 101 (98%)   | 2 (2%)   | 50          | 67  |
| 12  | BF    | 104/105 (99%)     | 102 (98%)   | 2 (2%)   | 50          | 67  |
| All | All   | 37084/66670 (56%) | 36199 (98%) | 885 (2%) | 43          | 63  |

All (885) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | GLN  |
| 1   | A     | 35  | THR  |
| 1   | A     | 46  | VAL  |
| 1   | A     | 58  | ILE  |
| 1   | A     | 85  | ASN  |
| 1   | A     | 106 | PHE  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 195 | VAL  |
| 1   | B     | 32  | GLN  |
| 1   | B     | 35  | THR  |
| 1   | B     | 46  | VAL  |
| 1   | B     | 58  | ILE  |
| 1   | B     | 85  | ASN  |
| 1   | B     | 106 | PHE  |
| 1   | B     | 113 | LEU  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 195 | VAL  |
| 1   | C     | 32  | GLN  |
| 1   | C     | 35  | THR  |
| 1   | C     | 46  | VAL  |
| 1   | C     | 58  | ILE  |
| 1   | C     | 85  | ASN  |
| 1   | C     | 106 | PHE  |
| 1   | C     | 113 | LEU  |
| 1   | C     | 133 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 195 | VAL  |
| 1   | D     | 32  | GLN  |
| 1   | D     | 35  | THR  |
| 1   | D     | 46  | VAL  |
| 1   | D     | 58  | ILE  |
| 1   | D     | 85  | ASN  |
| 1   | D     | 106 | PHE  |
| 1   | D     | 113 | LEU  |
| 1   | D     | 133 | ASN  |
| 1   | D     | 195 | VAL  |
| 1   | E     | 32  | GLN  |
| 1   | E     | 35  | THR  |
| 1   | E     | 46  | VAL  |
| 1   | E     | 58  | ILE  |
| 1   | E     | 85  | ASN  |
| 1   | E     | 106 | PHE  |
| 1   | E     | 113 | LEU  |
| 1   | E     | 133 | ASN  |
| 1   | E     | 195 | VAL  |
| 1   | F     | 32  | GLN  |
| 1   | F     | 35  | THR  |
| 1   | F     | 46  | VAL  |
| 1   | F     | 58  | ILE  |
| 1   | F     | 85  | ASN  |
| 1   | F     | 106 | PHE  |
| 1   | F     | 113 | LEU  |
| 1   | F     | 133 | ASN  |
| 1   | F     | 195 | VAL  |
| 1   | G     | 32  | GLN  |
| 1   | G     | 35  | THR  |
| 1   | G     | 46  | VAL  |
| 1   | G     | 58  | ILE  |
| 1   | G     | 85  | ASN  |
| 1   | G     | 106 | PHE  |
| 1   | G     | 113 | LEU  |
| 1   | G     | 133 | ASN  |
| 1   | G     | 195 | VAL  |
| 1   | H     | 32  | GLN  |
| 1   | H     | 35  | THR  |
| 1   | H     | 46  | VAL  |
| 1   | H     | 58  | ILE  |
| 1   | H     | 85  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 106 | PHE  |
| 1   | H     | 113 | LEU  |
| 1   | H     | 133 | ASN  |
| 1   | H     | 195 | VAL  |
| 1   | I     | 32  | GLN  |
| 1   | I     | 35  | THR  |
| 1   | I     | 46  | VAL  |
| 1   | I     | 58  | ILE  |
| 1   | I     | 85  | ASN  |
| 1   | I     | 106 | PHE  |
| 1   | I     | 113 | LEU  |
| 1   | I     | 133 | ASN  |
| 1   | I     | 195 | VAL  |
| 1   | J     | 32  | GLN  |
| 1   | J     | 35  | THR  |
| 1   | J     | 46  | VAL  |
| 1   | J     | 58  | ILE  |
| 1   | J     | 85  | ASN  |
| 1   | J     | 106 | PHE  |
| 1   | J     | 113 | LEU  |
| 1   | J     | 133 | ASN  |
| 1   | J     | 195 | VAL  |
| 1   | K     | 32  | GLN  |
| 1   | K     | 35  | THR  |
| 1   | K     | 46  | VAL  |
| 1   | K     | 58  | ILE  |
| 1   | K     | 85  | ASN  |
| 1   | K     | 106 | PHE  |
| 1   | K     | 113 | LEU  |
| 1   | K     | 133 | ASN  |
| 1   | K     | 195 | VAL  |
| 1   | L     | 32  | GLN  |
| 1   | L     | 35  | THR  |
| 1   | L     | 46  | VAL  |
| 1   | L     | 58  | ILE  |
| 1   | L     | 85  | ASN  |
| 1   | L     | 106 | PHE  |
| 1   | L     | 113 | LEU  |
| 1   | L     | 133 | ASN  |
| 1   | L     | 195 | VAL  |
| 1   | M     | 32  | GLN  |
| 1   | M     | 35  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 46  | VAL  |
| 1   | M     | 58  | ILE  |
| 1   | M     | 85  | ASN  |
| 1   | M     | 106 | PHE  |
| 1   | M     | 113 | LEU  |
| 1   | M     | 133 | ASN  |
| 1   | M     | 195 | VAL  |
| 1   | N     | 32  | GLN  |
| 1   | N     | 35  | THR  |
| 1   | N     | 46  | VAL  |
| 1   | N     | 58  | ILE  |
| 1   | N     | 85  | ASN  |
| 1   | N     | 106 | PHE  |
| 1   | N     | 113 | LEU  |
| 1   | N     | 133 | ASN  |
| 1   | N     | 195 | VAL  |
| 1   | O     | 32  | GLN  |
| 1   | O     | 35  | THR  |
| 1   | O     | 46  | VAL  |
| 1   | O     | 58  | ILE  |
| 1   | O     | 85  | ASN  |
| 1   | O     | 106 | PHE  |
| 1   | O     | 113 | LEU  |
| 1   | O     | 133 | ASN  |
| 1   | O     | 195 | VAL  |
| 1   | P     | 32  | GLN  |
| 1   | P     | 35  | THR  |
| 1   | P     | 46  | VAL  |
| 1   | P     | 58  | ILE  |
| 1   | P     | 85  | ASN  |
| 1   | P     | 106 | PHE  |
| 1   | P     | 113 | LEU  |
| 1   | P     | 133 | ASN  |
| 1   | P     | 195 | VAL  |
| 1   | Q     | 32  | GLN  |
| 1   | Q     | 35  | THR  |
| 1   | Q     | 46  | VAL  |
| 1   | Q     | 58  | ILE  |
| 1   | Q     | 85  | ASN  |
| 1   | Q     | 106 | PHE  |
| 1   | Q     | 113 | LEU  |
| 1   | Q     | 133 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 195 | VAL  |
| 1   | R     | 32  | GLN  |
| 1   | R     | 35  | THR  |
| 1   | R     | 46  | VAL  |
| 1   | R     | 58  | ILE  |
| 1   | R     | 85  | ASN  |
| 1   | R     | 106 | PHE  |
| 1   | R     | 113 | LEU  |
| 1   | R     | 133 | ASN  |
| 1   | R     | 195 | VAL  |
| 1   | S     | 32  | GLN  |
| 1   | S     | 35  | THR  |
| 1   | S     | 46  | VAL  |
| 1   | S     | 58  | ILE  |
| 1   | S     | 85  | ASN  |
| 1   | S     | 106 | PHE  |
| 1   | S     | 113 | LEU  |
| 1   | S     | 133 | ASN  |
| 1   | S     | 195 | VAL  |
| 1   | T     | 32  | GLN  |
| 1   | T     | 35  | THR  |
| 1   | T     | 46  | VAL  |
| 1   | T     | 58  | ILE  |
| 1   | T     | 85  | ASN  |
| 1   | T     | 106 | PHE  |
| 1   | T     | 113 | LEU  |
| 1   | T     | 133 | ASN  |
| 1   | T     | 195 | VAL  |
| 1   | U     | 32  | GLN  |
| 1   | U     | 35  | THR  |
| 1   | U     | 46  | VAL  |
| 1   | U     | 58  | ILE  |
| 1   | U     | 85  | ASN  |
| 1   | U     | 106 | PHE  |
| 1   | U     | 113 | LEU  |
| 1   | U     | 133 | ASN  |
| 1   | U     | 195 | VAL  |
| 1   | V     | 32  | GLN  |
| 1   | V     | 35  | THR  |
| 1   | V     | 46  | VAL  |
| 1   | V     | 58  | ILE  |
| 1   | V     | 85  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 106 | PHE  |
| 1   | V     | 113 | LEU  |
| 1   | V     | 133 | ASN  |
| 1   | V     | 195 | VAL  |
| 1   | W     | 32  | GLN  |
| 1   | W     | 35  | THR  |
| 1   | W     | 46  | VAL  |
| 1   | W     | 58  | ILE  |
| 1   | W     | 85  | ASN  |
| 1   | W     | 106 | PHE  |
| 1   | W     | 113 | LEU  |
| 1   | W     | 133 | ASN  |
| 1   | W     | 195 | VAL  |
| 1   | X     | 32  | GLN  |
| 1   | X     | 35  | THR  |
| 1   | X     | 46  | VAL  |
| 1   | X     | 58  | ILE  |
| 1   | X     | 85  | ASN  |
| 1   | X     | 106 | PHE  |
| 1   | X     | 113 | LEU  |
| 1   | X     | 133 | ASN  |
| 1   | X     | 195 | VAL  |
| 1   | Y     | 32  | GLN  |
| 1   | Y     | 35  | THR  |
| 1   | Y     | 46  | VAL  |
| 1   | Y     | 58  | ILE  |
| 1   | Y     | 85  | ASN  |
| 1   | Y     | 106 | PHE  |
| 1   | Y     | 113 | LEU  |
| 1   | Y     | 133 | ASN  |
| 1   | Y     | 195 | VAL  |
| 1   | Z     | 32  | GLN  |
| 1   | Z     | 35  | THR  |
| 1   | Z     | 46  | VAL  |
| 1   | Z     | 58  | ILE  |
| 1   | Z     | 85  | ASN  |
| 1   | Z     | 106 | PHE  |
| 1   | Z     | 113 | LEU  |
| 1   | Z     | 133 | ASN  |
| 1   | Z     | 195 | VAL  |
| 2   | a     | 20  | GLU  |
| 2   | a     | 110 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | a     | 114 | LYS  |
| 2   | a     | 192 | GLU  |
| 2   | a     | 199 | GLN  |
| 2   | a     | 244 | VAL  |
| 2   | a     | 248 | PRO  |
| 2   | b     | 20  | GLU  |
| 2   | b     | 110 | MET  |
| 2   | b     | 114 | LYS  |
| 2   | b     | 192 | GLU  |
| 2   | b     | 199 | GLN  |
| 2   | b     | 244 | VAL  |
| 2   | b     | 248 | PRO  |
| 2   | c     | 20  | GLU  |
| 2   | c     | 110 | MET  |
| 2   | c     | 114 | LYS  |
| 2   | c     | 192 | GLU  |
| 2   | c     | 199 | GLN  |
| 2   | c     | 244 | VAL  |
| 2   | c     | 248 | PRO  |
| 2   | d     | 20  | GLU  |
| 2   | d     | 110 | MET  |
| 2   | d     | 114 | LYS  |
| 2   | d     | 192 | GLU  |
| 2   | d     | 199 | GLN  |
| 2   | d     | 244 | VAL  |
| 2   | d     | 248 | PRO  |
| 2   | e     | 20  | GLU  |
| 2   | e     | 110 | MET  |
| 2   | e     | 114 | LYS  |
| 2   | e     | 192 | GLU  |
| 2   | e     | 199 | GLN  |
| 2   | e     | 244 | VAL  |
| 2   | e     | 248 | PRO  |
| 2   | f     | 20  | GLU  |
| 2   | f     | 110 | MET  |
| 2   | f     | 114 | LYS  |
| 2   | f     | 192 | GLU  |
| 2   | f     | 199 | GLN  |
| 2   | f     | 244 | VAL  |
| 2   | f     | 248 | PRO  |
| 2   | g     | 20  | GLU  |
| 2   | g     | 110 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | g     | 114 | LYS  |
| 2   | g     | 192 | GLU  |
| 2   | g     | 199 | GLN  |
| 2   | g     | 244 | VAL  |
| 2   | g     | 248 | PRO  |
| 2   | h     | 20  | GLU  |
| 2   | h     | 110 | MET  |
| 2   | h     | 114 | LYS  |
| 2   | h     | 192 | GLU  |
| 2   | h     | 199 | GLN  |
| 2   | h     | 244 | VAL  |
| 2   | h     | 248 | PRO  |
| 2   | i     | 20  | GLU  |
| 2   | i     | 110 | MET  |
| 2   | i     | 114 | LYS  |
| 2   | i     | 192 | GLU  |
| 2   | i     | 199 | GLN  |
| 2   | i     | 244 | VAL  |
| 2   | i     | 248 | PRO  |
| 2   | j     | 20  | GLU  |
| 2   | j     | 110 | MET  |
| 2   | j     | 114 | LYS  |
| 2   | j     | 192 | GLU  |
| 2   | j     | 199 | GLN  |
| 2   | j     | 244 | VAL  |
| 2   | j     | 248 | PRO  |
| 2   | k     | 20  | GLU  |
| 2   | k     | 110 | MET  |
| 2   | k     | 114 | LYS  |
| 2   | k     | 192 | GLU  |
| 2   | k     | 199 | GLN  |
| 2   | k     | 244 | VAL  |
| 2   | k     | 248 | PRO  |
| 2   | l     | 20  | GLU  |
| 2   | l     | 110 | MET  |
| 2   | l     | 114 | LYS  |
| 2   | l     | 192 | GLU  |
| 2   | l     | 199 | GLN  |
| 2   | l     | 244 | VAL  |
| 2   | l     | 248 | PRO  |
| 2   | m     | 20  | GLU  |
| 2   | m     | 110 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | m     | 114 | LYS  |
| 2   | m     | 192 | GLU  |
| 2   | m     | 199 | GLN  |
| 2   | m     | 244 | VAL  |
| 2   | m     | 248 | PRO  |
| 2   | n     | 20  | GLU  |
| 2   | n     | 110 | MET  |
| 2   | n     | 114 | LYS  |
| 2   | n     | 192 | GLU  |
| 2   | n     | 199 | GLN  |
| 2   | n     | 244 | VAL  |
| 2   | n     | 248 | PRO  |
| 2   | o     | 20  | GLU  |
| 2   | o     | 110 | MET  |
| 2   | o     | 114 | LYS  |
| 2   | o     | 192 | GLU  |
| 2   | o     | 199 | GLN  |
| 2   | o     | 244 | VAL  |
| 2   | o     | 248 | PRO  |
| 2   | p     | 20  | GLU  |
| 2   | p     | 110 | MET  |
| 2   | p     | 114 | LYS  |
| 2   | p     | 192 | GLU  |
| 2   | p     | 199 | GLN  |
| 2   | p     | 244 | VAL  |
| 2   | p     | 248 | PRO  |
| 2   | q     | 20  | GLU  |
| 2   | q     | 110 | MET  |
| 2   | q     | 114 | LYS  |
| 2   | q     | 192 | GLU  |
| 2   | q     | 199 | GLN  |
| 2   | q     | 244 | VAL  |
| 2   | q     | 248 | PRO  |
| 2   | r     | 20  | GLU  |
| 2   | r     | 110 | MET  |
| 2   | r     | 114 | LYS  |
| 2   | r     | 192 | GLU  |
| 2   | r     | 199 | GLN  |
| 2   | r     | 244 | VAL  |
| 2   | r     | 248 | PRO  |
| 2   | s     | 20  | GLU  |
| 2   | s     | 110 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | s     | 114 | LYS  |
| 2   | s     | 192 | GLU  |
| 2   | s     | 199 | GLN  |
| 2   | s     | 244 | VAL  |
| 2   | s     | 248 | PRO  |
| 2   | t     | 20  | GLU  |
| 2   | t     | 110 | MET  |
| 2   | t     | 114 | LYS  |
| 2   | t     | 192 | GLU  |
| 2   | t     | 199 | GLN  |
| 2   | t     | 244 | VAL  |
| 2   | t     | 248 | PRO  |
| 2   | u     | 20  | GLU  |
| 2   | u     | 110 | MET  |
| 2   | u     | 114 | LYS  |
| 2   | u     | 192 | GLU  |
| 2   | u     | 199 | GLN  |
| 2   | u     | 244 | VAL  |
| 2   | u     | 248 | PRO  |
| 2   | v     | 20  | GLU  |
| 2   | v     | 110 | MET  |
| 2   | v     | 114 | LYS  |
| 2   | v     | 192 | GLU  |
| 2   | v     | 199 | GLN  |
| 2   | v     | 244 | VAL  |
| 2   | v     | 248 | PRO  |
| 2   | w     | 20  | GLU  |
| 2   | w     | 110 | MET  |
| 2   | w     | 114 | LYS  |
| 2   | w     | 192 | GLU  |
| 2   | w     | 199 | GLN  |
| 2   | w     | 244 | VAL  |
| 2   | w     | 248 | PRO  |
| 2   | x     | 20  | GLU  |
| 2   | x     | 110 | MET  |
| 2   | x     | 114 | LYS  |
| 2   | x     | 192 | GLU  |
| 2   | x     | 199 | GLN  |
| 2   | x     | 244 | VAL  |
| 2   | x     | 248 | PRO  |
| 2   | y     | 20  | GLU  |
| 2   | y     | 110 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | y     | 114 | LYS  |
| 2   | y     | 192 | GLU  |
| 2   | y     | 199 | GLN  |
| 2   | y     | 244 | VAL  |
| 2   | y     | 248 | PRO  |
| 2   | z     | 20  | GLU  |
| 2   | z     | 110 | MET  |
| 2   | z     | 114 | LYS  |
| 2   | z     | 192 | GLU  |
| 2   | z     | 199 | GLN  |
| 2   | z     | 244 | VAL  |
| 2   | z     | 248 | PRO  |
| 3   | 0     | 1   | MET  |
| 3   | 0     | 9   | LYS  |
| 3   | 0     | 36  | ARG  |
| 3   | 0     | 50  | ARG  |
| 3   | 0     | 52  | PRO  |
| 3   | 0     | 73  | ARG  |
| 3   | 1     | 1   | MET  |
| 3   | 1     | 42  | GLU  |
| 3   | 1     | 75  | VAL  |
| 3   | 2     | 179 | MET  |
| 3   | 3     | 43  | ASP  |
| 3   | 4     | 2   | ILE  |
| 3   | 4     | 137 | GLN  |
| 3   | 4     | 209 | ASN  |
| 3   | 5     | 73  | ARG  |
| 3   | 5     | 85  | ASN  |
| 3   | 5     | 109 | ASP  |
| 3   | 5     | 245 | LYS  |
| 3   | 6     | 59  | GLN  |
| 3   | 6     | 78  | GLU  |
| 3   | 6     | 203 | GLU  |
| 3   | 7     | 59  | GLN  |
| 3   | 8     | 17  | THR  |
| 3   | 8     | 58  | GLU  |
| 3   | 8     | 100 | GLN  |
| 3   | 8     | 194 | GLU  |
| 3   | 8     | 195 | THR  |
| 3   | 8     | 256 | LYS  |
| 3   | 9     | 66  | LEU  |
