



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:29 AM UTC

PDB ID : 7TNQ / pdb\_00007tnq  
EMDB ID : EMD-26018  
Title : The symmetry-released subpellicular microtubule map from detergent-extracted Toxoplasma cells  
Authors : Sun, S.Y.; Pintilie, G.D.; Chen, M.  
Deposited on : 2022-01-21  
Resolution : 8.40 Å(reported)  
Based on initial model : 7MIZ

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

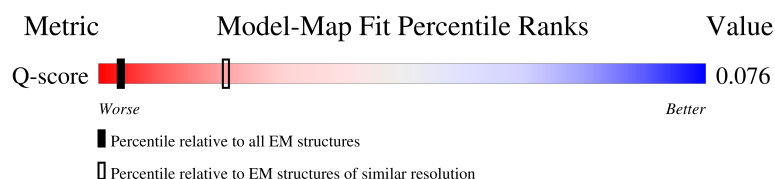
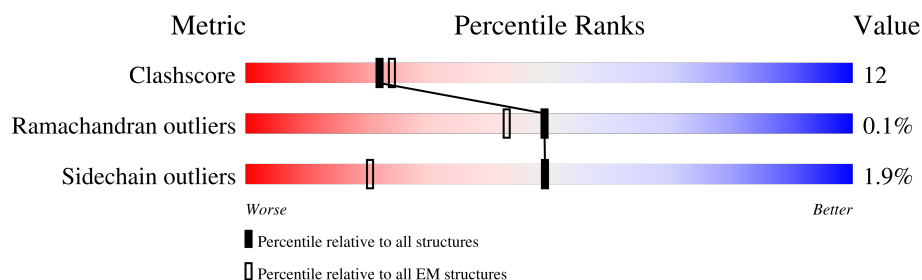
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

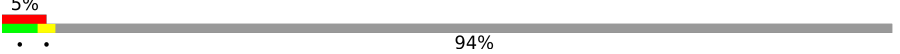
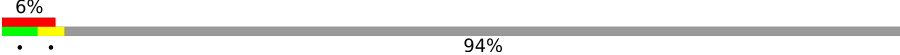
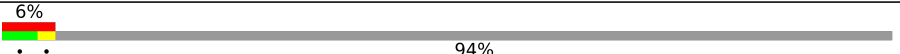
The reported resolution of this entry is 8.40 Å.

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                       | 298 ( 7.90 - 8.90 )                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 0     | 351    |  |
| 1   | 1     | 351    |  |
| 1   | 10    | 351    |  |
| 1   | 11    | 351    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 12    | 351    |                  |
| 1   | 13    | 351    |                  |
| 1   | 14    | 351    |                  |
| 1   | 15    | 351    |                  |
| 1   | 16    | 351    |                  |
| 1   | 17    | 351    |                  |
| 1   | 18    | 351    |                  |
| 1   | 19    | 351    |                  |
| 1   | 2     | 351    |                  |
| 1   | 20    | 351    |                  |
| 1   | 21    | 351    |                  |
| 1   | 22    | 351    |                  |
| 1   | 23    | 351    |                  |
| 1   | 3     | 351    |                  |
| 1   | 4     | 351    |                  |
| 1   | 5     | 351    |                  |
| 1   | 6     | 351    |                  |
| 1   | 7     | 351    |                  |
| 1   | 8     | 351    |                  |
| 1   | 9     | 351    |                  |
| 2   | A0    | 453    |                  |
| 2   | A2    | 453    |                  |
| 2   | A4    | 453    |                  |
| 2   | A6    | 453    |                  |
| 2   | A8    | 453    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B0    | 453    |                  |
| 2   | B2    | 453    |                  |
| 2   | B4    | 453    |                  |
| 2   | B6    | 453    |                  |
| 2   | B8    | 453    |                  |
| 2   | C0    | 453    |                  |
| 2   | C2    | 453    |                  |
| 2   | C4    | 453    |                  |
| 2   | C6    | 453    |                  |
| 2   | C8    | 453    |                  |
| 2   | D0    | 453    |                  |
| 2   | D2    | 453    |                  |
| 2   | D4    | 453    |                  |
| 2   | D6    | 453    |                  |
| 2   | D8    | 453    |                  |
| 2   | E0    | 453    |                  |
| 2   | E2    | 453    |                  |
| 2   | E4    | 453    |                  |
| 2   | E6    | 453    |                  |
| 2   | E8    | 453    |                  |
| 2   | F0    | 453    |                  |
| 3   | A1    | 449    |                  |
| 3   | A3    | 449    |                  |
| 3   | A5    | 449    |                  |
| 3   | A7    | 449    |                  |