| 3   | 9     | 226 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | ZA    | 50  | ARG  |
| 3   | ZB    | 95  | VAL  |
| 3   | ZB    | 100 | GLN  |
| 3   | ZC    | 43  | ASP  |
| 3   | ZC    | 249 | THR  |
| 3   | ZC    | 260 | LEU  |
| 3   | ZD    | 1   | MET  |
| 3   | ZD    | 2   | ILE  |
| 3   | ZD    | 142 | ILE  |
| 3   | ZD    | 162 | GLN  |
| 3   | ZD    | 196 | GLN  |
| 3   | ZD    | 233 | MET  |
| 3   | ZD    | 238 | ARG  |
| 3   | ZE    | 37  | GLN  |
| 3   | ZE    | 50  | ARG  |
| 3   | ZE    | 121 | GLN  |
| 3   | ZE    | 137 | GLN  |
| 3   | ZE    | 141 | THR  |
| 4   | ZF    | 134 | PRO  |
| 4   | ZF    | 154 | MET  |
| 4   | ZF    | 229 | THR  |
| 4   | ZF    | 352 | ASN  |
| 4   | ZF    | 355 | LYS  |
| 4   | ZF    | 392 | GLN  |
| 4   | ZG    | 3   | PHE  |
| 4   | ZG    | 103 | ASP  |
| 4   | ZG    | 104 | GLU  |
| 4   | ZG    | 234 | GLU  |
| 4   | ZG    | 332 | ASN  |
| 4   | ZG    | 395 | ILE  |
| 4   | ZH    | 71  | ARG  |
| 4   | ZH    | 128 | ILE  |
| 4   | ZH    | 288 | ASP  |
| 4   | ZH    | 355 | LYS  |
| 4   | ZH    | 399 | LEU  |
| 4   | ZI    | 52  | VAL  |
| 4   | ZI    | 99  | GLN  |
| 4   | ZI    | 105 | ASN  |
| 4   | ZI    | 288 | ASP  |
| 4   | ZI    | 352 | ASN  |
| 4   | ZJ    | 53  | LYS  |
| 4   | ZJ    | 96  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZJ    | 395 | ILE  |
| 4   | ZK    | 134 | PRO  |
| 4   | ZK    | 338 | GLN  |
| 4   | ZL    | 338 | GLN  |
| 4   | ZL    | 368 | LEU  |
| 4   | ZL    | 370 | LYS  |
| 4   | ZM    | 89  | ASN  |
| 4   | ZM    | 156 | ILE  |
| 4   | ZM    | 369 | SER  |
| 4   | ZN    | 240 | SER  |
| 4   | ZN    | 379 | GLN  |
| 4   | ZN    | 396 | LEU  |
| 4   | ZN    | 402 | LEU  |
| 4   | ZO    | 141 | ASN  |
| 4   | ZO    | 235 | ASN  |
| 4   | ZO    | 237 | ILE  |
| 4   | ZP    | 333 | VAL  |
| 4   | ZP    | 369 | SER  |
| 4   | ZP    | 370 | LYS  |
| 4   | ZQ    | 367 | ASP  |
| 4   | ZQ    | 370 | LYS  |
| 4   | ZR    | 156 | ILE  |
| 4   | ZS    | 367 | ASP  |
| 4   | ZT    | 5   | GLN  |
| 4   | ZT    | 73  | LEU  |
| 4   | ZT    | 133 | ASN  |
| 4   | ZU    | 237 | ILE  |
| 4   | ZU    | 337 | THR  |
| 4   | ZU    | 380 | ARG  |
| 4   | ZV    | 397 | ASN  |
| 4   | ZV    | 399 | LEU  |
| 4   | ZW    | 42  | MET  |
| 4   | ZX    | 63  | ASP  |
| 4   | ZX    | 195 | ASP  |
| 4   | Za    | 96  | ARG  |
| 4   | Zb    | 36  | THR  |
| 4   | Zb    | 89  | ASN  |
| 4   | Zb    | 331 | ASP  |
| 4   | Zc    | 369 | SER  |
| 4   | Zc    | 370 | LYS  |
| 4   | Zc    | 399 | LEU  |
| 4   | Zd    | 397 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Ze    | 96  | ARG  |
| 4   | Ze    | 395 | ILE  |
| 4   | Zf    | 395 | ILE  |
| 4   | Zf    | 396 | LEU  |
| 4   | Zg    | 375 | MET  |
| 5   | AA    | 37  | GLN  |
| 5   | AA    | 39  | ASN  |
| 5   | AA    | 123 | GLU  |
| 5   | AA    | 247 | LEU  |
| 5   | AB    | 49  | LEU  |
| 5   | AB    | 53  | THR  |
| 5   | AB    | 153 | ASN  |
| 5   | AB    | 201 | ILE  |
| 5   | AB    | 225 | ARG  |
| 5   | AC    | 184 | GLU  |
| 5   | AD    | 47  | ASP  |
| 5   | AD    | 49  | LEU  |
| 5   | AD    | 160 | ARG  |
| 5   | AD    | 189 | ARG  |
| 5   | AE    | 51  | LEU  |
| 5   | AE    | 146 | LEU  |
| 5   | AE    | 155 | VAL  |
| 5   | AE    | 163 | LEU  |
| 5   | AE    | 235 | THR  |
| 3   | AF    | 36  | ARG  |
| 3   | AF    | 256 | LYS  |
| 3   | AG    | 6   | TRP  |
| 3   | AG    | 16  | GLN  |
| 3   | AG    | 17  | THR  |
| 3   | AG    | 128 | LEU  |
| 3   | AG    | 137 | GLN  |
| 3   | AG    | 138 | PRO  |
| 3   | AG    | 251 | ASP  |
| 3   | AG    | 257 | LEU  |
| 3   | AH    | 1   | MET  |
| 3   | AH    | 66  | LEU  |
| 3   | AH    | 100 | GLN  |
| 3   | AH    | 135 | GLN  |
| 3   | AH    | 179 | MET  |
| 3   | AH    | 195 | THR  |
| 3   | AH    | 208 | LEU  |
| 3   | AI    | 4   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AI    | 61  | THR  |
| 3   | AI    | 173 | LEU  |
| 3   | AI    | 179 | MET  |
| 3   | AI    | 194 | GLU  |
| 3   | AI    | 195 | THR  |
| 3   | AJ    | 73  | ARG  |
| 3   | AJ    | 127 | GLN  |
| 3   | AJ    | 140 | ILE  |
| 3   | AJ    | 161 | GLN  |
| 3   | AJ    | 198 | SER  |
| 3   | AJ    | 206 | PRO  |
| 3   | AK    | 5   | LEU  |
| 3   | AK    | 100 | GLN  |
| 3   | AK    | 137 | GLN  |
| 3   | AK    | 203 | GLU  |
| 3   | AL    | 1   | MET  |
| 3   | AL    | 73  | ARG  |
| 3   | AL    | 170 | VAL  |
| 3   | AM    | 1   | MET  |
| 3   | AM    | 36  | ARG  |
| 3   | AM    | 50  | ARG  |
| 3   | AM    | 208 | LEU  |
| 3   | AM    | 209 | ASN  |
| 3   | AN    | 1   | MET  |
| 3   | AN    | 3   | SER  |
| 3   | AN    | 179 | MET  |
| 3   | AN    | 252 | GLN  |
| 6   | AR    | 295 | SER  |
| 6   | AS    | 295 | SER  |
| 6   | AT    | 295 | SER  |
| 6   | AU    | 295 | SER  |
| 6   | AV    | 295 | SER  |
| 6   | AW    | 295 | SER  |
| 6   | AX    | 295 | SER  |
| 6   | AY    | 295 | SER  |
| 6   | AZ    | 295 | SER  |
| 6   | Aa    | 295 | SER  |
| 7   | Ab    | 7   | MET  |
| 7   | Ab    | 15  | LYS  |
| 7   | Ab    | 69  | MET  |
| 7   | Ab    | 73  | LEU  |
| 7   | Ab    | 75  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Ab    | 85  | PRO  |
| 7   | Ab    | 87  | ILE  |
| 6   | Ac    | 295 | SER  |
| 6   | Ad    | 295 | SER  |
| 6   | Ae    | 295 | SER  |
| 6   | Af    | 295 | SER  |
| 6   | Ag    | 295 | SER  |
| 6   | Ah    | 295 | SER  |
| 6   | Ai    | 295 | SER  |
| 6   | Aj    | 295 | SER  |
| 6   | Ak    | 295 | SER  |
| 6   | Al    | 295 | SER  |
| 6   | Am    | 295 | SER  |
| 6   | An    | 295 | SER  |
| 6   | Ao    | 295 | SER  |
| 6   | Ap    | 295 | SER  |
| 6   | AO    | 295 | SER  |
| 6   | AP    | 295 | SER  |
| 6   | AQ    | 295 | SER  |
| 7   | Aq    | 2   | THR  |
| 7   | Aq    | 6   | VAL  |
| 8   | At    | 214 | PHE  |
| 9   | Au    | 160 | GLN  |
| 9   | Au    | 190 | PHE  |
| 9   | Au    | 217 | ILE  |
| 9   | Av    | 48  | ILE  |
| 9   | Av    | 140 | ARG  |
| 9   | Av    | 160 | GLN  |
| 9   | Av    | 162 | PRO  |
| 9   | Aw    | 135 | ARG  |
| 9   | Aw    | 152 | ARG  |
| 9   | Ax    | 125 | GLU  |
| 9   | Ax    | 152 | ARG  |
| 9   | Ax    | 187 | PHE  |
| 9   | Ax    | 241 | GLN  |
| 9   | Ay    | 65  | THR  |
| 9   | Ay    | 67  | ILE  |
| 9   | Ay    | 140 | ARG  |
| 9   | Ay    | 144 | GLU  |
| 9   | Ay    | 230 | ASP  |
| 10  | Az    | 15  | GLN  |
| 10  | Az    | 19  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A1    | 13  | GLN  |
| 10  | A1    | 15  | GLN  |
| 10  | A1    | 33  | SER  |
| 10  | A2    | 7   | ILE  |
| 10  | A2    | 11  | ILE  |
| 10  | A3    | 5   | GLN  |
| 10  | A3    | 15  | GLN  |
| 10  | A3    | 19  | MET  |
| 10  | A3    | 97  | GLN  |
| 10  | A4    | 15  | GLN  |
| 10  | A4    | 19  | MET  |
| 10  | A5    | 8   | GLU  |
| 10  | A5    | 15  | GLN  |
| 10  | A5    | 19  | MET  |
| 10  | A5    | 57  | GLU  |
| 10  | A5    | 91  | LYS  |
| 10  | A5    | 102 | MET  |
| 11  | A6    | 53  | MET  |
| 11  | A6    | 60  | THR  |
| 11  | A6    | 101 | ASP  |
| 11  | A6    | 125 | SER  |
| 11  | A8    | 5   | LEU  |
| 11  | A8    | 65  | LEU  |
| 11  | A8    | 69  | SER  |
| 11  | A8    | 71  | HIS  |
| 11  | A8    | 72  | HIS  |
| 11  | A9    | 76  | GLN  |
| 11  | A0    | 65  | LEU  |
| 11  | A0    | 104 | ARG  |
| 6   | UI    | 98  | LEU  |
| 6   | UI    | 127 | SER  |
| 6   | UI    | 154 | ARG  |
| 6   | UI    | 159 | MET  |
| 6   | UI    | 165 | PHE  |
| 6   | UI    | 219 | LEU  |
| 6   | UJ    | 98  | LEU  |
| 6   | UJ    | 103 | GLN  |
| 6   | UJ    | 127 | SER  |
| 6   | UJ    | 154 | ARG  |
| 6   | UJ    | 159 | MET  |
| 6   | UJ    | 165 | PHE  |
| 6   | UJ    | 268 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | UK    | 98  | LEU  |
| 6   | UK    | 127 | SER  |
| 6   | UK    | 154 | ARG  |
| 6   | UK    | 159 | MET  |
| 6   | UK    | 165 | PHE  |
| 6   | UK    | 219 | LEU  |
| 6   | UL    | 98  | LEU  |
| 6   | UL    | 127 | SER  |
| 6   | UL    | 154 | ARG  |
| 6   | UL    | 159 | MET  |
| 6   | UL    | 167 | ARG  |
| 6   | UL    | 219 | LEU  |
| 6   | UM    | 98  | LEU  |
| 6   | UM    | 127 | SER  |
| 6   | UM    | 154 | ARG  |
| 6   | UM    | 159 | MET  |
| 6   | UM    | 165 | PHE  |
| 6   | UM    | 219 | LEU  |
| 6   | UN    | 98  | LEU  |
| 6   | UN    | 127 | SER  |
| 6   | UN    | 154 | ARG  |
| 6   | UN    | 159 | MET  |
| 6   | UN    | 165 | PHE  |
| 6   | UN    | 219 | LEU  |
| 6   | UO    | 98  | LEU  |
| 6   | UO    | 127 | SER  |
| 6   | UO    | 154 | ARG  |
| 6   | UO    | 159 | MET  |
| 6   | UO    | 165 | PHE  |
| 6   | UO    | 219 | LEU  |
| 6   | UP    | 98  | LEU  |
| 6   | UP    | 127 | SER  |
| 6   | UP    | 154 | ARG  |
| 6   | UP    | 159 | MET  |
| 6   | UP    | 165 | PHE  |
| 6   | UP    | 167 | ARG  |
| 6   | UP    | 219 | LEU  |
| 12  | BB    | 3   | LEU  |
| 12  | BB    | 46  | GLN  |
| 12  | BB    | 84  | LEU  |
| 12  | BB    | 126 | MET  |
| 6   | WA    | 114 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | WA    | 123 | ILE  |
| 6   | WA    | 167 | ARG  |
| 6   | WA    | 170 | LYS  |
| 6   | WB    | 119 | GLU  |
| 6   | WB    | 120 | LYS  |
| 6   | WB    | 137 | GLU  |
| 6   | WB    | 159 | MET  |
| 6   | WB    | 164 | LEU  |
| 6   | WB    | 166 | VAL  |
| 6   | WB    | 169 | GLN  |
| 6   | WC    | 115 | LEU  |
| 6   | WC    | 120 | LYS  |
| 6   | WC    | 128 | GLU  |
| 6   | WC    | 134 | ARG  |
| 6   | WC    | 164 | LEU  |
| 6   | WC    | 166 | VAL  |
| 6   | WC    | 168 | GLU  |
| 6   | WC    | 170 | LYS  |
| 6   | WD    | 114 | GLU  |
| 6   | WD    | 115 | LEU  |
| 6   | WD    | 159 | MET  |
| 6   | WD    | 167 | ARG  |
| 6   | WE    | 114 | GLU  |
| 6   | WE    | 123 | ILE  |
| 6   | WE    | 128 | GLU  |
| 6   | WE    | 134 | ARG  |
| 6   | WE    | 160 | PRO  |
| 6   | WE    | 161 | LYS  |
| 6   | WE    | 164 | LEU  |
| 6   | WF    | 111 | VAL  |
| 6   | WF    | 113 | PHE  |
| 6   | WF    | 123 | ILE  |
| 6   | WF    | 134 | ARG  |
| 6   | WF    | 142 | ARG  |
| 6   | WF    | 159 | MET  |
| 6   | WF    | 161 | LYS  |
| 6   | WF    | 162 | PRO  |
| 6   | WF    | 166 | VAL  |
| 6   | WG    | 111 | VAL  |
| 6   | WG    | 114 | GLU  |
| 6   | WG    | 115 | LEU  |
| 6   | WG    | 120 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | WG    | 129 | GLN  |
| 6   | WG    | 134 | ARG  |
| 6   | WG    | 164 | LEU  |
| 6   | WG    | 170 | LYS  |
| 6   | WG    | 190 | GLN  |
| 6   | WH    | 134 | ARG  |
| 6   | WH    | 159 | MET  |
| 6   | WH    | 168 | GLU  |
| 6   | WH    | 221 | THR  |
| 6   | WI    | 165 | PHE  |
| 6   | WI    | 168 | GLU  |
| 6   | WI    | 169 | GLN  |
| 6   | WI    | 170 | LYS  |
| 6   | WJ    | 123 | ILE  |
| 6   | WJ    | 167 | ARG  |
| 6   | WJ    | 169 | GLN  |
| 6   | WK    | 129 | GLN  |
| 6   | WK    | 164 | LEU  |
| 6   | WK    | 165 | PHE  |
| 6   | WK    | 167 | ARG  |
| 6   | WK    | 170 | LYS  |
| 6   | WK    | 187 | ASP  |
| 6   | WL    | 159 | MET  |
| 6   | WL    | 221 | THR  |
| 6   | WM    | 159 | MET  |
| 6   | WM    | 221 | THR  |
| 6   | WN    | 159 | MET  |
| 6   | WN    | 221 | THR  |
| 6   | WO    | 159 | MET  |
| 6   | WO    | 169 | GLN  |
| 6   | WO    | 170 | LYS  |
| 6   | WO    | 221 | THR  |
| 6   | WP    | 154 | ARG  |
| 6   | WP    | 161 | LYS  |
| 6   | WP    | 165 | PHE  |
| 6   | WQ    | 114 | GLU  |
| 6   | WQ    | 134 | ARG  |
| 6   | WQ    | 159 | MET  |
| 6   | WR    | 114 | GLU  |
| 6   | WR    | 117 | ASP  |
| 6   | WR    | 128 | GLU  |
| 6   | WR    | 129 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | WR    | 164 | LEU  |
| 6   | WR    | 166 | VAL  |
| 6   | WR    | 169 | GLN  |
| 6   | WR    | 170 | LYS  |
| 6   | WS    | 114 | GLU  |
| 6   | WS    | 134 | ARG  |
| 6   | WS    | 159 | MET  |
| 6   | WS    | 221 | THR  |
| 6   | WT    | 119 | GLU  |
| 6   | WT    | 123 | ILE  |
| 6   | WT    | 134 | ARG  |
| 6   | WT    | 159 | MET  |
| 6   | WT    | 161 | LYS  |
| 6   | WT    | 165 | PHE  |
| 6   | WT    | 167 | ARG  |
| 6   | WU    | 114 | GLU  |
| 6   | WU    | 123 | ILE  |
| 6   | WU    | 134 | ARG  |
| 6   | WU    | 159 | MET  |
| 6   | WU    | 161 | LYS  |
| 6   | WU    | 164 | LEU  |
| 6   | WV    | 114 | GLU  |
| 6   | WV    | 120 | LYS  |
| 6   | WV    | 128 | GLU  |
| 6   | WV    | 129 | GLN  |
| 6   | WV    | 134 | ARG  |
| 6   | WV    | 164 | LEU  |
| 6   | WV    | 166 | VAL  |
| 6   | WV    | 169 | GLN  |
| 6   | WV    | 170 | LYS  |
| 6   | WV    | 187 | ASP  |
| 6   | WW    | 114 | GLU  |
| 6   | WW    | 115 | LEU  |
| 6   | WW    | 134 | ARG  |
| 6   | WW    | 159 | MET  |
| 6   | WW    | 167 | ARG  |
| 6   | WW    | 168 | GLU  |
| 6   | WW    | 169 | GLN  |
| 6   | WW    | 221 | THR  |
| 12  | BC    | 119 | LEU  |
| 12  | BC    | 128 | LYS  |
| 12  | BD    | 3   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | BD    | 4   | LEU  |
| 12  | BD    | 75  | LYS  |
| 12  | BD    | 101 | GLU  |
| 12  | BE    | 6   | ILE  |
| 12  | BE    | 127 | LEU  |
| 12  | BF    | 38  | ASP  |
| 12  | BF    | 123 | LYS  |
| 6   | BG    | 322 | PRO  |
| 6   | BI    | 318 | ASN  |
| 6   | BI    | 319 | GLN  |
| 6   | BO    | 319 | GLN  |
| 6   | BQ    | 318 | ASN  |
| 6   | BR    | 295 | SER  |
| 6   | BS    | 295 | SER  |
| 6   | BT    | 295 | SER  |
| 6   | BU    | 295 | SER  |
| 6   | BV    | 295 | SER  |
| 6   | BW    | 295 | SER  |
| 6   | BX    | 295 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1360) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | GLN  |
| 1   | A     | 130 | ASN  |
| 1   | A     | 142 | ASN  |
| 1   | A     | 160 | ASN  |
| 1   | A     | 173 | GLN  |
| 1   | A     | 214 | ASN  |
| 1   | A     | 217 | GLN  |