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| Mol | Chain | Length | Quality of chain                      |
|-----|-------|--------|---------------------------------------|
| 3   | A9    | 449    | <div>49%</div> <div>72% 21% 5%</div>  |
| 3   | B1    | 449    | <div>56%</div> <div>75% 19% 5%</div>  |
| 3   | B3    | 449    | <div>49%</div> <div>73% 20% 5%</div>  |
| 3   | B5    | 449    | <div>53%</div> <div>73% 20% 5%</div>  |
| 3   | B7    | 449    | <div>40%</div> <div>75% 19% 5%</div>  |
| 3   | B9    | 449    | <div>51%</div> <div>73% 20% 5%</div>  |
| 3   | C1    | 449    | <div>40%</div> <div>68% 25% 5%</div>  |
| 3   | C3    | 449    | <div>46%</div> <div>69% 25% 5%</div>  |
| 3   | C5    | 449    | <div>45%</div> <div>70% 23% 5%</div>  |
| 3   | C7    | 449    | <div>48%</div> <div>70% 23% 5%</div>  |
| 3   | C9    | 449    | <div>51%</div> <div>68% 25% 5%</div>  |
| 3   | D1    | 449    | <div>55%</div> <div>70% 23% 5%</div>  |
| 3   | D3    | 449    | <div>54%</div> <div>66% 27% 5%</div>  |
| 3   | D5    | 449    | <div>55%</div> <div>62% 29% 5%</div>  |
| 3   | D7    | 449    | <div>53%</div> <div>70% 23% 5%</div>  |
| 3   | D9    | 449    | <div>50%</div> <div>69% 24% 5%</div>  |
| 3   | E1    | 449    | <div>46%</div> <div>74% 20% 5%</div>  |
| 3   | E3    | 449    | <div>43%</div> <div>74% 19% 5%</div>  |
| 3   | E5    | 449    | <div>45%</div> <div>70% 24% 5%</div>  |
| 3   | E7    | 449    | <div>40%</div> <div>69% 24% 5%</div>  |
| 3   | E9    | 449    | <div>53%</div> <div>71% 23% 5%</div>  |
| 3   | F1    | 449    | <div>43%</div> <div>65% 28% 5%</div>  |
| 4   | a     | 220    | <div>43%</div> <div>45% 22% 32%</div> |
| 4   | b     | 220    | <div>48%</div> <div>48% 19% 32%</div> |
| 4   | c     | 220    | <div>41%</div> <div>65% 25% 9%</div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | d     | 220    |                  |
| 4   | e     | 220    |                  |
| 4   | f     | 220    |                  |
| 4   | g     | 220    |                  |
| 4   | h     | 220    |                  |
| 4   | i     | 220    |                  |
| 4   | j     | 220    |                  |
| 4   | m     | 220    |                  |
| 4   | n     | 220    |                  |
| 4   | o     | 220    |                  |
| 4   | p     | 220    |                  |
| 4   | q     | 220    |                  |
| 4   | r     | 220    |                  |
| 4   | s     | 220    |                  |
| 4   | t     | 220    |                  |
| 4   | u     | 220    |                  |
| 4   | v     | 220    |                  |
| 5   | k     | 189    |                  |
| 5   | l     | 189    |                  |
| 5   | w     | 189    |                  |
| 5   | x     | 189    |                  |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 213168 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 Microtubule associated protein SPM1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 1     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 10    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 11    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 12    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 13    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 14    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 15    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 16    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 17    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 18    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 19    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 2     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 20    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 21    | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 22    | 20       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 160   | 105 | 26 | 28 | 1 |         |       |
| 1   | 23    | 20       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 160   | 105 | 26 | 28 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 3     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 4     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 5     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 6     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 7     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 8     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |
| 1   | 9     | 22       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 174   | 114 | 28 | 31 | 1 |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 0     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 1     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 10    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 11    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 12    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 13    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 14    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 15    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 16    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 17    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 18    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 19    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 2     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 20    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 21    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 22    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 23    | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 3     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 4     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 5     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 6     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 7     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 8     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |
| 9     | 263     | ALA      | VAL    | conflict | UNP S8F1Y1 |

- Molecule 2 is a protein called Tubulin alpha chain.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2   | A0    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | A2    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | A4    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | A6    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | A8    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | B0    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | B2    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | B4    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | B6    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | B8    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | C0    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | C2    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | C4    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | C6    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | C8    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | D0    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | D2    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | D4    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | D6    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | D8    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |
| 2   | E0    | 428      | Total<br>3325 | C<br>2105 | N<br>569 | O<br>625 | S<br>26 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | E2    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E4    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E6    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E8    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | F0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |

- Molecule 3 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | A1    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A3    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A5    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A7    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A9    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B1    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B3    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B5    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B7    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B9    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | C1    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | C3    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | C5    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | C7    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 3   | C9    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D1    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D3    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D5    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D7    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D9    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E1    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E3    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E5    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E7    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E9    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | F1    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |

- Molecule 4 is a protein called PDI family protein.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 4   | a     | 150      | Total<br>1198 | C<br>763  | N<br>213 | O<br>217 | S<br>5 | 0       | 0     |
| 4   | b     | 150      | Total<br>1198 | C<br>763  | N<br>213 | O<br>217 | S<br>5 | 0       | 0     |
| 4   | c     | 201      | Total<br>1608 | C<br>1021 | N<br>283 | O<br>297 | S<br>7 | 0       | 0     |
| 4   | d     | 201      | Total<br>1608 | C<br>1021 | N<br>283 | O<br>297 | S<br>7 | 0       | 0     |
| 4   | e     | 201      | Total<br>1608 | C<br>1021 | N<br>283 | O<br>297 | S<br>7 | 0       | 0     |
| 4   | f     | 201      | Total<br>1608 | C<br>1021 | N<br>283 | O<br>297 | S<br>7 | 0       | 0     |
| 4   | g     | 201      | Total<br>1608 | C<br>1021 | N<br>283 | O<br>297 | S<br>7 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | h     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | i     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | j     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | m     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | n     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | o     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | p     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | q     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | r     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | s     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | t     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | u     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 4   | v     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |

- Molecule 5 is a protein called PDI family protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | k     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1140  | 738 | 203 | 195 | 4 |         |       |
| 5   | l     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1140  | 738 | 203 | 195 | 4 |         |       |
| 5   | w     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 755 | 207 | 205 | 5 |         |       |
| 5   | x     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1172  | 755 | 207 | 205 | 5 |         |       |







[illegible]

- Molecule 1: Microtubule associated protein SPM1

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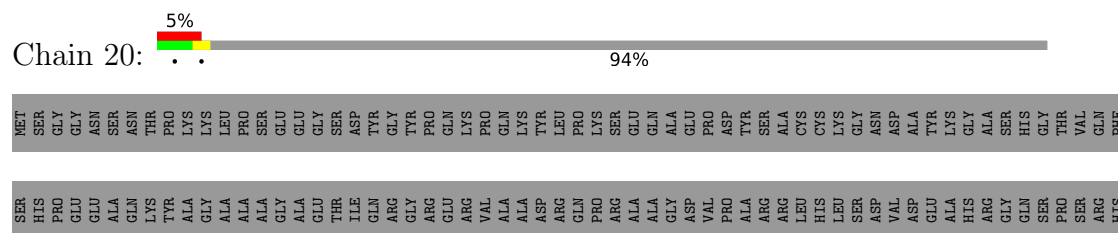
- Molecule 1: Microtubule associated protein SPM1

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- Molecule 1: Microtubule associated protein SPM1

- Molecule 1: Microtubule associated protein SPM1



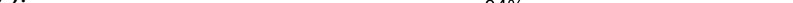
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| GLN | GLU | ASP | GLN |
| ASN | GLY | TYR | VAL |
| HIS | SER | PRO | SER |
| VAL | THR | PRO | VAL |
| PHE | THR | LYS | GLN |
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|     | LYS | LYS |     |
|     | THR | THR |     |
|     | VAL | VAL |     |
|     | GLU | GLU |     |
|     | LEU | LEU |     |
|     | PRO | PRO |     |
|     | THR | THR |     |
|     | PRO | PRO |     |
|     | LEU | LEU |     |
|     | VAL | VAL |     |
|     | THR | THR |     |
|     | GLY | GLY |     |
|     | ASP | ASP |     |
|     | THR | THR |     |
|     | VAL | VAL |     |
|     | GLN | GLN |     |
|     | LYS | LYS |     |
|     | THR | THR |     |
|     | VAL | VAL |     |
|     | GLU | GLU |     |
|     | LEU | LEU |     |
|     | PRO | PRO |     |
|     | THR | THR |     |
|     | PRO | PRO |     |
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- Molecule 1: Microtubule associated protein SPM1

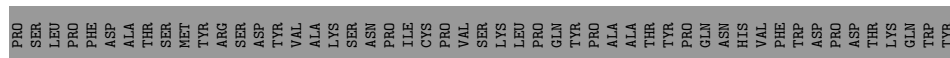
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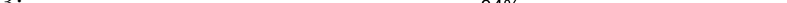
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| V252 | SER | ALA | ALA |
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| A253 | TYR | HIS | HIS |
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|      | ASN | THR | THR |
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| P258 | PRO | ARG | ARG |
|      | CYS | ALA | ALA |
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|      | THR | VAL | VAL |
| THR  | VAL | VAL | VAL |
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| GLU  | LYS | THR | THR |
|      | LEU | THR | THR |
| GLN  | GLN | THR | THR |
|      | TYR | GLN | GLN |
| PRO  | PRO | TYR | TYR |
|      | PRO | GLN | GLN |
| ALA  | ALA | ARG | ARG |
|      | THR | GLN | GLN |
| THR  | THR | PHE | PHE |
|      | PRO | VAL | VAL |
| GLY  | GLY | VAL | VAL |
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| GLN  | GLN | PRO | PRO |
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|      | HIS | HIS | HIS |
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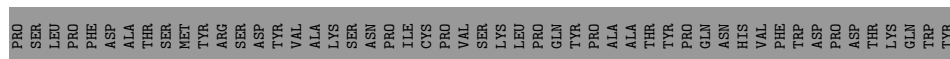
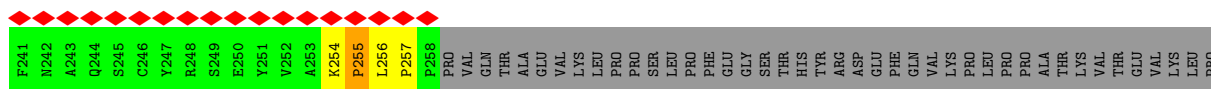
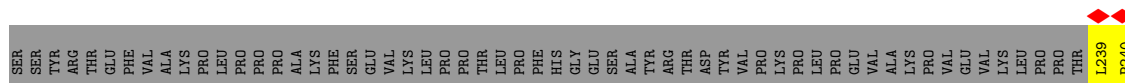
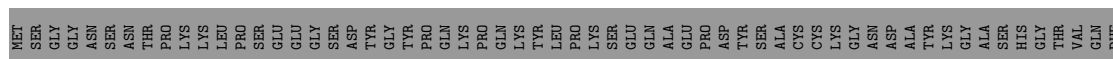
- Molecule 1: Microtubule associated protein SPM1

Chain 22: 