| 1   | A     | 223 | GLN  |
| 1   | B     | 83  | GLN  |
| 1   | B     | 130 | ASN  |
| 1   | B     | 142 | ASN  |
| 1   | B     | 160 | ASN  |
| 1   | B     | 173 | GLN  |
| 1   | B     | 214 | ASN  |
| 1   | B     | 217 | GLN  |
| 1   | B     | 223 | GLN  |
| 1   | C     | 83  | GLN  |
| 1   | C     | 130 | ASN  |
| 1   | C     | 142 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 160 | ASN  |
| 1   | C     | 173 | GLN  |
| 1   | C     | 214 | ASN  |
| 1   | C     | 217 | GLN  |
| 1   | C     | 223 | GLN  |
| 1   | D     | 83  | GLN  |
| 1   | D     | 130 | ASN  |
| 1   | D     | 142 | ASN  |
| 1   | D     | 160 | ASN  |
| 1   | D     | 173 | GLN  |
| 1   | D     | 214 | ASN  |
| 1   | D     | 217 | GLN  |
| 1   | D     | 223 | GLN  |
| 1   | E     | 83  | GLN  |
| 1   | E     | 130 | ASN  |
| 1   | E     | 142 | ASN  |
| 1   | E     | 173 | GLN  |
| 1   | E     | 214 | ASN  |
| 1   | E     | 217 | GLN  |
| 1   | E     | 223 | GLN  |
| 1   | F     | 83  | GLN  |
| 1   | F     | 130 | ASN  |
| 1   | F     | 142 | ASN  |
| 1   | F     | 160 | ASN  |
| 1   | F     | 173 | GLN  |
| 1   | F     | 214 | ASN  |
| 1   | F     | 217 | GLN  |
| 1   | F     | 223 | GLN  |
| 1   | G     | 83  | GLN  |
| 1   | G     | 130 | ASN  |
| 1   | G     | 142 | ASN  |
| 1   | G     | 160 | ASN  |
| 1   | G     | 173 | GLN  |
| 1   | G     | 214 | ASN  |
| 1   | G     | 217 | GLN  |
| 1   | G     | 223 | GLN  |
| 1   | H     | 83  | GLN  |
| 1   | H     | 130 | ASN  |
| 1   | H     | 142 | ASN  |
| 1   | H     | 160 | ASN  |
| 1   | H     | 173 | GLN  |
| 1   | H     | 214 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 217 | GLN  |
| 1   | H     | 223 | GLN  |
| 1   | I     | 83  | GLN  |
| 1   | I     | 130 | ASN  |
| 1   | I     | 142 | ASN  |
| 1   | I     | 173 | GLN  |
| 1   | I     | 214 | ASN  |
| 1   | I     | 217 | GLN  |
| 1   | I     | 223 | GLN  |
| 1   | J     | 83  | GLN  |
| 1   | J     | 130 | ASN  |
| 1   | J     | 142 | ASN  |
| 1   | J     | 160 | ASN  |
| 1   | J     | 173 | GLN  |
| 1   | J     | 214 | ASN  |
| 1   | J     | 217 | GLN  |
| 1   | J     | 223 | GLN  |
| 1   | K     | 83  | GLN  |
| 1   | K     | 130 | ASN  |
| 1   | K     | 142 | ASN  |
| 1   | K     | 160 | ASN  |
| 1   | K     | 173 | GLN  |
| 1   | K     | 214 | ASN  |
| 1   | K     | 217 | GLN  |
| 1   | K     | 223 | GLN  |
| 1   | L     | 83  | GLN  |
| 1   | L     | 130 | ASN  |
| 1   | L     | 142 | ASN  |
| 1   | L     | 173 | GLN  |
| 1   | L     | 214 | ASN  |
| 1   | L     | 217 | GLN  |
| 1   | L     | 223 | GLN  |
| 1   | M     | 83  | GLN  |
| 1   | M     | 130 | ASN  |
| 1   | M     | 142 | ASN  |
| 1   | M     | 173 | GLN  |
| 1   | M     | 214 | ASN  |
| 1   | M     | 217 | GLN  |
| 1   | M     | 223 | GLN  |
| 1   | N     | 83  | GLN  |
| 1   | N     | 130 | ASN  |
| 1   | N     | 142 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 173 | GLN  |
| 1   | N     | 214 | ASN  |
| 1   | N     | 217 | GLN  |
| 1   | N     | 223 | GLN  |
| 1   | O     | 83  | GLN  |
| 1   | O     | 130 | ASN  |
| 1   | O     | 142 | ASN  |
| 1   | O     | 173 | GLN  |
| 1   | O     | 214 | ASN  |
| 1   | O     | 217 | GLN  |
| 1   | O     | 223 | GLN  |
| 1   | P     | 83  | GLN  |
| 1   | P     | 130 | ASN  |
| 1   | P     | 142 | ASN  |
| 1   | P     | 173 | GLN  |
| 1   | P     | 214 | ASN  |
| 1   | P     | 217 | GLN  |
| 1   | Q     | 83  | GLN  |
| 1   | Q     | 130 | ASN  |
| 1   | Q     | 142 | ASN  |
| 1   | Q     | 173 | GLN  |
| 1   | Q     | 214 | ASN  |
| 1   | Q     | 217 | GLN  |
| 1   | R     | 83  | GLN  |
| 1   | R     | 130 | ASN  |
| 1   | R     | 142 | ASN  |
| 1   | R     | 173 | GLN  |
| 1   | R     | 214 | ASN  |
| 1   | R     | 217 | GLN  |
| 1   | R     | 223 | GLN  |
| 1   | S     | 83  | GLN  |
| 1   | S     | 130 | ASN  |
| 1   | S     | 142 | ASN  |
| 1   | S     | 173 | GLN  |
| 1   | S     | 214 | ASN  |
| 1   | S     | 217 | GLN  |
| 1   | S     | 223 | GLN  |
| 1   | T     | 83  | GLN  |
| 1   | T     | 130 | ASN  |
| 1   | T     | 142 | ASN  |
| 1   | T     | 173 | GLN  |
| 1   | T     | 214 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 217 | GLN  |
| 1   | T     | 223 | GLN  |
| 1   | U     | 83  | GLN  |
| 1   | U     | 130 | ASN  |
| 1   | U     | 142 | ASN  |
| 1   | U     | 160 | ASN  |
| 1   | U     | 173 | GLN  |
| 1   | U     | 214 | ASN  |
| 1   | U     | 217 | GLN  |
| 1   | U     | 223 | GLN  |
| 1   | V     | 83  | GLN  |
| 1   | V     | 130 | ASN  |
| 1   | V     | 142 | ASN  |
| 1   | V     | 160 | ASN  |
| 1   | V     | 173 | GLN  |
| 1   | V     | 214 | ASN  |
| 1   | V     | 217 | GLN  |
| 1   | V     | 223 | GLN  |
| 1   | W     | 83  | GLN  |
| 1   | W     | 130 | ASN  |
| 1   | W     | 142 | ASN  |
| 1   | W     | 173 | GLN  |
| 1   | W     | 214 | ASN  |
| 1   | W     | 217 | GLN  |
| 1   | W     | 223 | GLN  |
| 1   | X     | 83  | GLN  |
| 1   | X     | 130 | ASN  |
| 1   | X     | 142 | ASN  |
| 1   | X     | 160 | ASN  |
| 1   | X     | 173 | GLN  |
| 1   | X     | 214 | ASN  |
| 1   | X     | 217 | GLN  |
| 1   | Y     | 83  | GLN  |
| 1   | Y     | 130 | ASN  |
| 1   | Y     | 142 | ASN  |
| 1   | Y     | 173 | GLN  |
| 1   | Y     | 214 | ASN  |
| 1   | Y     | 217 | GLN  |
| 1   | Y     | 223 | GLN  |
| 1   | Z     | 83  | GLN  |
| 1   | Z     | 130 | ASN  |
| 1   | Z     | 142 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 173 | GLN  |
| 1   | Z     | 214 | ASN  |
| 1   | Z     | 217 | GLN  |
| 1   | Z     | 223 | GLN  |
| 2   | a     | 80  | GLN  |
| 2   | a     | 140 | ASN  |
| 2   | a     | 159 | GLN  |
| 2   | a     | 161 | ASN  |
| 2   | a     | 178 | GLN  |
| 2   | a     | 188 | GLN  |
| 2   | a     | 249 | GLN  |
| 2   | a     | 277 | GLN  |
| 2   | b     | 54  | GLN  |
| 2   | b     | 140 | ASN  |
| 2   | b     | 159 | GLN  |
| 2   | b     | 161 | ASN  |
| 2   | b     | 178 | GLN  |
| 2   | b     | 188 | GLN  |
| 2   | b     | 229 | ASN  |
| 2   | b     | 249 | GLN  |
| 2   | b     | 277 | GLN  |
| 2   | b     | 327 | ASN  |
| 2   | b     | 350 | GLN  |
| 2   | c     | 54  | GLN  |
| 2   | c     | 80  | GLN  |
| 2   | c     | 140 | ASN  |
| 2   | c     | 159 | GLN  |
| 2   | c     | 178 | GLN  |
| 2   | c     | 188 | GLN  |
| 2   | c     | 249 | GLN  |
| 2   | c     | 277 | GLN  |
| 2   | c     | 327 | ASN  |
| 2   | d     | 80  | GLN  |
| 2   | d     | 140 | ASN  |
| 2   | d     | 159 | GLN  |
| 2   | d     | 161 | ASN  |
| 2   | d     | 178 | GLN  |
| 2   | d     | 188 | GLN  |
| 2   | d     | 249 | GLN  |
| 2   | d     | 277 | GLN  |
| 2   | d     | 327 | ASN  |
| 2   | e     | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | e     | 140 | ASN  |
| 2   | e     | 159 | GLN  |
| 2   | e     | 161 | ASN  |
| 2   | e     | 178 | GLN  |
| 2   | e     | 188 | GLN  |
| 2   | e     | 249 | GLN  |
| 2   | e     | 277 | GLN  |
| 2   | e     | 327 | ASN  |
| 2   | f     | 80  | GLN  |
| 2   | f     | 140 | ASN  |
| 2   | f     | 159 | GLN  |
| 2   | f     | 161 | ASN  |
| 2   | f     | 178 | GLN  |
| 2   | f     | 188 | GLN  |
| 2   | f     | 249 | GLN  |
| 2   | f     | 277 | GLN  |
| 2   | f     | 327 | ASN  |
| 2   | g     | 54  | GLN  |
| 2   | g     | 80  | GLN  |
| 2   | g     | 140 | ASN  |
| 2   | g     | 159 | GLN  |
| 2   | g     | 161 | ASN  |
| 2   | g     | 178 | GLN  |
| 2   | g     | 188 | GLN  |
| 2   | g     | 249 | GLN  |
| 2   | g     | 277 | GLN  |
| 2   | h     | 54  | GLN  |
| 2   | h     | 80  | GLN  |
| 2   | h     | 140 | ASN  |
| 2   | h     | 159 | GLN  |
| 2   | h     | 161 | ASN  |
| 2   | h     | 178 | GLN  |
| 2   | h     | 188 | GLN  |
| 2   | h     | 249 | GLN  |
| 2   | h     | 327 | ASN  |
| 2   | h     | 350 | GLN  |
| 2   | i     | 54  | GLN  |
| 2   | i     | 80  | GLN  |
| 2   | i     | 140 | ASN  |
| 2   | i     | 159 | GLN  |
| 2   | i     | 161 | ASN  |
| 2   | i     | 178 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | i     | 188 | GLN  |
| 2   | i     | 249 | GLN  |
| 2   | i     | 327 | ASN  |
| 2   | i     | 350 | GLN  |
| 2   | j     | 80  | GLN  |
| 2   | j     | 140 | ASN  |
| 2   | j     | 159 | GLN  |
| 2   | j     | 178 | GLN  |
| 2   | j     | 188 | GLN  |
| 2   | j     | 249 | GLN  |
| 2   | j     | 327 | ASN  |
| 2   | k     | 54  | GLN  |
| 2   | k     | 140 | ASN  |
| 2   | k     | 159 | GLN  |
| 2   | k     | 161 | ASN  |
| 2   | k     | 178 | GLN  |
| 2   | k     | 188 | GLN  |
| 2   | k     | 249 | GLN  |
| 2   | k     | 327 | ASN  |
| 2   | k     | 350 | GLN  |
| 2   | l     | 140 | ASN  |
| 2   | l     | 159 | GLN  |
| 2   | l     | 161 | ASN  |
| 2   | l     | 178 | GLN  |
| 2   | l     | 188 | GLN  |
| 2   | l     | 229 | ASN  |
| 2   | l     | 249 | GLN  |
| 2   | l     | 327 | ASN  |
| 2   | m     | 80  | GLN  |
| 2   | m     | 140 | ASN  |
| 2   | m     | 159 | GLN  |
| 2   | m     | 161 | ASN  |
| 2   | m     | 178 | GLN  |
| 2   | m     | 188 | GLN  |
| 2   | m     | 249 | GLN  |
| 2   | m     | 327 | ASN  |
| 2   | m     | 350 | GLN  |
| 2   | n     | 54  | GLN  |
| 2   | n     | 140 | ASN  |
| 2   | n     | 159 | GLN  |
| 2   | n     | 178 | GLN  |
| 2   | n     | 188 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | n     | 249 | GLN  |
| 2   | n     | 277 | GLN  |
| 2   | n     | 327 | ASN  |
| 2   | n     | 350 | GLN  |
| 2   | o     | 54  | GLN  |
| 2   | o     | 80  | GLN  |
| 2   | o     | 140 | ASN  |
| 2   | o     | 159 | GLN  |
| 2   | o     | 161 | ASN  |
| 2   | o     | 178 | GLN  |
| 2   | o     | 188 | GLN  |
| 2   | o     | 249 | GLN  |
| 2   | o     | 277 | GLN  |
| 2   | o     | 350 | GLN  |
| 2   | p     | 54  | GLN  |
| 2   | p     | 140 | ASN  |
| 2   | p     | 159 | GLN  |
| 2   | p     | 161 | ASN  |
| 2   | p     | 178 | GLN  |
| 2   | p     | 188 | GLN  |
| 2   | p     | 249 | GLN  |
| 2   | p     | 327 | ASN  |
| 2   | p     | 350 | GLN  |
| 2   | q     | 54  | GLN  |
| 2   | q     | 140 | ASN  |
| 2   | q     | 159 | GLN  |
| 2   | q     | 161 | ASN  |
| 2   | q     | 178 | GLN  |
| 2   | q     | 188 | GLN  |
| 2   | q     | 229 | ASN  |
| 2   | q     | 249 | GLN  |
| 2   | q     | 277 | GLN  |
| 2   | q     | 327 | ASN  |
| 2   | q     | 350 | GLN  |
| 2   | r     | 140 | ASN  |
| 2   | r     | 159 | GLN  |
| 2   | r     | 161 | ASN  |
| 2   | r     | 178 | GLN  |
| 2   | r     | 188 | GLN  |
| 2   | r     | 249 | GLN  |
| 2   | r     | 277 | GLN  |
| 2   | s     | 54  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | s     | 80  | GLN  |
| 2   | s     | 140 | ASN  |
| 2   | s     | 159 | GLN  |
| 2   | s     | 161 | ASN  |
| 2   | s     | 178 | GLN  |
| 2   | s     | 188 | GLN  |
| 2   | s     | 327 | ASN  |
| 2   | t     | 54  | GLN  |
| 2   | t     | 80  | GLN  |
| 2   | t     | 140 | ASN  |
| 2   | t     | 159 | GLN  |
| 2   | t     | 161 | ASN  |
| 2   | t     | 178 | GLN  |
| 2   | t     | 188 | GLN  |
| 2   | t     | 277 | GLN  |
| 2   | t     | 327 | ASN  |
| 2   | t     | 350 | GLN  |
| 2   | u     | 54  | GLN  |
| 2   | u     | 140 | ASN  |
| 2   | u     | 159 | GLN  |
| 2   | u     | 161 | ASN  |
| 2   | u     | 178 | GLN  |
| 2   | u     | 188 | GLN  |
| 2   | u     | 277 | GLN  |
| 2   | u     | 327 | ASN  |
| 2   | u     | 350 | GLN  |
| 2   | v     | 54  | GLN  |
| 2   | v     | 140 | ASN  |
| 2   | v     | 159 | GLN  |
| 2   | v     | 161 | ASN  |
| 2   | v     | 178 | GLN  |
| 2   | v     | 188 | GLN  |
| 2   | v     | 229 | ASN  |
| 2   | v     | 249 | GLN  |
| 2   | v     | 277 | GLN  |
| 2   | v     | 327 | ASN  |
| 2   | w     | 80  | GLN  |
| 2   | w     | 140 | ASN  |
| 2   | w     | 159 | GLN  |
| 2   | w     | 161 | ASN  |
| 2   | w     | 178 | GLN  |
| 2   | w     | 188 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | w     | 249 | GLN  |
| 2   | w     | 277 | GLN  |
| 2   | w     | 327 | ASN  |
| 2   | x     | 51  | GLN  |
| 2   | x     | 80  | GLN  |
| 2   | x     | 140 | ASN  |
| 2   | x     | 159 | GLN  |
| 2   | x     | 161 | ASN  |
| 2   | x     | 178 | GLN  |
| 2   | x     | 188 | GLN  |
| 2   | x     | 277 | GLN  |
| 2   | x     | 327 | ASN  |
| 2   | y     | 54  | GLN  |
| 2   | y     | 80  | GLN  |
| 2   | y     | 140 | ASN  |
| 2   | y     | 159 | GLN  |
| 2   | y     | 161 | ASN  |
| 2   | y     | 178 | GLN  |
| 2   | y     | 188 | GLN  |
| 2   | y     | 277 | GLN  |
| 2   | z     | 54  | GLN  |
| 2   | z     | 80  | GLN  |
| 2   | z     | 140 | ASN  |
| 2   | z     | 159 | GLN  |
| 2   | z     | 161 | ASN  |
| 2   | z     | 178 | GLN  |
| 2   | z     | 188 | GLN  |
| 2   | z     | 277 | GLN  |
| 2   | z     | 327 | ASN  |
| 3   | 0     | 16  | GLN  |
| 3   | 0     | 32  | ASN  |
| 3   | 0     | 47  | GLN  |
| 3   | 0     | 90  | ASN  |
| 3   | 0     | 135 | GLN  |
| 3   | 0     | 137 | GLN  |
| 3   | 0     | 180 | ASN  |
| 3   | 0     | 196 | GLN  |
| 3   | 0     | 255 | GLN  |
| 3   | 1     | 67  | GLN  |
| 3   | 1     | 83  | GLN  |
| 3   | 1     | 85  | ASN  |
| 3   | 1     | 162 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1     | 237 | GLN  |
| 3   | 1     | 252 | GLN  |
| 3   | 2     | 51  | GLN  |
| 3   | 2     | 83  | GLN  |
| 3   | 2     | 145 | ASN  |
| 3   | 2     | 164 | GLN  |
| 3   | 2     | 235 | GLN  |
| 3   | 2     | 255 | GLN  |
| 3   | 3     | 32  | ASN  |
| 3   | 3     | 37  | GLN  |
| 3   | 3     | 67  | GLN  |
| 3   | 3     | 88  | GLN  |
| 3   | 3     | 121 | GLN  |
| 3   | 3     | 137 | GLN  |
| 3   | 3     | 255 | GLN  |
| 3   | 4     | 32  | ASN  |
| 3   | 4     | 37  | GLN  |
| 3   | 4     | 81  | HIS  |
| 3   | 4     | 88  | GLN  |
| 3   | 4     | 104 | GLN  |
| 3   | 4     | 125 | ASN  |
| 3   | 4     | 127 | GLN  |
| 3   | 4     | 174 | ASN  |
| 3   | 4     | 216 | GLN  |
| 3   | 4     | 235 | GLN  |
| 3   | 4     | 255 | GLN  |
| 3   | 5     | 55  | GLN  |
| 3   | 5     | 100 | GLN  |
| 3   | 5     | 121 | GLN  |
| 3   | 5     | 164 | GLN  |
| 3   | 5     | 237 | GLN  |
| 3   | 6     | 59  | GLN  |
| 3   | 6     | 91  | ASN  |
| 3   | 6     | 127 | GLN  |
| 3   | 6     | 135 | GLN  |
| 3   | 6     | 137 | GLN  |
| 3   | 6     | 161 | GLN  |
| 3   | 6     | 209 | ASN  |
| 3   | 6     | 237 | GLN  |
| 3   | 7     | 55  | GLN  |
| 3   | 7     | 81  | HIS  |
| 3   | 7     | 125 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 7     | 164 | GLN  |
| 3   | 7     | 190 | ASN  |
| 3   | 7     | 235 | GLN  |
| 3   | 8     | 83  | GLN  |
| 3   | 8     | 172 | GLN  |
| 3   | 8     | 209 | ASN  |
| 3   | 8     | 255 | GLN  |
| 3   | 9     | 37  | GLN  |
| 3   | 9     | 85  | ASN  |
| 3   | 9     | 88  | GLN  |
| 3   | 9     | 91  | ASN  |
| 3   | 9     | 127 | GLN  |
| 3   | 9     | 259 | GLN  |
| 3   | ZA    | 32  | ASN  |
| 3   | ZA    | 37  | GLN  |
| 3   | ZA    | 81  | HIS  |
| 3   | ZA    | 83  | GLN  |
| 3   | ZA    | 137 | GLN  |
| 3   | ZA    | 235 | GLN  |
| 3   | ZB    | 24  | ASN  |
| 3   | ZB    | 25  | ASN  |
| 3   | ZB    | 28  | ASN  |
| 3   | ZB    | 37  | GLN  |
| 3   | ZB    | 135 | GLN  |
| 3   | ZB    | 137 | GLN  |
| 3   | ZB    | 237 | GLN  |
| 3   | ZB    | 243 | ASN  |
| 3   | ZC    | 16  | GLN  |
| 3   | ZC    | 37  | GLN  |
| 3   | ZC    | 55  | GLN  |
| 3   | ZC    | 83  | GLN  |
| 3   | ZC    | 88  | GLN  |
| 3   | ZC    | 100 | GLN  |
| 3   | ZC    | 125 | ASN  |
| 3   | ZC    | 127 | GLN  |
| 3   | ZC    | 137 | GLN  |
| 3   | ZC    | 202 | ASN  |
| 3   | ZC    | 255 | GLN  |
| 3   | ZD    | 24  | ASN  |
| 3   | ZD    | 32  | ASN  |
| 3   | ZD    | 67  | GLN  |
| 3   | ZD    | 88  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | ZD    | 91  | ASN  |
| 3   | ZD    | 124 | GLN  |
| 3   | ZD    | 135 | GLN  |
| 3   | ZD    | 237 | GLN  |
| 3   | ZE    | 24  | ASN  |
| 3   | ZE    | 67  | GLN  |
| 3   | ZE    | 85  | ASN  |
| 3   | ZE    | 91  | ASN  |
| 3   | ZE    | 121 | GLN  |
| 3   | ZE    | 252 | GLN  |
| 4   | ZF    | 5   | GLN  |
| 4   | ZF    | 107 | ASN  |
| 4   | ZF    | 155 | GLN  |
| 4   | ZF    | 194 | HIS  |
| 4   | ZF    | 197 | ASN  |
| 4   | ZF    | 280 | ASN  |
| 4   | ZF    | 282 | ASN  |
| 4   | ZF    | 310 | GLN  |
| 4   | ZF    | 358 | ASN  |
| 4   | ZF    | 385 | ASN  |
| 4   | ZF    | 392 | GLN  |
| 4   | ZF    | 401 | ASN  |
| 4   | ZG    | 22  | ASN  |
| 4   | ZG    | 89  | ASN  |
| 4   | ZG    | 107 | ASN  |
| 4   | ZG    | 130 | GLN  |
| 4   | ZG    | 133 | ASN  |
| 4   | ZG    | 233 | ASN  |
| 4   | ZG    | 265 | ASN  |
| 4   | ZG    | 293 | GLN  |
| 4   | ZG    | 303 | ASN  |
| 4   | ZG    | 322 | ASN  |
| 4   | ZG    | 332 | ASN  |
| 4   | ZG    | 385 | ASN  |
| 4   | ZG    | 387 | GLN  |
| 4   | ZG    | 394 | GLN  |
| 4   | ZH    | 157 | ASN  |
| 4   | ZH    | 206 | ASN  |
| 4   | ZH    | 252 | ASN  |
| 4   | ZH    | 296 | ASN  |
| 4   | ZH    | 329 | GLN  |
| 4   | ZH    | 352 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZH    | 365 | ASN  |
| 4   | ZH    | 379 | GLN  |
| 4   | ZI    | 22  | ASN  |
| 4   | ZI    | 79  | GLN  |
| 4   | ZI    | 89  | ASN  |
| 4   | ZI    | 130 | GLN  |
| 4   | ZI    | 197 | ASN  |
| 4   | ZI    | 245 | ASN  |
| 4   | ZI    | 252 | ASN  |
| 4   | ZI    | 265 | ASN  |
| 4   | ZI    | 269 | GLN  |
| 4   | ZI    | 310 | GLN  |
| 4   | ZI    | 385 | ASN  |
| 4   | ZI    | 392 | GLN  |
| 4   | ZI    | 394 | GLN  |
| 4   | ZI    | 401 | ASN  |
| 4   | ZJ    | 22  | ASN  |
| 4   | ZJ    | 89  | ASN  |
| 4   | ZJ    | 133 | ASN  |
| 4   | ZJ    | 159 | ASN  |
| 4   | ZJ    | 197 | ASN  |
| 4   | ZJ    | 265 | ASN  |
| 4   | ZJ    | 282 | ASN  |
| 4   | ZJ    | 293 | GLN  |
| 4   | ZJ    | 310 | GLN  |
| 4   | ZJ    | 379 | GLN  |
| 4   | ZJ    | 385 | ASN  |
| 4   | ZJ    | 392 | GLN  |
| 4   | ZJ    | 401 | ASN  |
| 4   | ZK    | 89  | ASN  |
| 4   | ZK    | 99  | GLN  |
| 4   | ZK    | 107 | ASN  |
| 4   | ZK    | 197 | ASN  |
| 4   | ZK    | 252 | ASN  |
| 4   | ZK    | 270 | ASN  |
| 4   | ZK    | 274 | ASN  |
| 4   | ZK    | 303 | ASN  |
| 4   | ZK    | 319 | ASN  |
| 4   | ZK    | 332 | ASN  |
| 4   | ZK    | 379 | GLN  |
| 4   | ZK    | 392 | GLN  |
| 4   | ZK    | 401 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZL    | 5   | GLN  |
| 4   | ZL    | 99  | GLN  |
| 4   | ZL    | 179 | ASN  |
| 4   | ZL    | 190 | GLN  |
| 4   | ZL    | 197 | ASN  |
| 4   | ZL    | 252 | ASN  |
| 4   | ZL    | 269 | GLN  |
| 4   | ZL    | 282 | ASN  |
| 4   | ZL    | 293 | GLN  |
| 4   | ZL    | 303 | ASN  |
| 4   | ZL    | 306 | ASN  |
| 4   | ZL    | 310 | GLN  |
| 4   | ZL    | 338 | GLN  |
| 4   | ZL    | 401 | ASN  |
| 4   | ZM    | 5   | GLN  |
| 4   | ZM    | 22  | ASN  |
| 4   | ZM    | 59  | GLN  |
| 4   | ZM    | 89  | ASN  |
| 4   | ZM    | 197 | ASN  |
| 4   | ZM    | 206 | ASN  |
| 4   | ZM    | 213 | HIS  |
| 4   | ZM    | 235 | ASN  |
| 4   | ZM    | 252 | ASN  |
| 4   | ZM    | 381 | ASN  |
| 4   | ZM    | 397 | ASN  |
| 4   | ZN    | 5   | GLN  |
| 4   | ZN    | 22  | ASN  |
| 4   | ZN    | 79  | GLN  |
| 4   | ZN    | 107 | ASN  |
| 4   | ZN    | 112 | GLN  |
| 4   | ZN    | 129 | GLN  |
| 4   | ZN    | 133 | ASN  |
| 4   | ZN    | 157 | ASN  |
| 4   | ZN    | 190 | GLN  |
| 4   | ZN    | 197 | ASN  |
| 4   | ZN    | 213 | HIS  |
| 4   | ZN    | 270 | ASN  |
| 4   | ZN    | 293 | GLN  |
| 4   | ZN    | 310 | GLN  |
| 4   | ZN    | 319 | ASN  |
| 4   | ZN    | 332 | ASN  |
| 4   | ZN    | 379 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZN    | 381 | ASN  |
| 4   | ZN    | 385 | ASN  |
| 4   | ZN    | 394 | GLN  |
| 4   | ZN    | 401 | ASN  |
| 4   | ZO    | 5   | GLN  |
| 4   | ZO    | 22  | ASN  |
| 4   | ZO    | 89  | ASN  |
| 4   | ZO    | 141 | ASN  |
| 4   | ZO    | 235 | ASN  |
| 4   | ZO    | 268 | GLN  |
| 4   | ZO    | 296 | ASN  |
| 4   | ZO    | 322 | ASN  |
| 4   | ZO    | 332 | ASN  |
| 4   | ZP    | 11  | ASN  |
| 4   | ZP    | 107 | ASN  |
| 4   | ZP    | 129 | GLN  |
| 4   | ZP    | 194 | HIS  |
| 4   | ZP    | 213 | HIS  |
| 4   | ZP    | 245 | ASN  |
| 4   | ZP    | 270 | ASN  |
| 4   | ZP    | 293 | GLN  |
| 4   | ZP    | 314 | GLN  |
| 4   | ZP    | 322 | ASN  |
| 4   | ZP    | 338 | GLN  |
| 4   | ZP    | 379 | GLN  |
| 4   | ZP    | 381 | ASN  |
| 4   | ZP    | 385 | ASN  |
| 4   | ZP    | 392 | GLN  |
| 4   | ZQ    | 5   | GLN  |
| 4   | ZQ    | 89  | ASN  |
| 4   | ZQ    | 97  | ASN  |
| 4   | ZQ    | 105 | ASN  |
| 4   | ZQ    | 133 | ASN  |
| 4   | ZQ    | 141 | ASN  |
| 4   | ZQ    | 155 | GLN  |
| 4   | ZQ    | 157 | ASN  |
| 4   | ZQ    | 197 | ASN  |
| 4   | ZQ    | 213 | HIS  |
| 4   | ZQ    | 233 | ASN  |
| 4   | ZQ    | 265 | ASN  |
| 4   | ZQ    | 387 | GLN  |
| 4   | ZQ    | 397 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZR    | 5   | GLN  |
| 4   | ZR    | 89  | ASN  |
| 4   | ZR    | 107 | ASN  |
| 4   | ZR    | 112 | GLN  |
| 4   | ZR    | 157 | ASN  |
| 4   | ZR    | 197 | ASN  |
| 4   | ZR    | 268 | GLN  |
| 4   | ZR    | 269 | GLN  |
| 4   | ZR    | 293 | GLN  |
| 4   | ZR    | 295 | ASN  |
| 4   | ZR    | 310 | GLN  |
| 4   | ZR    | 401 | ASN  |
| 4   | ZS    | 22  | ASN  |
| 4   | ZS    | 133 | ASN  |
| 4   | ZS    | 197 | ASN  |
| 4   | ZS    | 206 | ASN  |
| 4   | ZS    | 303 | ASN  |
| 4   | ZS    | 387 | GLN  |
| 4   | ZS    | 394 | GLN  |
| 4   | ZT    | 26  | ASN  |
| 4   | ZT    | 99  | GLN  |
| 4   | ZT    | 129 | GLN  |
| 4   | ZT    | 197 | ASN  |
| 4   | ZT    | 206 | ASN  |
| 4   | ZT    | 213 | HIS  |
| 4   | ZT    | 235 | ASN  |
| 4   | ZT    | 252 | ASN  |
| 4   | ZT    | 270 | ASN  |
| 4   | ZT    | 275 | ASN  |
| 4   | ZT    | 293 | GLN  |
| 4   | ZT    | 303 | ASN  |
| 4   | ZT    | 310 | GLN  |
| 4   | ZT    | 314 | GLN  |
| 4   | ZT    | 352 | ASN  |
| 4   | ZU    | 22  | ASN  |
| 4   | ZU    | 97  | ASN  |
| 4   | ZU    | 107 | ASN  |
| 4   | ZU    | 129 | GLN  |
| 4   | ZU    | 133 | ASN  |
| 4   | ZU    | 159 | ASN  |
| 4   | ZU    | 190 | GLN  |
| 4   | ZU    | 197 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZU    | 268 | GLN  |
| 4   | ZU    | 269 | GLN  |
| 4   | ZU    | 293 | GLN  |
| 4   | ZU    | 310 | GLN  |
| 4   | ZU    | 379 | GLN  |
| 4   | ZU    | 401 | ASN  |
| 4   | ZV    | 5   | GLN  |
| 4   | ZV    | 89  | ASN  |
| 4   | ZV    | 107 | ASN  |
| 4   | ZV    | 130 | GLN  |
| 4   | ZV    | 133 | ASN  |
| 4   | ZV    | 157 | ASN  |
| 4   | ZV    | 159 | ASN  |
| 4   | ZV    | 197 | ASN  |
| 4   | ZV    | 213 | HIS  |
| 4   | ZV    | 252 | ASN  |
| 4   | ZV    | 269 | GLN  |
| 4   | ZV    | 280 | ASN  |
| 4   | ZV    | 293 | GLN  |
| 4   | ZV    | 295 | ASN  |
| 4   | ZV    | 303 | ASN  |
| 4   | ZV    | 314 | GLN  |
| 4   | ZV    | 381 | ASN  |
| 4   | ZV    | 394 | GLN  |
| 4   | ZW    | 5   | GLN  |
| 4   | ZW    | 26  | ASN  |
| 4   | ZW    | 107 | ASN  |
| 4   | ZW    | 129 | GLN  |
| 4   | ZW    | 133 | ASN  |
| 4   | ZW    | 213 | HIS  |
| 4   | ZW    | 252 | ASN  |
| 4   | ZW    | 270 | ASN  |
| 4   | ZW    | 310 | GLN  |
| 4   | ZW    | 314 | GLN  |
| 4   | ZW    | 332 | ASN  |
| 4   | ZX    | 11  | ASN  |
| 4   | ZX    | 22  | ASN  |
| 4   | ZX    | 133 | ASN  |
| 4   | ZX    | 159 | ASN  |
| 4   | ZX    | 314 | GLN  |
| 4   | ZX    | 387 | GLN  |
| 4   | ZX    | 401 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | ZY    | 5   | GLN  |
| 4   | ZY    | 26  | ASN  |
| 4   | ZY    | 80  | ASN  |
| 4   | ZY    | 115 | GLN  |
| 4   | ZY    | 159 | ASN  |
| 4   | ZY    | 197 | ASN  |
| 4   | ZY    | 245 | ASN  |
| 4   | ZY    | 265 | ASN  |
| 4   | ZY    | 268 | GLN  |
| 4   | ZY    | 303 | ASN  |
| 4   | ZY    | 308 | GLN  |
| 4   | ZY    | 314 | GLN  |
| 4   | ZY    | 332 | ASN  |
| 4   | ZY    | 392 | GLN  |
| 4   | ZZ    | 5   | GLN  |
| 4   | ZZ    | 99  | GLN  |
| 4   | ZZ    | 107 | ASN  |
| 4   | ZZ    | 133 | ASN  |
| 4   | ZZ    | 194 | HIS  |
| 4   | ZZ    | 197 | ASN  |
| 4   | ZZ    | 213 | HIS  |
| 4   | ZZ    | 293 | GLN  |
| 4   | ZZ    | 303 | ASN  |
| 4   | ZZ    | 314 | GLN  |
| 4   | ZZ    | 332 | ASN  |
| 4   | ZZ    | 401 | ASN  |
| 4   | Za    | 129 | GLN  |
| 4   | Za    | 157 | ASN  |
| 4   | Za    | 190 | GLN  |
| 4   | Za    | 197 | ASN  |
| 4   | Za    | 293 | GLN  |
| 4   | Za    | 332 | ASN  |
| 4   | Za    | 385 | ASN  |
| 4   | Zb    | 5   | GLN  |
| 4   | Zb    | 79  | GLN  |
| 4   | Zb    | 107 | ASN  |
| 4   | Zb    | 129 | GLN  |
| 4   | Zb    | 130 | GLN  |
| 4   | Zb    | 159 | ASN  |
| 4   | Zb    | 190 | GLN  |
| 4   | Zb    | 197 | ASN  |
| 4   | Zb    | 293 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Zb    | 308 | GLN  |
| 4   | Zb    | 314 | GLN  |
| 4   | Zb    | 322 | ASN  |
| 4   | Zb    | 332 | ASN  |
| 4   | Zb    | 358 | ASN  |
| 4   | Zb    | 381 | ASN  |
| 4   | Zb    | 387 | GLN  |
| 4   | Zb    | 401 | ASN  |
| 4   | Zc    | 5   | GLN  |
| 4   | Zc    | 107 | ASN  |
| 4   | Zc    | 115 | GLN  |
| 4   | Zc    | 129 | GLN  |
| 4   | Zc    | 133 | ASN  |
| 4   | Zc    | 159 | ASN  |
| 4   | Zc    | 197 | ASN  |
| 4   | Zc    | 293 | GLN  |
| 4   | Zc    | 379 | GLN  |
| 4   | Zc    | 387 | GLN  |
| 4   | Zc    | 397 | ASN  |
| 4   | Zd    | 5   | GLN  |
| 4   | Zd    | 22  | ASN  |
| 4   | Zd    | 105 | ASN  |
| 4   | Zd    | 129 | GLN  |
| 4   | Zd    | 130 | GLN  |
| 4   | Zd    | 293 | GLN  |
| 4   | Zd    | 295 | ASN  |
| 4   | Zd    | 303 | ASN  |
| 4   | Zd    | 322 | ASN  |
| 4   | Zd    | 397 | ASN  |
| 4   | Ze    | 22  | ASN  |
| 4   | Ze    | 99  | GLN  |
| 4   | Ze    | 107 | ASN  |
| 4   | Ze    | 133 | ASN  |
| 4   | Ze    | 194 | HIS  |
| 4   | Ze    | 197 | ASN  |
| 4   | Ze    | 252 | ASN  |
| 4   | Ze    | 303 | ASN  |
| 4   | Ze    | 358 | ASN  |
| 4   | Ze    | 394 | GLN  |
| 4   | Zf    | 22  | ASN  |
| 4   | Zf    | 105 | ASN  |
| 4   | Zf    | 107 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Zf    | 115 | GLN  |
| 4   | Zf    | 133 | ASN  |
| 4   | Zf    | 159 | ASN  |
| 4   | Zf    | 197 | ASN  |
| 4   | Zf    | 252 | ASN  |
| 4   | Zf    | 293 | GLN  |
| 4   | Zf    | 303 | ASN  |
| 4   | Zf    | 308 | GLN  |
| 4   | Zf    | 314 | GLN  |
| 4   | Zf    | 332 | ASN  |
| 4   | Zf    | 397 | ASN  |
| 4   | Zg    | 5   | GLN  |
| 4   | Zg    | 107 | ASN  |
| 4   | Zg    | 115 | GLN  |
| 4   | Zg    | 129 | GLN  |
| 4   | Zg    | 133 | ASN  |
| 4   | Zg    | 159 | ASN  |
| 4   | Zg    | 179 | ASN  |
| 4   | Zg    | 197 | ASN  |
| 4   | Zg    | 213 | HIS  |
| 4   | Zg    | 310 | GLN  |
| 4   | Zg    | 381 | ASN  |
| 4   | Zh    | 5   | GLN  |
| 4   | Zh    | 97  | ASN  |
| 4   | Zh    | 99  | GLN  |
| 4   | Zh    | 115 | GLN  |
| 4   | Zh    | 129 | GLN  |
| 4   | Zh    | 197 | ASN  |
| 4   | Zh    | 303 | ASN  |
| 4   | Zh    | 383 | GLN  |
| 4   | Zh    | 385 | ASN  |
| 4   | Zh    | 392 | GLN  |
| 5   | AA    | 18  | GLN  |
| 5   | AA    | 37  | GLN  |
| 5   | AA    | 102 | ASN  |
| 5   | AA    | 112 | GLN  |
| 5   | AB    | 18  | GLN  |
| 5   | AB    | 70  | GLN  |
| 5   | AB    | 106 | GLN  |
| 5   | AB    | 116 | GLN  |
| 5   | AB    | 172 | GLN  |
| 5   | AB    | 210 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AB    | 223 | ASN  |
| 5   | AB    | 240 | ASN  |
| 5   | AC    | 14  | GLN  |
| 5   | AC    | 18  | GLN  |
| 5   | AC    | 28  | ASN  |
| 5   | AC    | 70  | GLN  |
| 5   | AC    | 83  | GLN  |
| 5   | AC    | 104 | ASN  |
| 5   | AC    | 106 | GLN  |