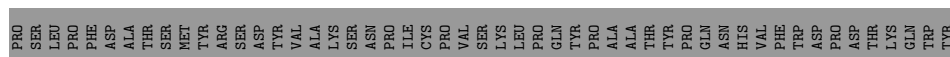
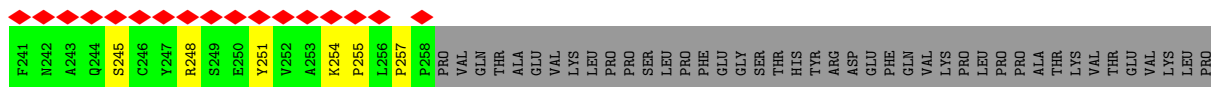
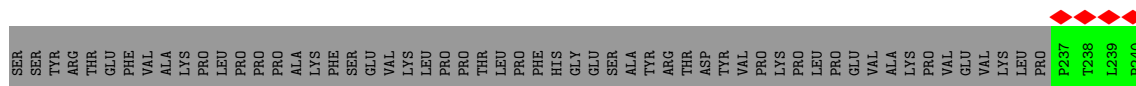
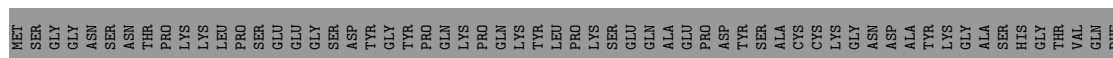
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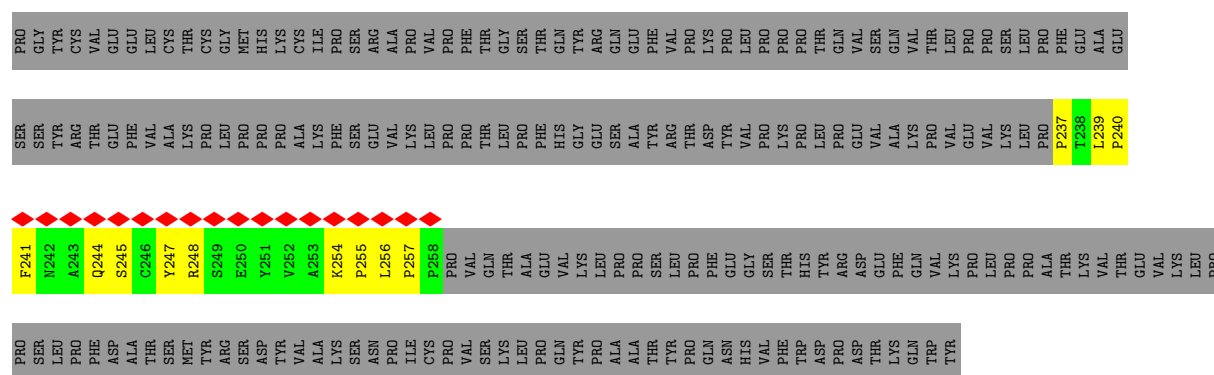
Chain 23:  94%