| 5   | AC    | 186 | GLN  |
| 5   | AC    | 230 | GLN  |
| 5   | AD    | 14  | GLN  |
| 5   | AD    | 17  | ASN  |
| 5   | AD    | 28  | ASN  |
| 5   | AD    | 84  | GLN  |
| 5   | AD    | 104 | ASN  |
| 5   | AD    | 106 | GLN  |
| 5   | AD    | 210 | ASN  |
| 5   | AD    | 240 | ASN  |
| 5   | AE    | 18  | GLN  |
| 5   | AE    | 106 | GLN  |
| 5   | AE    | 112 | GLN  |
| 5   | AE    | 116 | GLN  |
| 5   | AE    | 118 | HIS  |
| 5   | AE    | 153 | ASN  |
| 5   | AE    | 240 | ASN  |
| 3   | AF    | 47  | GLN  |
| 3   | AF    | 121 | GLN  |
| 3   | AF    | 135 | GLN  |
| 3   | AF    | 161 | GLN  |
| 3   | AF    | 169 | GLN  |
| 3   | AF    | 172 | GLN  |
| 3   | AF    | 223 | ASN  |
| 3   | AF    | 252 | GLN  |
| 3   | AG    | 16  | GLN  |
| 3   | AG    | 28  | ASN  |
| 3   | AG    | 37  | GLN  |
| 3   | AG    | 88  | GLN  |
| 3   | AG    | 145 | ASN  |
| 3   | AG    | 172 | GLN  |
| 3   | AG    | 174 | ASN  |
| 3   | AG    | 180 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AG    | 223 | ASN  |
| 3   | AG    | 259 | GLN  |
| 3   | AH    | 85  | ASN  |
| 3   | AH    | 90  | ASN  |
| 3   | AH    | 104 | GLN  |
| 3   | AH    | 127 | GLN  |
| 3   | AH    | 137 | GLN  |
| 3   | AH    | 172 | GLN  |
| 3   | AH    | 196 | GLN  |
| 3   | AH    | 223 | ASN  |
| 3   | AH    | 259 | GLN  |
| 3   | AI    | 16  | GLN  |
| 3   | AI    | 32  | ASN  |
| 3   | AI    | 37  | GLN  |
| 3   | AI    | 47  | GLN  |
| 3   | AI    | 125 | ASN  |
| 3   | AI    | 162 | GLN  |
| 3   | AI    | 202 | ASN  |
| 3   | AI    | 209 | ASN  |
| 3   | AI    | 235 | GLN  |
| 3   | AI    | 252 | GLN  |
| 3   | AJ    | 47  | GLN  |
| 3   | AJ    | 90  | ASN  |
| 3   | AJ    | 125 | ASN  |
| 3   | AJ    | 127 | GLN  |
| 3   | AJ    | 137 | GLN  |
| 3   | AJ    | 169 | GLN  |
| 3   | AJ    | 172 | GLN  |
| 3   | AJ    | 174 | ASN  |
| 3   | AJ    | 180 | ASN  |
| 3   | AJ    | 202 | ASN  |
| 3   | AJ    | 232 | ASN  |
| 3   | AK    | 28  | ASN  |
| 3   | AK    | 32  | ASN  |
| 3   | AK    | 47  | GLN  |
| 3   | AK    | 104 | GLN  |
| 3   | AK    | 121 | GLN  |
| 3   | AK    | 135 | GLN  |
| 3   | AK    | 145 | ASN  |
| 3   | AK    | 172 | GLN  |
| 3   | AK    | 174 | ASN  |
| 3   | AK    | 196 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AK    | 202 | ASN  |
| 3   | AK    | 223 | ASN  |
| 3   | AK    | 235 | GLN  |
| 3   | AL    | 32  | ASN  |
| 3   | AL    | 37  | GLN  |
| 3   | AL    | 47  | GLN  |
| 3   | AL    | 81  | HIS  |
| 3   | AL    | 83  | GLN  |
| 3   | AL    | 88  | GLN  |
| 3   | AL    | 104 | GLN  |
| 3   | AL    | 127 | GLN  |
| 3   | AL    | 145 | ASN  |
| 3   | AL    | 209 | ASN  |
| 3   | AM    | 16  | GLN  |
| 3   | AM    | 25  | ASN  |
| 3   | AM    | 37  | GLN  |
| 3   | AM    | 51  | GLN  |
| 3   | AM    | 67  | GLN  |
| 3   | AM    | 91  | ASN  |
| 3   | AM    | 125 | ASN  |
| 3   | AM    | 127 | GLN  |
| 3   | AM    | 137 | GLN  |
| 3   | AM    | 196 | GLN  |
| 3   | AM    | 209 | ASN  |
| 3   | AM    | 223 | ASN  |
| 3   | AM    | 252 | GLN  |
| 3   | AN    | 24  | ASN  |
| 3   | AN    | 67  | GLN  |
| 3   | AN    | 125 | ASN  |
| 3   | AN    | 137 | GLN  |
| 3   | AN    | 161 | GLN  |
| 3   | AN    | 162 | GLN  |
| 6   | AR    | 231 | ASN  |
| 6   | AR    | 234 | GLN  |
| 6   | AR    | 246 | GLN  |
| 6   | AR    | 281 | HIS  |
| 6   | AR    | 303 | GLN  |
| 6   | AR    | 374 | HIS  |
| 6   | AR    | 378 | ASN  |
| 6   | AR    | 434 | ASN  |
| 6   | AS    | 231 | ASN  |
| 6   | AS    | 234 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AS    | 263 | HIS  |
| 6   | AS    | 297 | GLN  |
| 6   | AS    | 299 | ASN  |
| 6   | AS    | 303 | GLN  |
| 6   | AS    | 374 | HIS  |
| 6   | AS    | 378 | ASN  |
| 6   | AS    | 434 | ASN  |
| 6   | AT    | 231 | ASN  |
| 6   | AT    | 234 | GLN  |
| 6   | AT    | 303 | GLN  |
| 6   | AT    | 374 | HIS  |
| 6   | AT    | 378 | ASN  |
| 6   | AT    | 434 | ASN  |
| 6   | AU    | 231 | ASN  |
| 6   | AU    | 234 | GLN  |
| 6   | AU    | 281 | HIS  |
| 6   | AU    | 303 | GLN  |
| 6   | AU    | 374 | HIS  |
| 6   | AU    | 378 | ASN  |
| 6   | AU    | 434 | ASN  |
| 6   | AV    | 231 | ASN  |
| 6   | AV    | 234 | GLN  |
| 6   | AV    | 303 | GLN  |
| 6   | AV    | 374 | HIS  |
| 6   | AV    | 378 | ASN  |
| 6   | AV    | 434 | ASN  |
| 6   | AW    | 231 | ASN  |
| 6   | AW    | 234 | GLN  |
| 6   | AW    | 281 | HIS  |
| 6   | AW    | 297 | GLN  |
| 6   | AW    | 299 | ASN  |
| 6   | AW    | 303 | GLN  |
| 6   | AW    | 374 | HIS  |
| 6   | AW    | 378 | ASN  |
| 6   | AW    | 434 | ASN  |
| 6   | AX    | 231 | ASN  |
| 6   | AX    | 234 | GLN  |
| 6   | AX    | 281 | HIS  |
| 6   | AX    | 297 | GLN  |
| 6   | AX    | 303 | GLN  |
| 6   | AX    | 374 | HIS  |
| 6   | AX    | 378 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AX    | 434 | ASN  |
| 6   | AY    | 231 | ASN  |
| 6   | AY    | 234 | GLN  |
| 6   | AY    | 299 | ASN  |
| 6   | AY    | 303 | GLN  |
| 6   | AY    | 374 | HIS  |
| 6   | AY    | 378 | ASN  |
| 6   | AY    | 434 | ASN  |
| 6   | AZ    | 231 | ASN  |
| 6   | AZ    | 234 | GLN  |
| 6   | AZ    | 281 | HIS  |
| 6   | AZ    | 303 | GLN  |
| 6   | AZ    | 374 | HIS  |
| 6   | AZ    | 378 | ASN  |
| 6   | AZ    | 434 | ASN  |
| 6   | Aa    | 231 | ASN  |
| 6   | Aa    | 234 | GLN  |
| 6   | Aa    | 303 | GLN  |
| 6   | Aa    | 374 | HIS  |
| 6   | Aa    | 378 | ASN  |
| 6   | Aa    | 434 | ASN  |
| 6   | Ac    | 231 | ASN  |
| 6   | Ac    | 234 | GLN  |
| 6   | Ac    | 281 | HIS  |
| 6   | Ac    | 374 | HIS  |
| 6   | Ac    | 378 | ASN  |
| 6   | Ac    | 434 | ASN  |
| 6   | Ad    | 231 | ASN  |
| 6   | Ad    | 234 | GLN  |
| 6   | Ad    | 246 | GLN  |
| 6   | Ad    | 265 | GLN  |
| 6   | Ad    | 303 | GLN  |
| 6   | Ad    | 374 | HIS  |
| 6   | Ad    | 378 | ASN  |
| 6   | Ad    | 434 | ASN  |
| 6   | Ae    | 231 | ASN  |
| 6   | Ae    | 234 | GLN  |
| 6   | Ae    | 303 | GLN  |
| 6   | Ae    | 374 | HIS  |
| 6   | Ae    | 378 | ASN  |
| 6   | Ae    | 434 | ASN  |
| 6   | Af    | 231 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | Af    | 234 | GLN  |
| 6   | Af    | 281 | HIS  |
| 6   | Af    | 297 | GLN  |
| 6   | Af    | 303 | GLN  |
| 6   | Af    | 365 | ASN  |
| 6   | Af    | 374 | HIS  |
| 6   | Af    | 378 | ASN  |
| 6   | Af    | 434 | ASN  |
| 6   | Ag    | 231 | ASN  |
| 6   | Ag    | 234 | GLN  |
| 6   | Ag    | 281 | HIS  |
| 6   | Ag    | 297 | GLN  |
| 6   | Ag    | 303 | GLN  |
| 6   | Ag    | 374 | HIS  |
| 6   | Ag    | 378 | ASN  |
| 6   | Ag    | 434 | ASN  |
| 6   | Ah    | 231 | ASN  |
| 6   | Ah    | 234 | GLN  |
| 6   | Ah    | 303 | GLN  |
| 6   | Ah    | 374 | HIS  |
| 6   | Ah    | 378 | ASN  |
| 6   | Ah    | 434 | ASN  |
| 6   | Ai    | 234 | GLN  |
| 6   | Ai    | 281 | HIS  |
| 6   | Ai    | 303 | GLN  |
| 6   | Ai    | 378 | ASN  |
| 6   | Ai    | 434 | ASN  |
| 6   | Aj    | 231 | ASN  |
| 6   | Aj    | 234 | GLN  |
| 6   | Aj    | 303 | GLN  |
| 6   | Aj    | 374 | HIS  |
| 6   | Aj    | 378 | ASN  |
| 6   | Aj    | 434 | ASN  |
| 6   | Ak    | 231 | ASN  |
| 6   | Ak    | 234 | GLN  |
| 6   | Ak    | 303 | GLN  |
| 6   | Ak    | 374 | HIS  |
| 6   | Ak    | 378 | ASN  |
| 6   | Ak    | 434 | ASN  |
| 6   | Al    | 234 | GLN  |
| 6   | Al    | 281 | HIS  |
| 6   | Al    | 303 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | Al    | 374 | HIS  |
| 6   | Al    | 378 | ASN  |
| 6   | Al    | 434 | ASN  |
| 6   | Am    | 234 | GLN  |
| 6   | Am    | 303 | GLN  |
| 6   | Am    | 374 | HIS  |
| 6   | Am    | 378 | ASN  |
| 6   | Am    | 434 | ASN  |
| 6   | An    | 234 | GLN  |
| 6   | An    | 303 | GLN  |
| 6   | An    | 378 | ASN  |
| 6   | An    | 434 | ASN  |
| 6   | Ao    | 234 | GLN  |
| 6   | Ao    | 374 | HIS  |
| 6   | Ao    | 378 | ASN  |
| 6   | Ao    | 434 | ASN  |
| 6   | Ap    | 234 | GLN  |
| 6   | Ap    | 374 | HIS  |
| 6   | Ap    | 378 | ASN  |
| 6   | Ap    | 434 | ASN  |
| 6   | AO    | 234 | GLN  |
| 6   | AO    | 297 | GLN  |
| 6   | AO    | 303 | GLN  |
| 6   | AO    | 374 | HIS  |
| 6   | AO    | 378 | ASN  |
| 6   | AO    | 434 | ASN  |
| 6   | AP    | 234 | GLN  |
| 6   | AP    | 297 | GLN  |
| 6   | AP    | 299 | ASN  |
| 6   | AP    | 303 | GLN  |
| 6   | AP    | 374 | HIS  |
| 6   | AP    | 378 | ASN  |
| 6   | AP    | 434 | ASN  |
| 6   | AQ    | 234 | GLN  |
| 6   | AQ    | 303 | GLN  |
| 6   | AQ    | 374 | HIS  |
| 6   | AQ    | 378 | ASN  |
| 6   | AQ    | 434 | ASN  |
| 7   | As    | 39  | GLN  |
| 8   | At    | 119 | HIS  |
| 8   | At    | 141 | ASN  |
| 8   | At    | 162 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | At    | 182 | ASN  |
| 8   | At    | 205 | ASN  |
| 9   | Au    | 119 | GLN  |
| 9   | Au    | 124 | GLN  |
| 9   | Au    | 141 | GLN  |
| 9   | Au    | 160 | GLN  |
| 9   | Av    | 87  | GLN  |
| 9   | Av    | 124 | GLN  |
| 9   | Av    | 160 | GLN  |
| 9   | Av    | 241 | GLN  |
| 9   | Aw    | 160 | GLN  |
| 9   | Aw    | 184 | GLN  |
| 9   | Ax    | 160 | GLN  |
| 9   | Ax    | 184 | GLN  |
| 9   | Ay    | 87  | GLN  |
| 9   | Ay    | 114 | GLN  |
| 9   | Ay    | 155 | ASN  |
| 9   | Ay    | 241 | GLN  |
| 10  | Az    | 69  | ASN  |
| 10  | Az    | 83  | GLN  |
| 10  | Az    | 103 | GLN  |
| 10  | A2    | 13  | GLN  |
| 10  | A2    | 15  | GLN  |
| 10  | A2    | 103 | GLN  |
| 10  | A3    | 87  | GLN  |
| 10  | A4    | 39  | HIS  |
| 10  | A4    | 55  | GLN  |
| 10  | A4    | 83  | GLN  |
| 10  | A4    | 87  | GLN  |
| 10  | A5    | 55  | GLN  |
| 10  | A5    | 87  | GLN  |
| 11  | A6    | 17  | ASN  |
| 11  | A6    | 71  | HIS  |
| 11  | A7    | 21  | GLN  |
| 11  | A7    | 29  | ASN  |
| 11  | A7    | 92  | GLN  |
| 11  | A7    | 98  | ASN  |
| 11  | A7    | 117 | GLN  |
| 11  | A8    | 29  | ASN  |
| 11  | A8    | 32  | ASN  |
| 11  | A8    | 76  | GLN  |
| 11  | A8    | 92  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A9    | 21  | GLN  |
| 11  | A9    | 32  | ASN  |
| 11  | A9    | 39  | GLN  |
| 11  | A9    | 72  | HIS  |
| 11  | A9    | 76  | GLN  |
| 11  | A9    | 98  | ASN  |
| 11  | A9    | 117 | GLN  |
| 11  | A0    | 72  | HIS  |
| 11  | A0    | 76  | GLN  |
| 11  | A0    | 112 | ASN  |
| 6   | UI    | 69  | GLN  |
| 6   | UI    | 94  | HIS  |
| 6   | UI    | 196 | HIS  |
| 6   | UJ    | 94  | HIS  |
| 6   | UJ    | 245 | HIS  |
| 6   | UK    | 94  | HIS  |
| 6   | UK    | 196 | HIS  |
| 6   | UL    | 69  | GLN  |
| 6   | UL    | 94  | HIS  |
| 6   | UL    | 196 | HIS  |
| 6   | UM    | 94  | HIS  |
| 6   | UM    | 196 | HIS  |
| 6   | UN    | 69  | GLN  |
| 6   | UN    | 94  | HIS  |
| 6   | UN    | 196 | HIS  |
| 6   | UO    | 94  | HIS  |
| 6   | UO    | 196 | HIS  |
| 6   | UP    | 94  | HIS  |
| 6   | UP    | 196 | HIS  |
| 12  | BA    | 30  | ASN  |
| 12  | BB    | 5   | ASN  |
| 12  | BB    | 22  | ASN  |
| 12  | BB    | 30  | ASN  |
| 6   | WA    | 156 | HIS  |
| 6   | WB    | 169 | GLN  |
| 6   | WC    | 129 | GLN  |
| 6   | WC    | 190 | GLN  |
| 6   | WE    | 156 | HIS  |
| 6   | WE    | 209 | ASN  |
| 6   | WF    | 118 | GLN  |
| 6   | WG    | 118 | GLN  |
| 6   | WH    | 156 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | WI    | 129 | GLN  |
| 6   | WI    | 156 | HIS  |
| 6   | WI    | 209 | ASN  |
| 6   | WJ    | 169 | GLN  |
| 6   | WJ    | 209 | ASN  |
| 6   | WO    | 209 | ASN  |
| 6   | WP    | 169 | GLN  |
| 6   | WP    | 209 | ASN  |
| 6   | WR    | 129 | GLN  |
| 6   | WR    | 156 | HIS  |
| 6   | WT    | 156 | HIS  |
| 6   | WT    | 209 | ASN  |
| 6   | WV    | 118 | GLN  |
| 6   | WV    | 169 | GLN  |
| 12  | BC    | 40  | GLN  |
| 12  | BC    | 50  | GLN  |
| 12  | BC    | 57  | GLN  |
| 12  | BC    | 134 | GLN  |
| 12  | BD    | 22  | ASN  |
| 12  | BD    | 82  | ASN  |
| 12  | BD    | 113 | GLN  |
| 12  | BE    | 17  | GLN  |
| 12  | BE    | 22  | ASN  |
| 12  | BE    | 30  | ASN  |
| 12  | BE    | 115 | ASN  |
| 12  | BF    | 30  | ASN  |
| 12  | BF    | 57  | GLN  |
| 12  | BF    | 115 | ASN  |
| 6   | BG    | 318 | ASN  |
| 6   | BG    | 319 | GLN  |
| 6   | BI    | 319 | GLN  |
| 6   | BJ    | 318 | ASN  |
| 6   | BJ    | 324 | ASN  |
| 6   | BN    | 318 | ASN  |
| 6   | BO    | 318 | ASN  |
| 6   | BQ    | 319 | GLN  |
| 6   | BQ    | 324 | ASN  |
| 6   | BR    | 234 | GLN  |
| 6   | BR    | 303 | GLN  |
| 6   | BR    | 374 | HIS  |
| 6   | BR    | 378 | ASN  |
| 6   | BR    | 434 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | BS    | 234 | GLN  |
| 6   | BS    | 303 | GLN  |
| 6   | BS    | 374 | HIS  |
| 6   | BS    | 378 | ASN  |
| 6   | BS    | 434 | ASN  |
| 6   | BT    | 231 | ASN  |
| 6   | BT    | 234 | GLN  |
| 6   | BT    | 303 | GLN  |
| 6   | BT    | 374 | HIS  |
| 6   | BT    | 378 | ASN  |
| 6   | BT    | 434 | ASN  |
| 6   | BU    | 231 | ASN  |
| 6   | BU    | 234 | GLN  |
| 6   | BU    | 281 | HIS  |
| 6   | BU    | 303 | GLN  |
| 6   | BU    | 374 | HIS  |
| 6   | BU    | 378 | ASN  |
| 6   | BU    | 434 | ASN  |
| 6   | BV    | 231 | ASN  |
| 6   | BV    | 234 | GLN  |
| 6   | BV    | 281 | HIS  |
| 6   | BV    | 303 | GLN  |
| 6   | BV    | 374 | HIS  |
| 6   | BV    | 378 | ASN  |
| 6   | BV    | 434 | ASN  |
| 6   | BW    | 231 | ASN  |
| 6   | BW    | 234 | GLN  |
| 6   | BW    | 303 | GLN  |
| 6   | BW    | 374 | HIS  |
| 6   | BW    | 378 | ASN  |
| 6   | BW    | 431 | ASN  |
| 6   | BW    | 434 | ASN  |
| 6   | BX    | 231 | ASN  |
| 6   | BX    | 234 | GLN  |
| 6   | BX    | 281 | HIS  |
| 6   | BX    | 303 | GLN  |
| 6   | BX    | 374 | HIS  |
| 6   | BX    | 378 | ASN  |
| 6   | BX    | 434 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