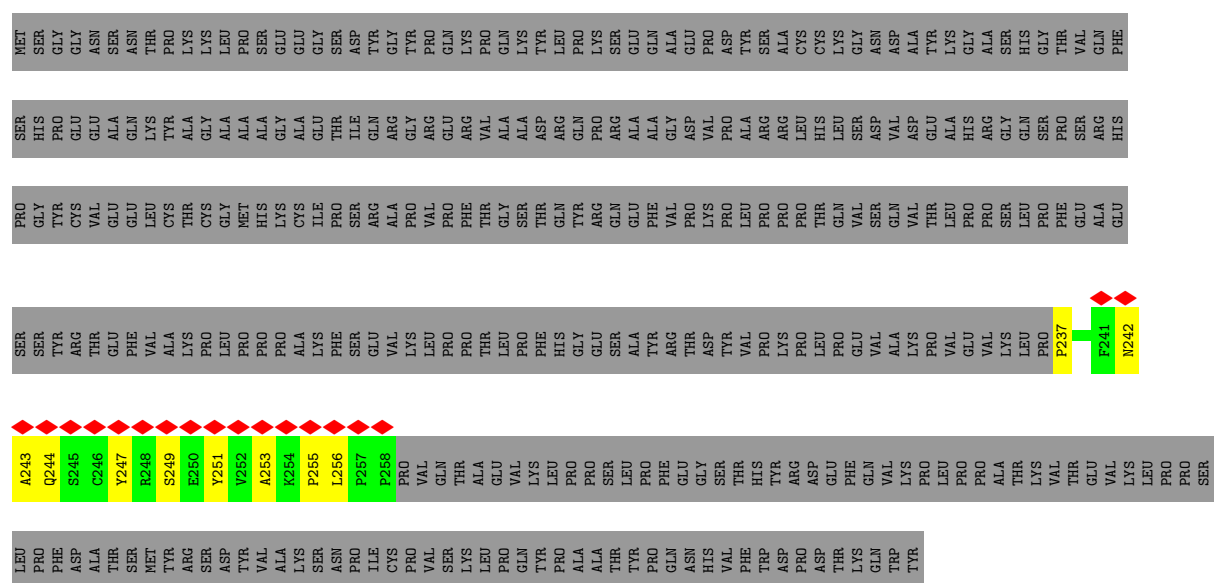
Chain 3: 6% 5% 94%



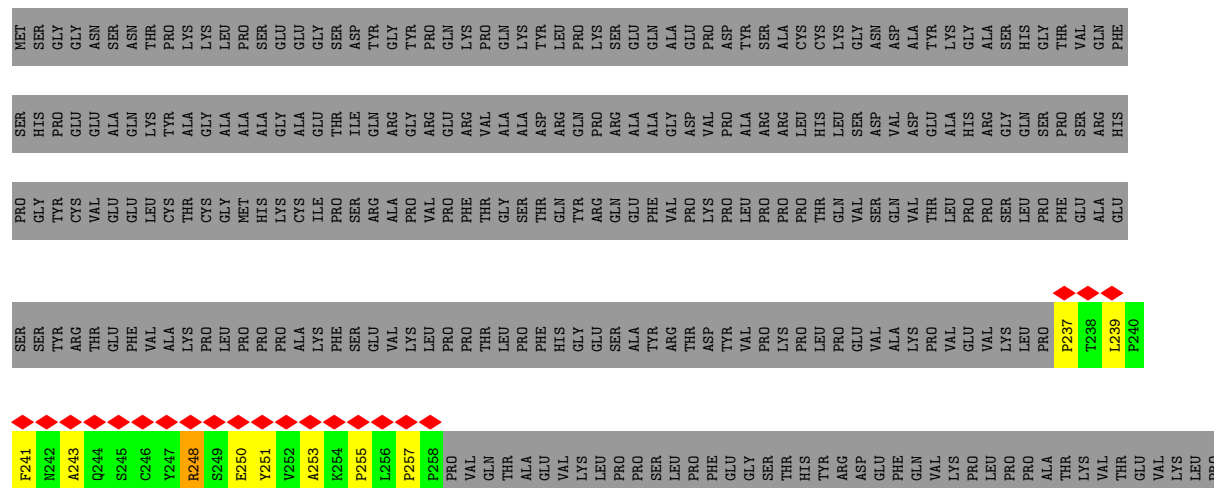




- Molecule 1: Microtubule associated protein SPM1



- Molecule 1: Microtubule associated protein SPM1

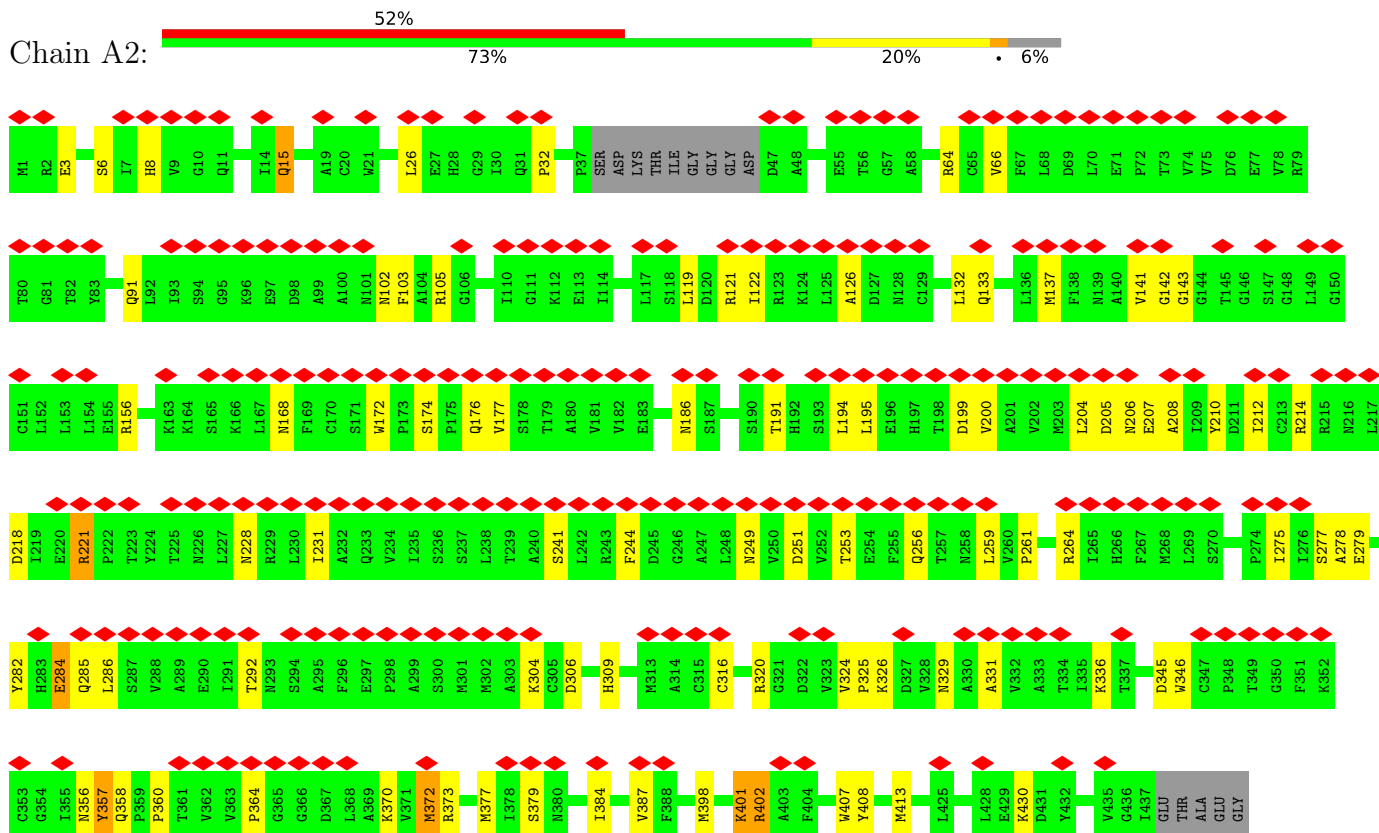




GLU  
TYR

• Molecule 2: Tubulin alpha chain

Chain A2:

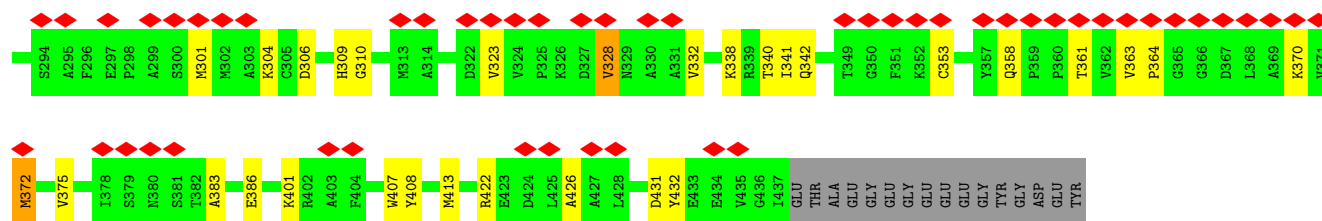


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TYR

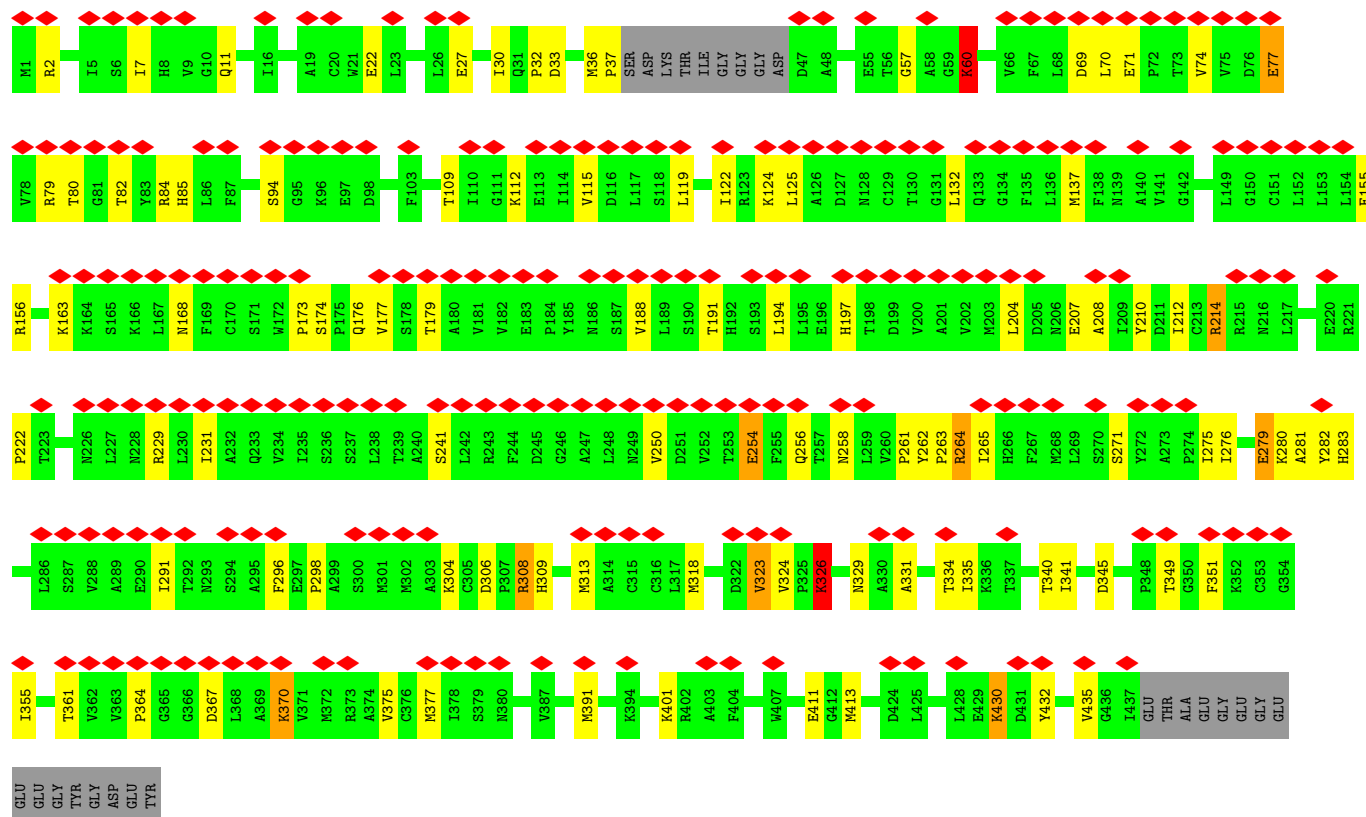
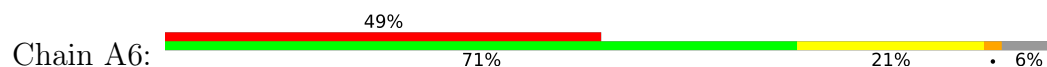
• Molecule 2: Tubulin alpha chain

Chain A4:

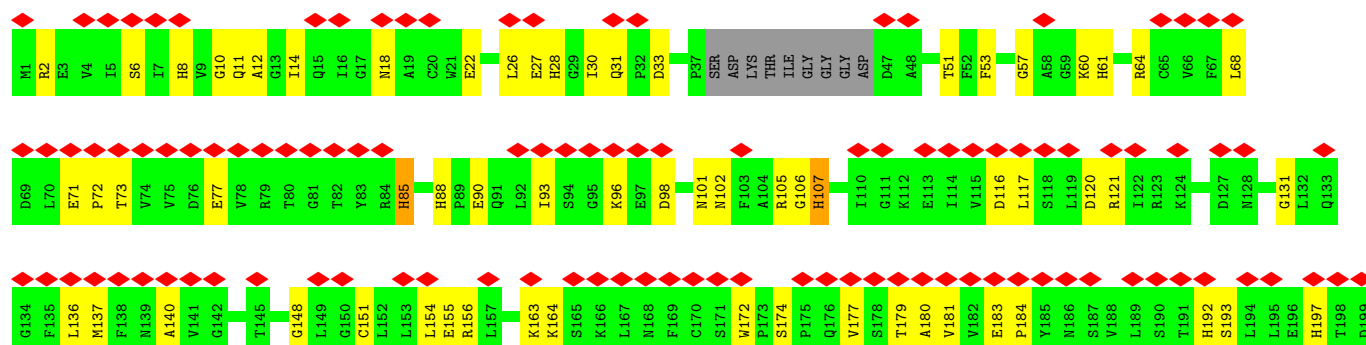


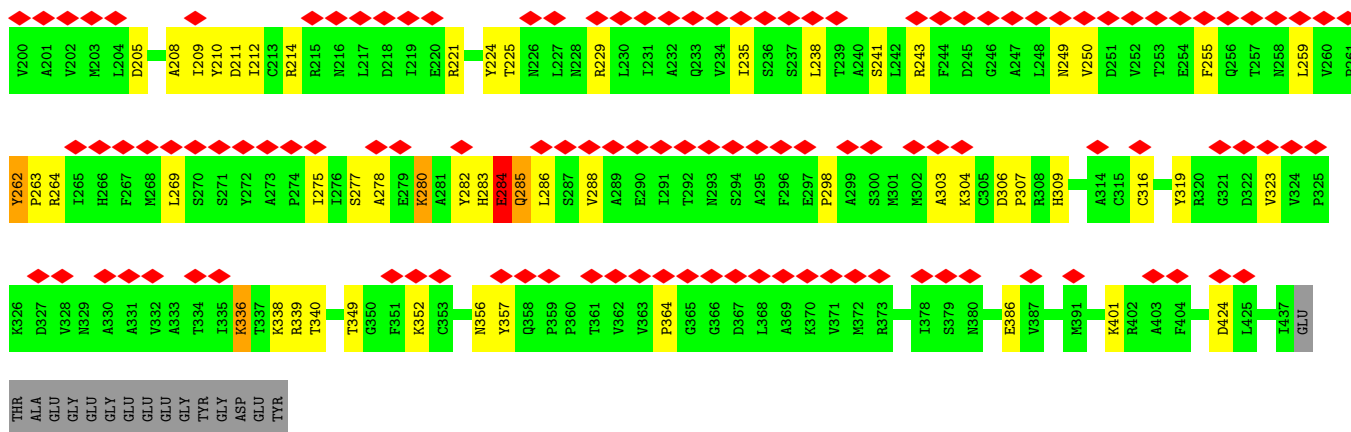


• Molecule 2: Tubulin alpha chain

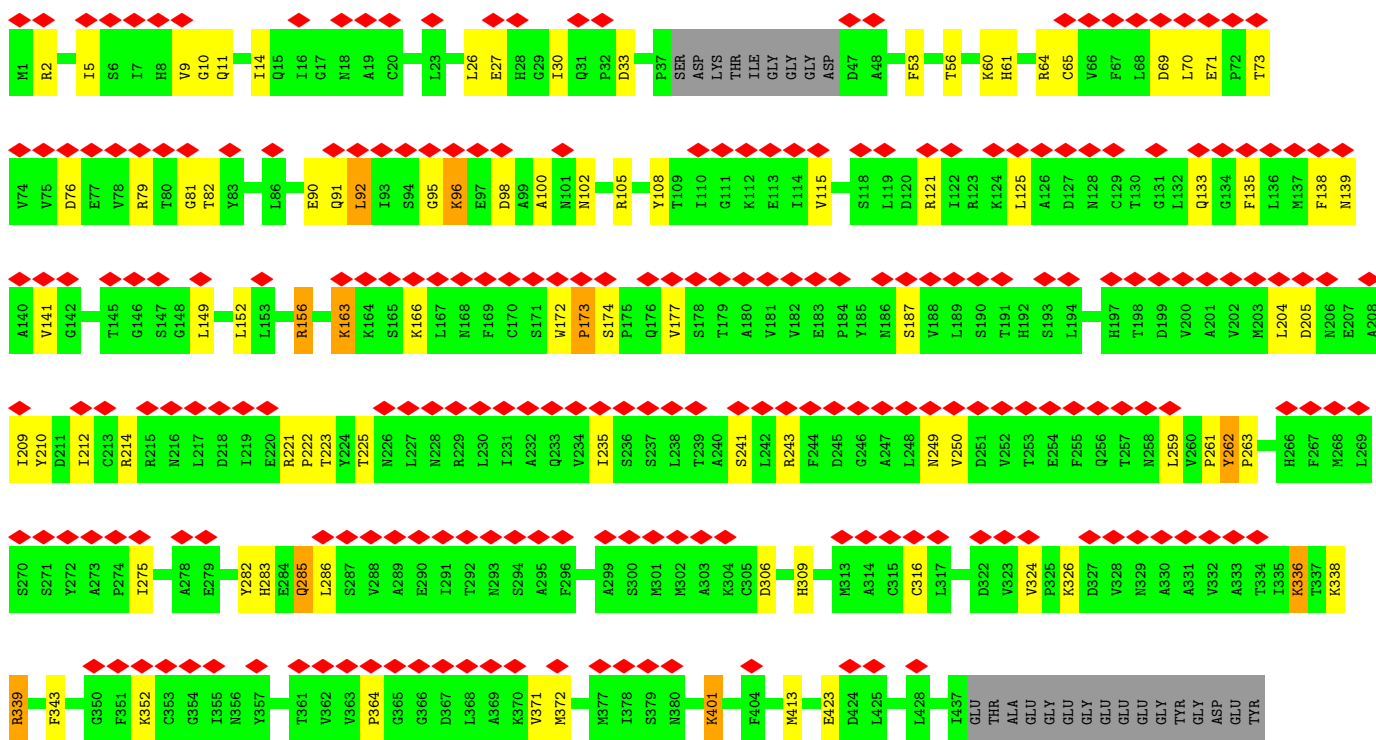
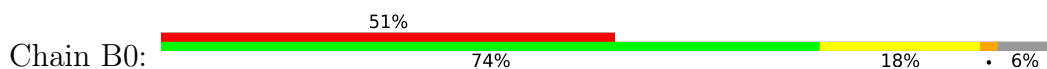