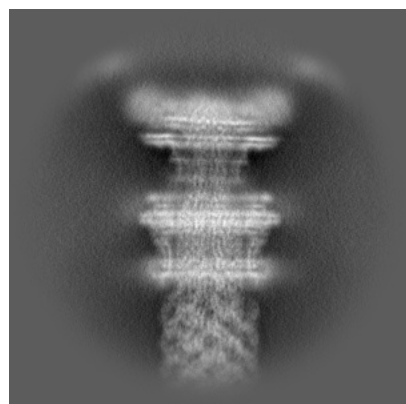
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37630. These allow visual inspection of the internal detail of the map and identification of artifacts.

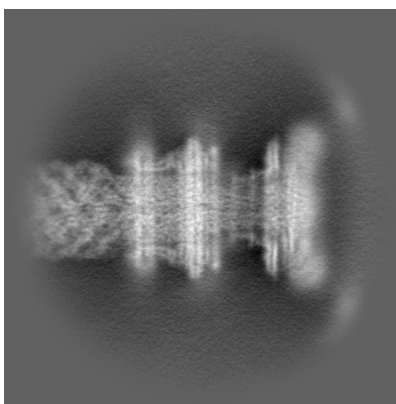
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

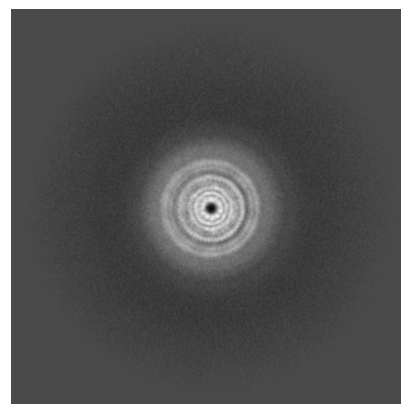
#### 6.1.1 Primary map



X

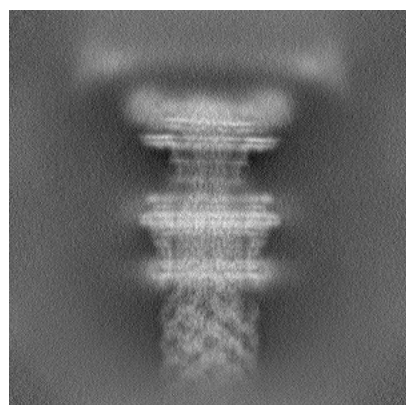


Y

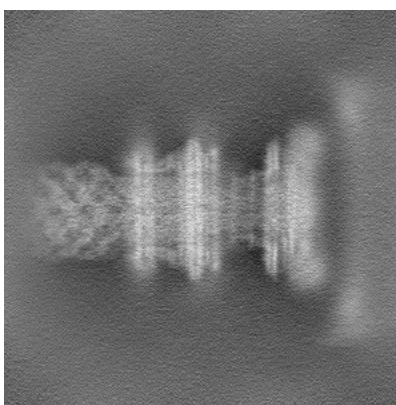


Z

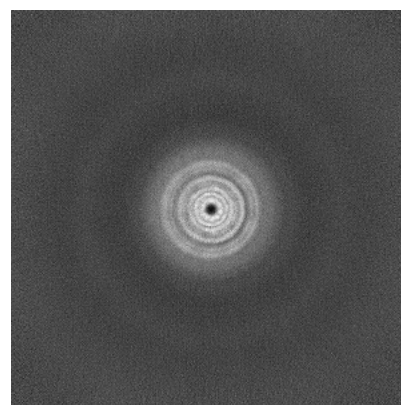
#### 6.1.2 Raw map



X



Y

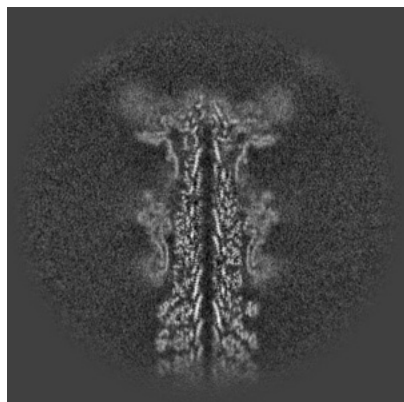


Z

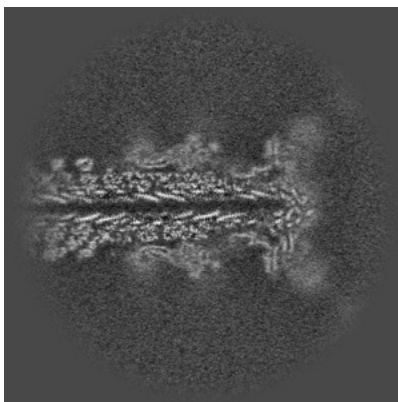
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

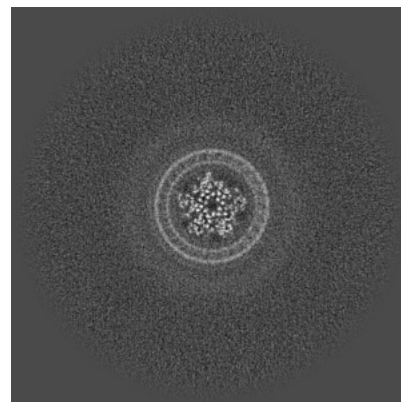
### 6.2.1 Primary map



X Index: 256

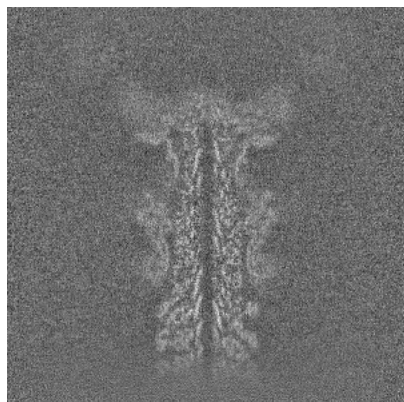


Y Index: 256

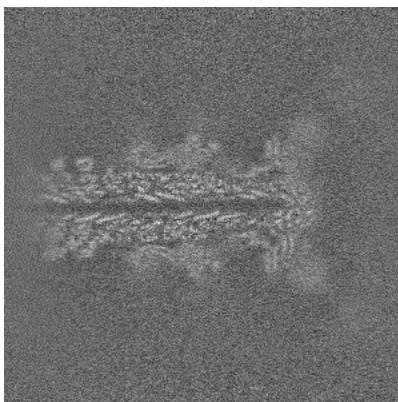


Z Index: 256

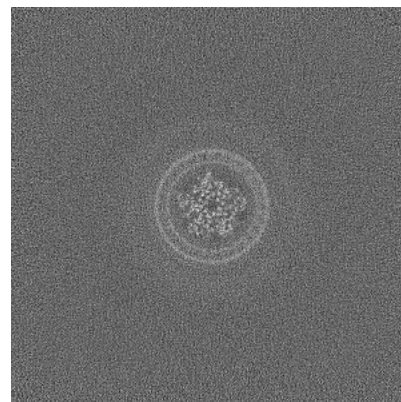
### 6.2.2 Raw map



X Index: 256



Y Index: 256



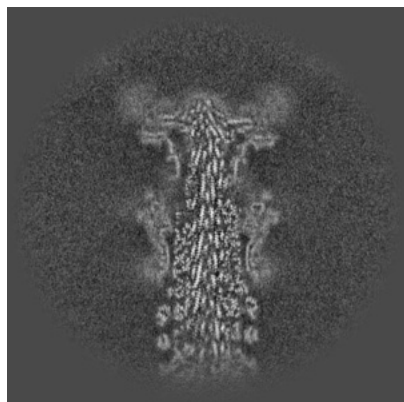
Z Index: 256

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

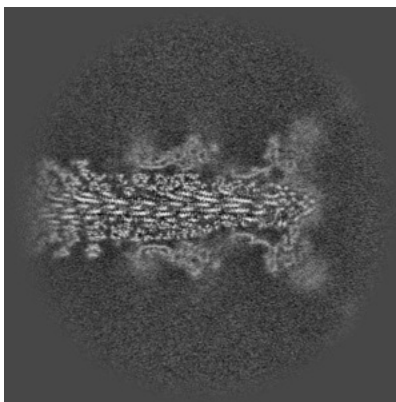


## 6.3 Largest variance slices [i](#)

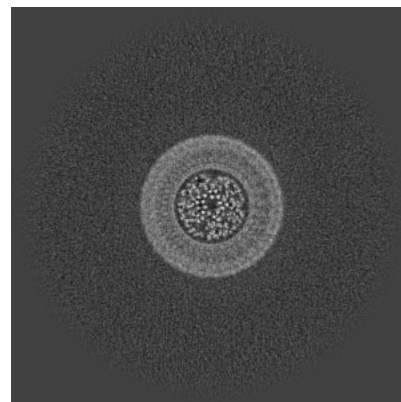
### 6.3.1 Primary map



X Index: 247

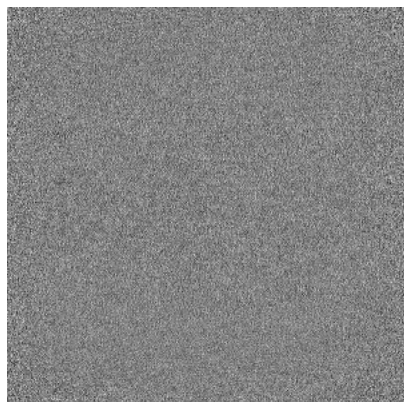


Y Index: 246

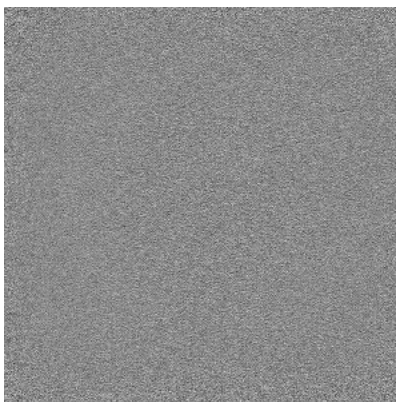


Z Index: 239

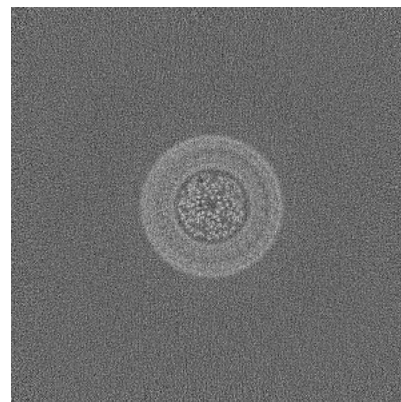
### 6.3.2 Raw map



X Index: 0



Y Index: 0

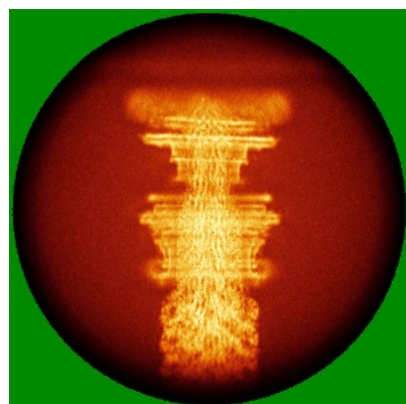


Z Index: 240

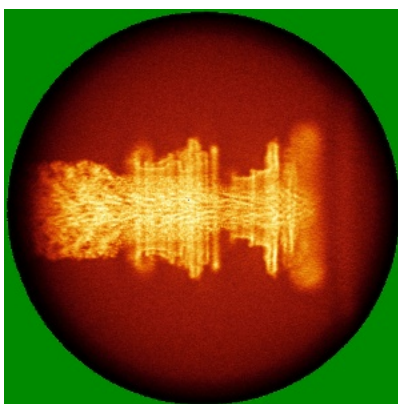
The images above show the largest variance slices of the map in three orthogonal directions.

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

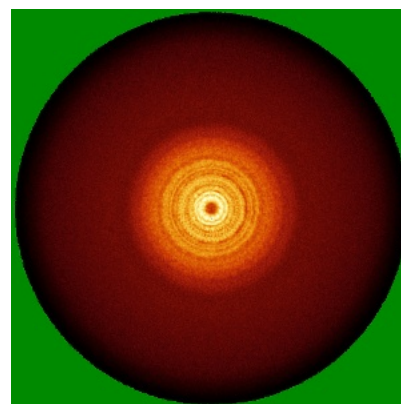
### 6.4.1 Primary map



X

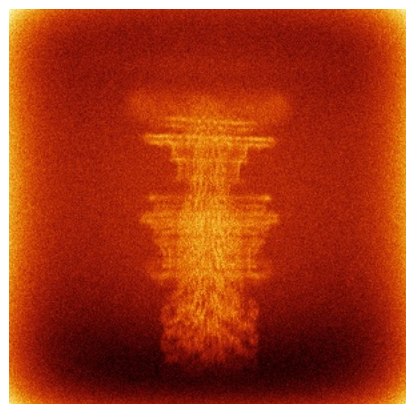


Y

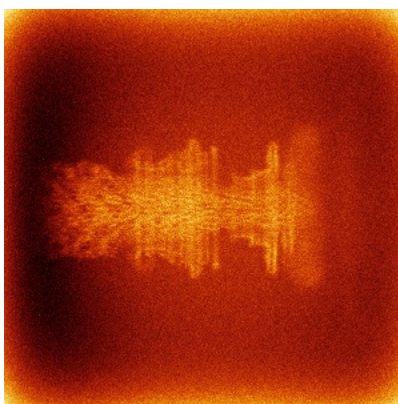


Z

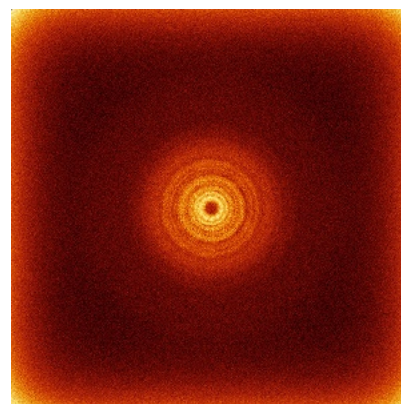
### 6.4.2 Raw map



X



Y



Z

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

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

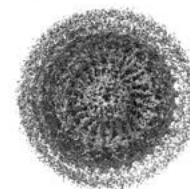
### 6.5.1 Primary map



X



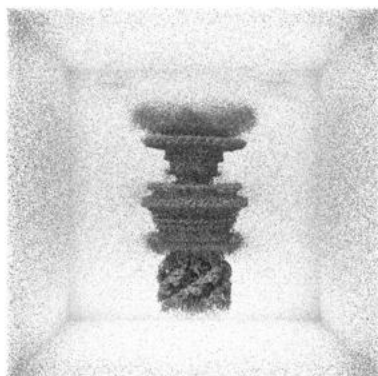
Y



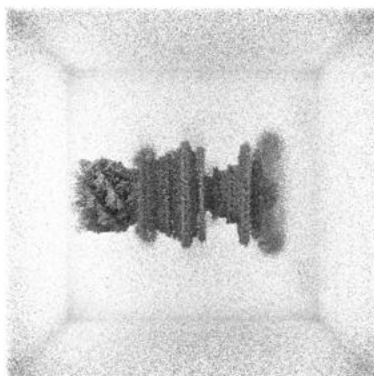
Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

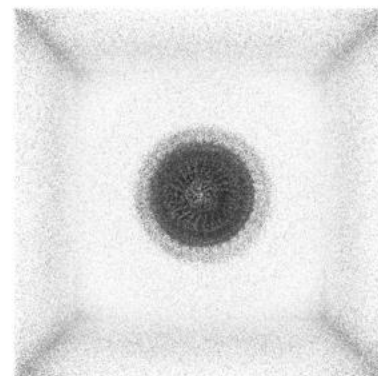
### 6.5.2 Raw map



X



Y



Z

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

## 6.6 Mask visualisation [i](#)

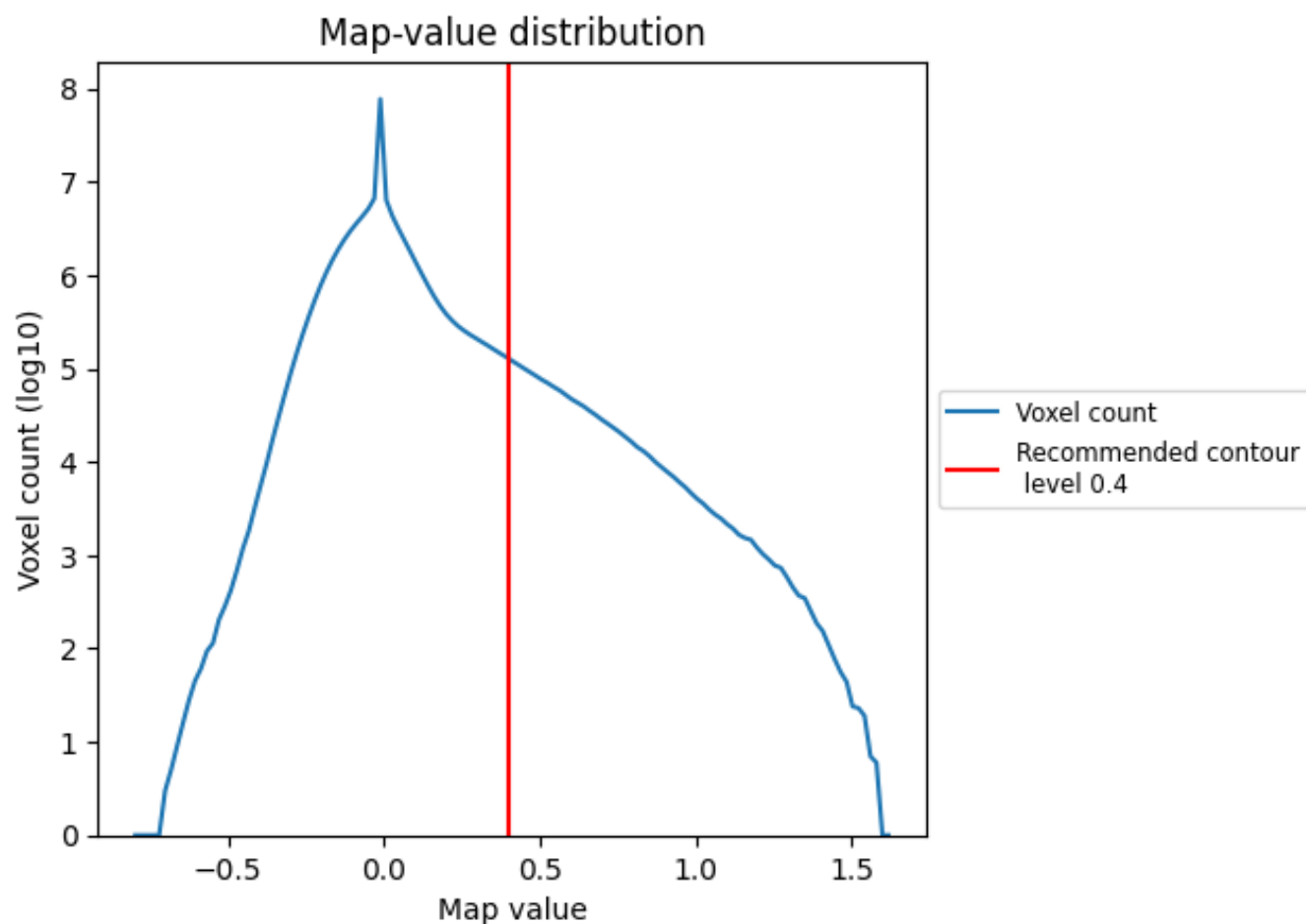
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

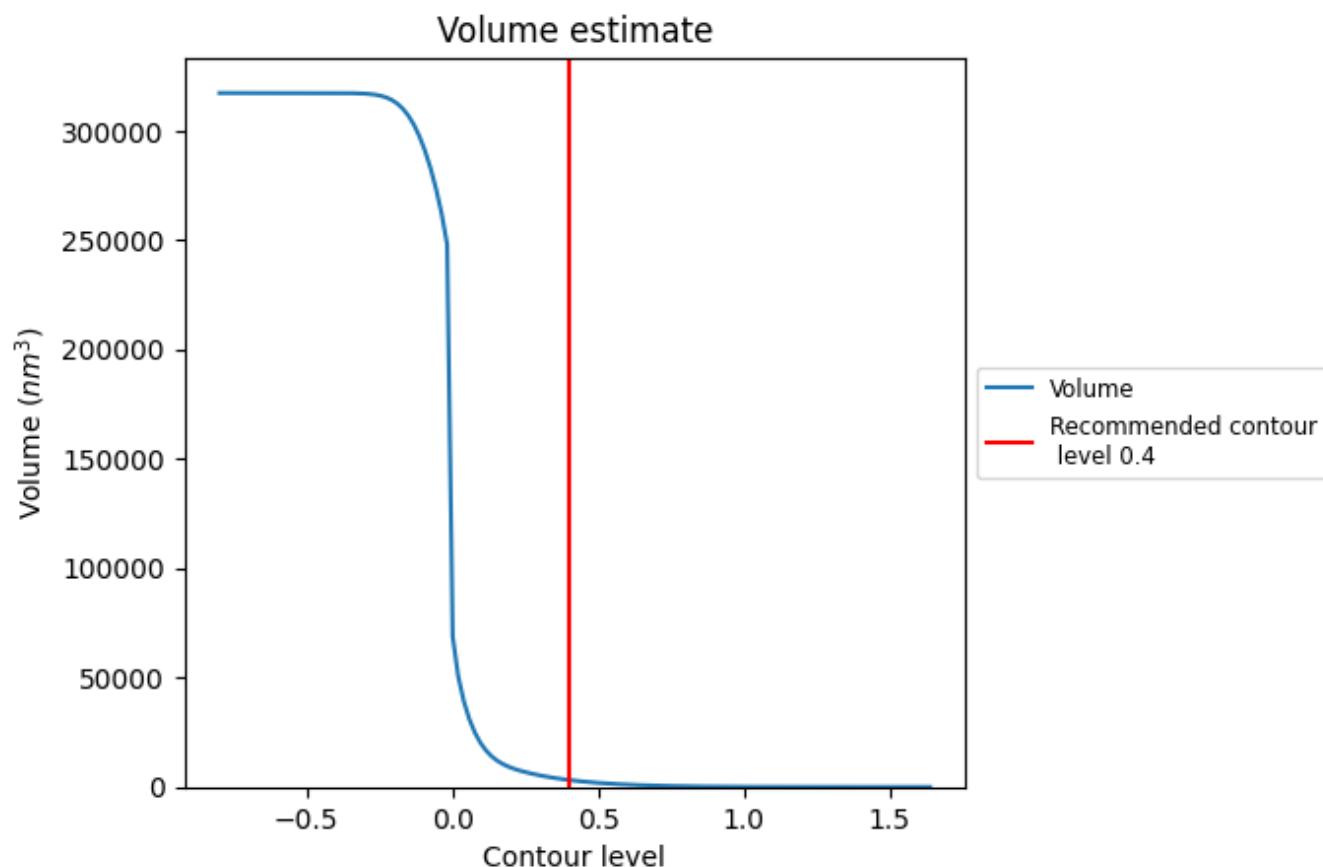
This section contains the results of statistical analysis of the map.

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



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

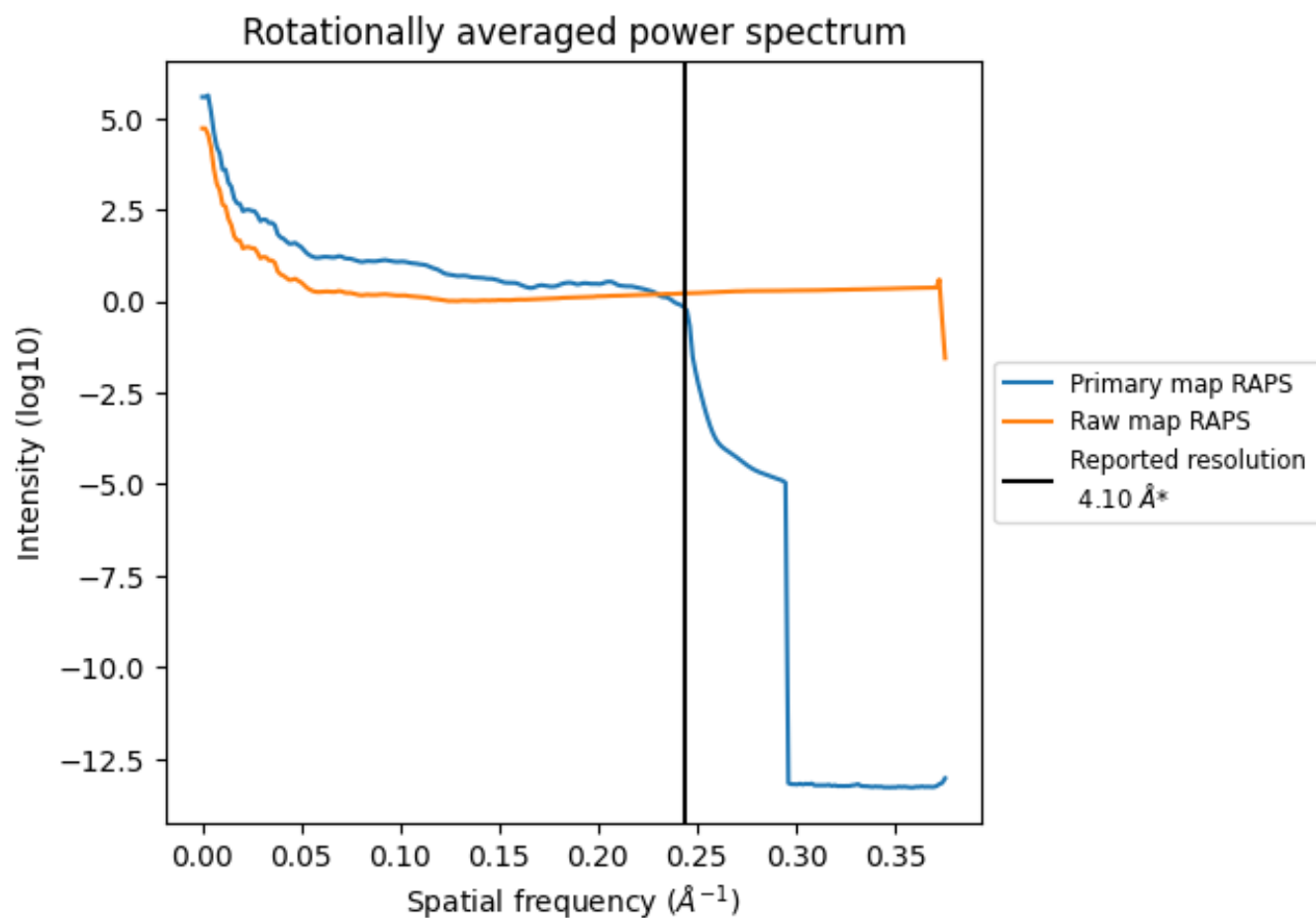
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3185 nm<sup>3</sup>; this corresponds to an approximate mass of 2877 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 ⓘ

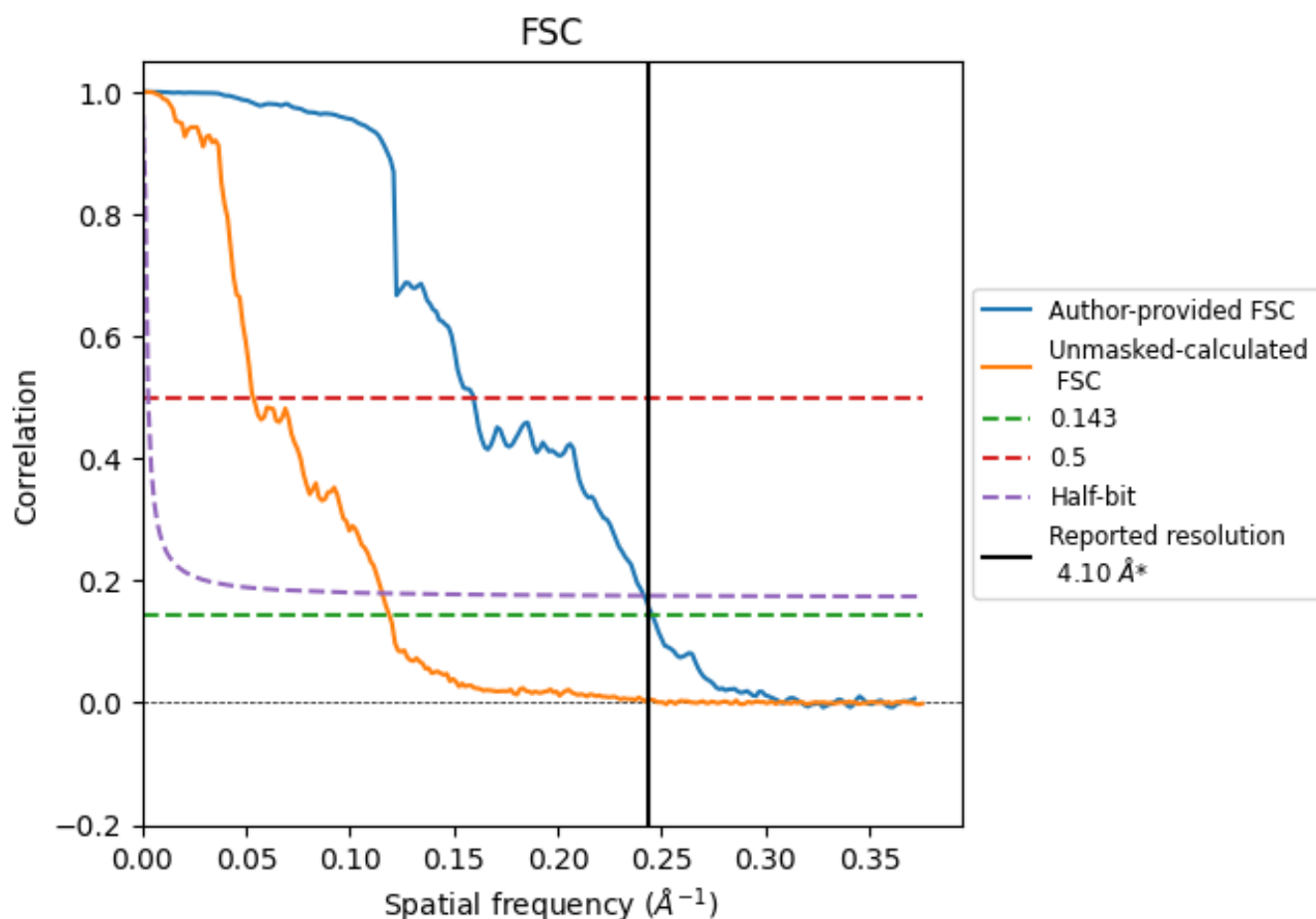


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.244 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

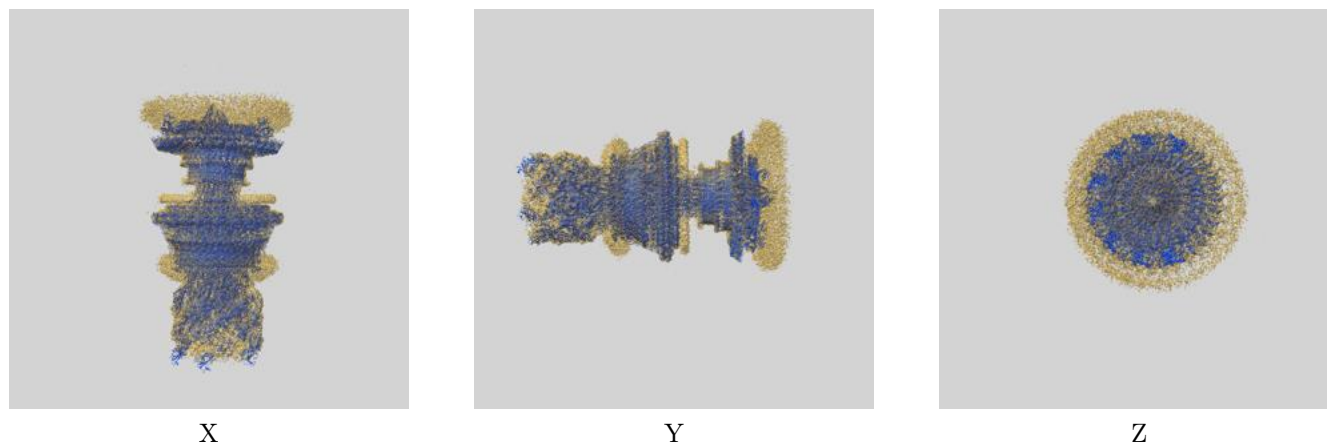
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.10                               | -     | -        |
| Author-provided FSC curve | 4.07                               | 6.28  | 4.14     |
| Unmasked-calculated*      | 8.41                               | 18.73 | 8.66     |

\*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 8.41 differs from the reported value 4.1 by more than 10 %

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

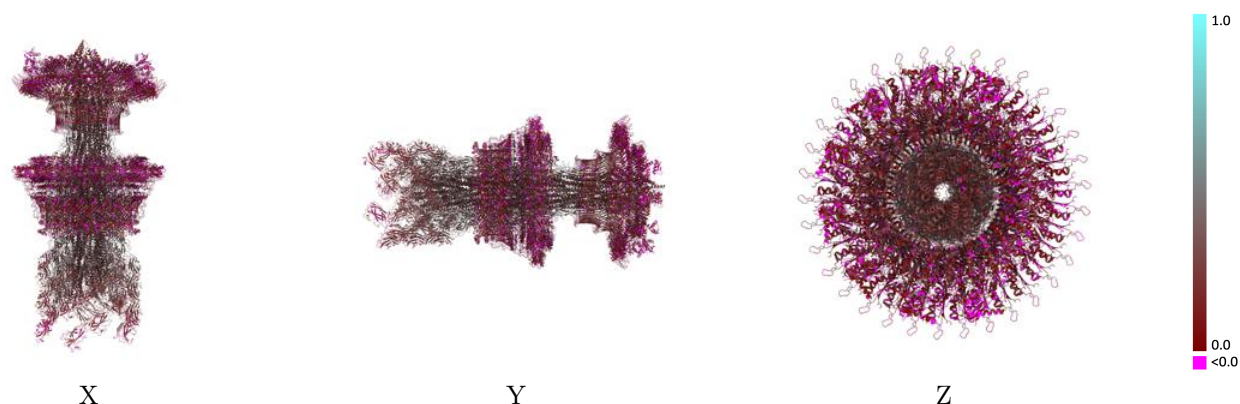
This section contains information regarding the fit between EMDB map EMD-37630 and PDB model 8WLT. Per-residue inclusion information can be found in section [3](#) on page [24](#).

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



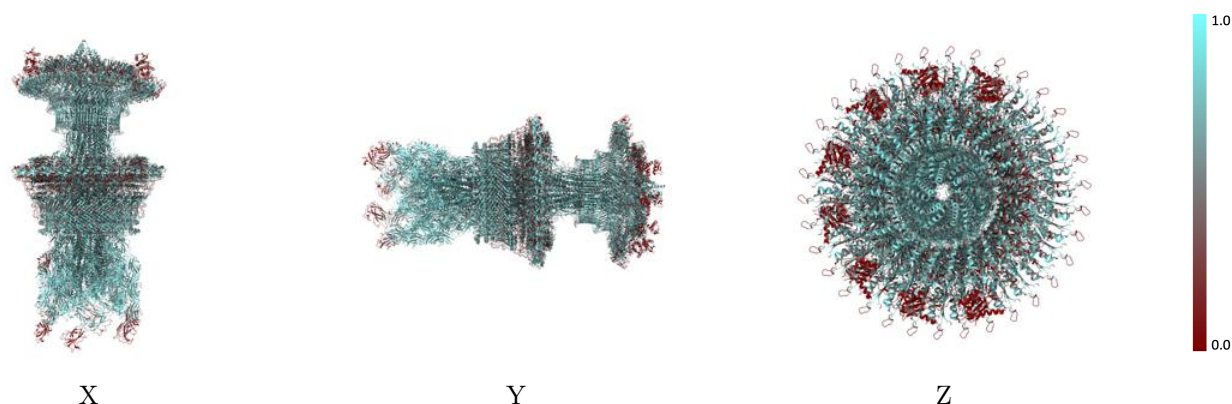
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



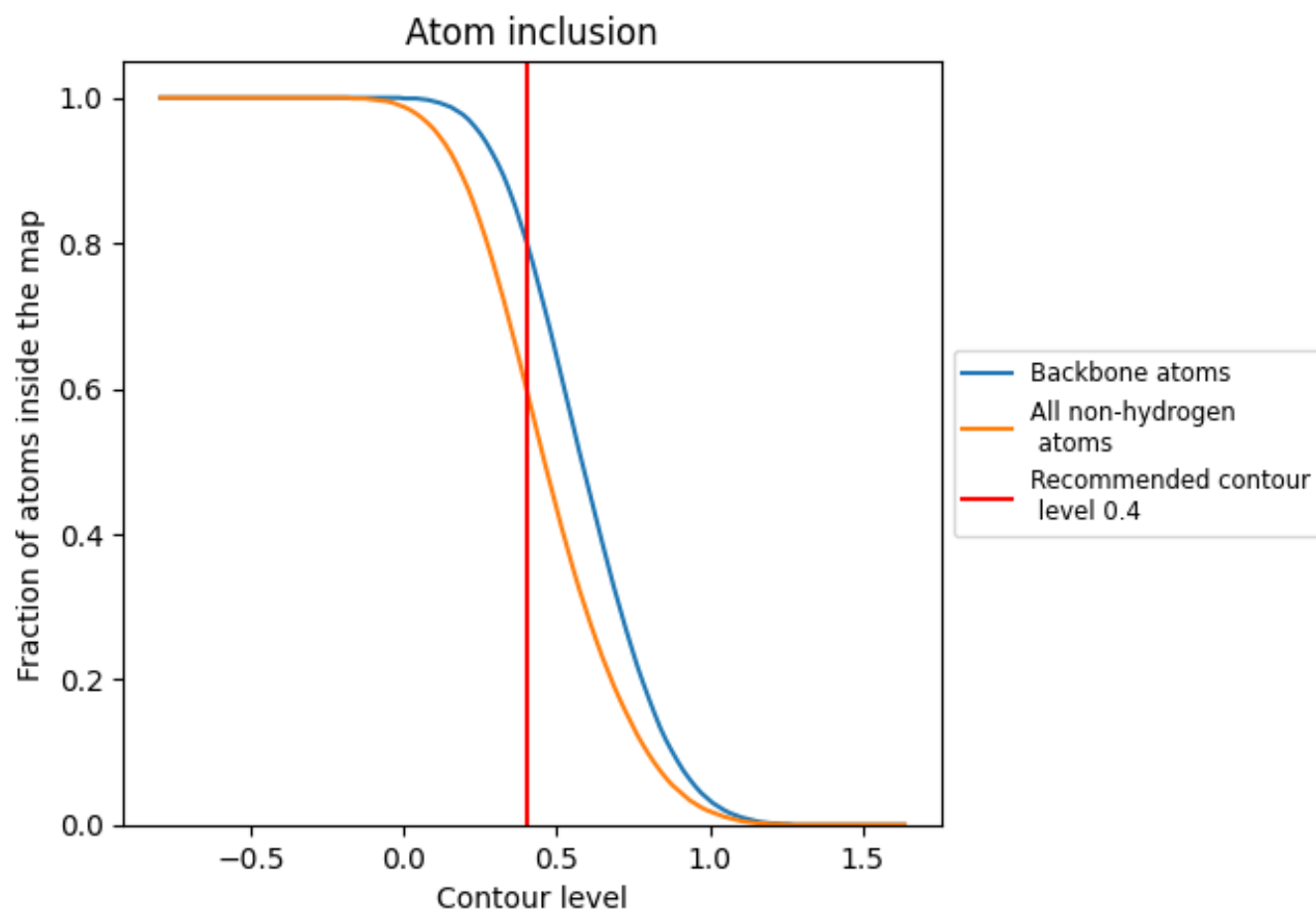
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 60% 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 (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6010   |  0.2210   |
| 0     |  0.6940   |  0.3430   |
| 1     |  0.6920   |  0.3390   |
| 2     |  0.6780   |  0.3430   |
| 3     |  0.6990   |  0.3360   |
| 4     |  0.7050   |  0.3390   |
| 5     |  0.6890   |  0.3410   |
| 6     |  0.7000   |  0.3430   |
| 7     |  0.7050   |  0.3460   |
| 8     |  0.7000   |  0.3440   |
| 9     |  0.6990   |  0.3440   |
| A     |  0.5000   |  0.1420   |
| A0    |  0.6570   |  0.3040   |
| A1    |  0.6240   |  0.2630   |
| A2    |  0.6620  |  0.2750  |
| A3    |  0.6410 |  0.2660 |
| A4    |  0.6090 |  0.2540 |
| A5    |  0.6020 |  0.2560 |
| A6    |  0.6260 |  0.2980 |
| A7    |  0.6680 |  0.2990 |
| A8    |  0.6560 |  0.2990 |
| A9    |  0.6780 |  0.2950 |
| AA    |  0.6770 |  0.3340 |
| AB    |  0.7270 |  0.3410 |
| AC    |  0.7260 |  0.3560 |
| AD    |  0.7180 |  0.3410 |
| AE    |  0.7100 |  0.3340 |
| AF    |  0.6820 |  0.3310 |
| AG    |  0.7090 |  0.3440 |
| AH    |  0.7040 |  0.3490 |
| AI    |  0.7050 |  0.3470 |
| AJ    |  0.6920 |  0.3430 |
| AK    |  0.6950 |  0.3430 |
| AL    |  0.6840 |  0.3310 |
| AM    |  0.6980 |  0.3480 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| AN    |  0.6980   |  0.3400   |
| AO    |  0.6000   |  0.1490   |
| AP    |  0.5970   |  0.1380   |
| AQ    |  0.5990   |  0.1500   |
| AR    |  0.6430   |  0.1560   |
| AS    |  0.6100   |  0.1490   |
| AT    |  0.6400   |  0.1730   |
| AU    |  0.6380   |  0.1670   |
| AV    |  0.6220   |  0.1490   |
| AW    |  0.6150   |  0.1550   |
| AX    |  0.6250   |  0.1600   |
| AY    |  0.6250   |  0.1370   |
| AZ    |  0.6350   |  0.1560   |
| Aa    |  0.6330   |  0.1520   |
| Ab    |  0.5990   |  0.2220   |
| Ac    |  0.6450   |  0.1550   |
| Ad    |  0.6390   |  0.1510   |
| Ae    |  0.6260   |  0.1520   |
| Af    |  0.6320   |  0.1300   |
| Ag    |  0.6360  |  0.1470  |
| Ah    |  0.6350 |  0.1320 |
| Ai    |  0.6330 |  0.1440 |
| Aj    |  0.6180 |  0.1450 |
| Ak    |  0.6020 |  0.1370 |
| Al    |  0.6030 |  0.1530 |
| Am    |  0.6070 |  0.1450 |
| An    |  0.6020 |  0.1370 |
| Ao    |  0.5850 |  0.1270 |
| Ap    |  0.5980 |  0.1500 |
| Aq    |  0.6660 |  0.2410 |
| Ar    |  0.6660 |  0.2290 |
| As    |  0.6500 |  0.2090 |
| At    |  0.6460 |  0.2490 |
| Au    |  0.6580 |  0.2420 |
| Av    |  0.6730 |  0.2690 |
| Aw    |  0.6880 |  0.2770 |
| Ax    |  0.6800 |  0.2750 |
| Ay    |  0.6610 |  0.2730 |
| Az    |  0.5230 |  0.2200 |
| B     |  0.4930 |  0.1220 |
| BA    |  0.6650 |  0.3090 |
| BB    |  0.6940 |  0.3290 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| BC    |  0.7000   |  0.3350   |
| BD    |  0.6860   |  0.3390   |
| BE    |  0.6960   |  0.3350   |
| BF    |  0.6890   |  0.3090   |
| BG    |  0.5430   |  0.3200   |
| BH    |  0.6410   |  0.3630   |
| BI    |  0.6240   |  0.3380   |
| BJ    |  0.7670   |  0.3940   |
| BK    |  0.7360   |  0.3660   |
| BL    |  0.6800   |  0.3550   |
| BM    |  0.7290   |  0.3910   |
| BN    |  0.6800   |  0.3410   |
| BO    |  0.7520   |  0.4020   |
| BP    |  0.6700   |  0.3130   |
| BQ    |  0.6500   |  0.3280   |
| BR    |  0.5940   |  0.1420   |
| BS    |  0.5910   |  0.1320   |
| BT    |  0.6110   |  0.1480   |
| BU    |  0.6150  |  0.1570  |
| BV    |  0.6070 |  0.1450 |
| BW    |  0.6270 |  0.1610 |
| BX    |  0.6100 |  0.1560 |
| C     |  0.5140 |  0.1440 |
| D     |  0.5180 |  0.1420 |
| E     |  0.5030 |  0.1370 |
| F     |  0.5050 |  0.1320 |
| G     |  0.5180 |  0.1380 |
| H     |  0.5290 |  0.1420 |
| I     |  0.5420 |  0.1350 |
| J     |  0.5330 |  0.1450 |
| K     |  0.5290 |  0.1490 |
| L     |  0.5400 |  0.1490 |
| M     |  0.5420 |  0.1610 |
| N     |  0.5320 |  0.1480 |
| O     |  0.5220 |  0.1300 |
| P     |  0.5240 |  0.1450 |
| Q     |  0.5360 |  0.1470 |
| R     |  0.5220 |  0.1420 |
| S     |  0.5400 |  0.1290 |
| T     |  0.5110 |  0.1390 |
| U     |  0.5270 |  0.1470 |
| UI    |  0.1300 |  0.0680 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| UJ    |  0.1340   |  0.0770   |
| UK    |  0.1080   |  0.0850   |
| UL    |  0.1020   |  0.0320   |
| UM    |  0.0690   |  0.0500   |
| UN    |  0.1330   |  0.0700   |
| UO    |  0.1360   |  0.0810   |
| UP    |  0.1950   |  0.0760   |
| V     |  0.5270   |  0.1490   |
| W     |  0.5200   |  0.1430   |
| WA    |  0.6210   |  0.1920   |
| WB    |  0.6410   |  0.2010   |
| WC    |  0.6490   |  0.2210   |
| WD    |  0.6120   |  0.1780   |
| WE    |  0.6320   |  0.1860   |
| WF    |  0.5930   |  0.1650   |
| WG    |  0.5140   |  0.1550   |
| WH    |  0.4740   |  0.1420   |
| WI    |  0.4840   |  0.1480   |
| WJ    |  0.4820   |  0.1460   |
| WK    |  0.3380  |  0.1160  |
| WL    |  0.3880 |  0.1150 |
| WM    |  0.4870 |  0.1190 |
| WN    |  0.4520 |  0.1200 |
| WO    |  0.4240 |  0.1050 |
| WP    |  0.5660 |  0.1610 |
| WQ    |  0.5480 |  0.1810 |
| WR    |  0.5700 |  0.1690 |
| WS    |  0.6120 |  0.2160 |
| WT    |  0.6190 |  0.1870 |
| WU    |  0.5990 |  0.2010 |
| WV    |  0.6180 |  0.2050 |
| WW    |  0.6090 |  0.1940 |
| X     |  0.5190 |  0.1620 |
| Y     |  0.5070 |  0.1390 |
| Z     |  0.5150 |  0.1530 |
| ZA    |  0.7070 |  0.3440 |
| ZB    |  0.7120 |  0.3440 |
| ZC    |  0.7230 |  0.3510 |
| ZD    |  0.7050 |  0.3420 |
| ZE    |  0.6980 |  0.3410 |
| ZF    |  0.5380 |  0.2920 |
| ZG    |  0.7300 |  0.3270 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| ZH    |  0.7480   |  0.3250   |
| ZI    |  0.7530   |  0.3290   |
| ZJ    |  0.7500   |  0.3260   |
| ZK    |  0.7630   |  0.3230   |
| ZL    |  0.7550   |  0.3280   |
| ZM    |  0.7440   |  0.3180   |
| ZN    |  0.7530   |  0.3170   |
| ZO    |  0.7570   |  0.3160   |
| ZP    |  0.7510   |  0.3160   |
| ZQ    |  0.7460   |  0.3080   |
| ZR    |  0.7440   |  0.3050   |
| ZS    |  0.7540   |  0.3060   |
| ZT    |  0.7450   |  0.3010   |
| ZU    |  0.7320   |  0.2980   |
| ZV    |  0.7400   |  0.2950   |
| ZW    |  0.7290   |  0.2830   |
| ZX    |  0.7140   |  0.2830   |
| ZY    |  0.7090   |  0.2760   |
| ZZ    |  0.6810  |  0.2700  |
| Za    |  0.6710 |  0.2720 |
| Zb    |  0.6320 |  0.2480 |
| Zc    |  0.6290 |  0.2530 |
| Zd    |  0.5790 |  0.2460 |
| Ze    |  0.5240 |  0.2320 |
| Zf    |  0.5060 |  0.2320 |
| Zg    |  0.4670 |  0.2100 |
| Zh    |  0.4390 |  0.2040 |
| a     |  0.4680 |  0.1160 |
| b     |  0.4770 |  0.1300 |
| c     |  0.4540 |  0.1230 |
| d     |  0.4850 |  0.1250 |
| e     |  0.4730 |  0.1230 |
| f     |  0.4860 |  0.1360 |
| g     |  0.5150 |  0.1260 |
| h     |  0.5190 |  0.1440 |
| i     |  0.5260 |  0.1450 |
| j     |  0.5220 |  0.1390 |
| k     |  0.5320 |  0.1400 |
| l     |  0.5100 |  0.1340 |
| m     |  0.5050 |  0.1400 |
| n     |  0.4890 |  0.1230 |
| o     |  0.5040 |  0.1430 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| p     |  0.5020 |  0.1290 |
| q     |  0.4840 |  0.1170 |
| r     |  0.4790 |  0.1220 |
| s     |  0.4910 |  0.1180 |
| t     |  0.4890 |  0.1330 |
| u     |  0.4570 |  0.1090 |
| v     |  0.4730 |  0.1200 |
| w     |  0.4790 |  0.1150 |
| x     |  0.4520 |  0.1060 |
| y     |  0.4510 |  0.1040 |
| z     |  0.4600 |  0.1200 |