• Molecule 2: Tubulin alpha chain

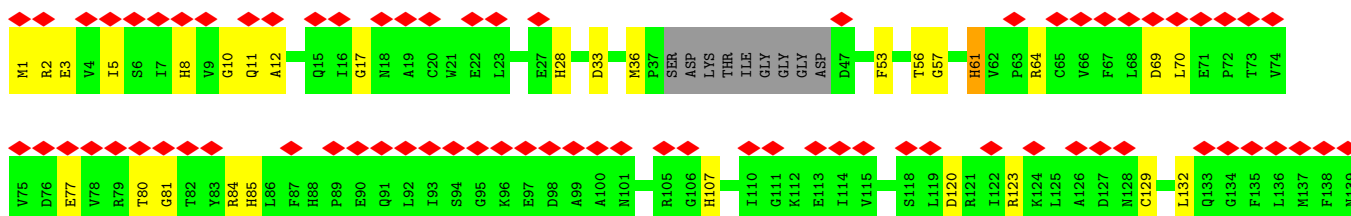
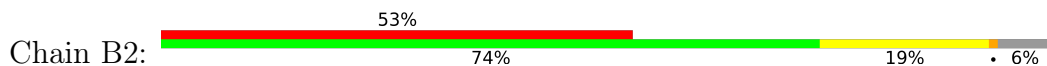


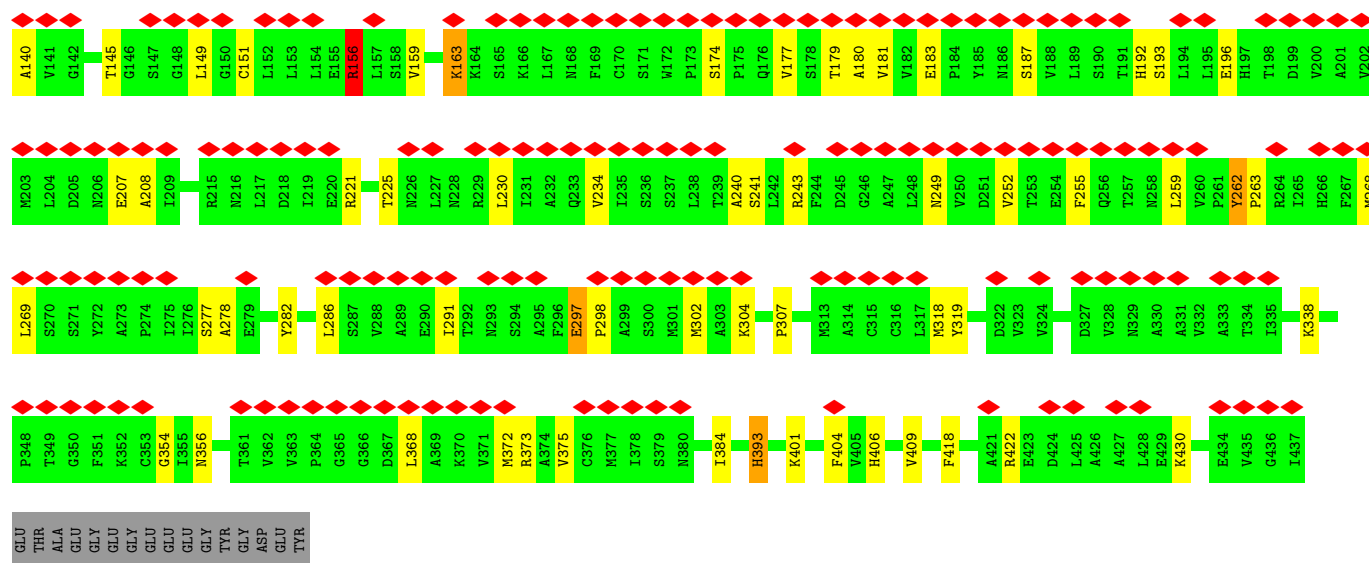


• Molecule 2: Tubulin alpha chain



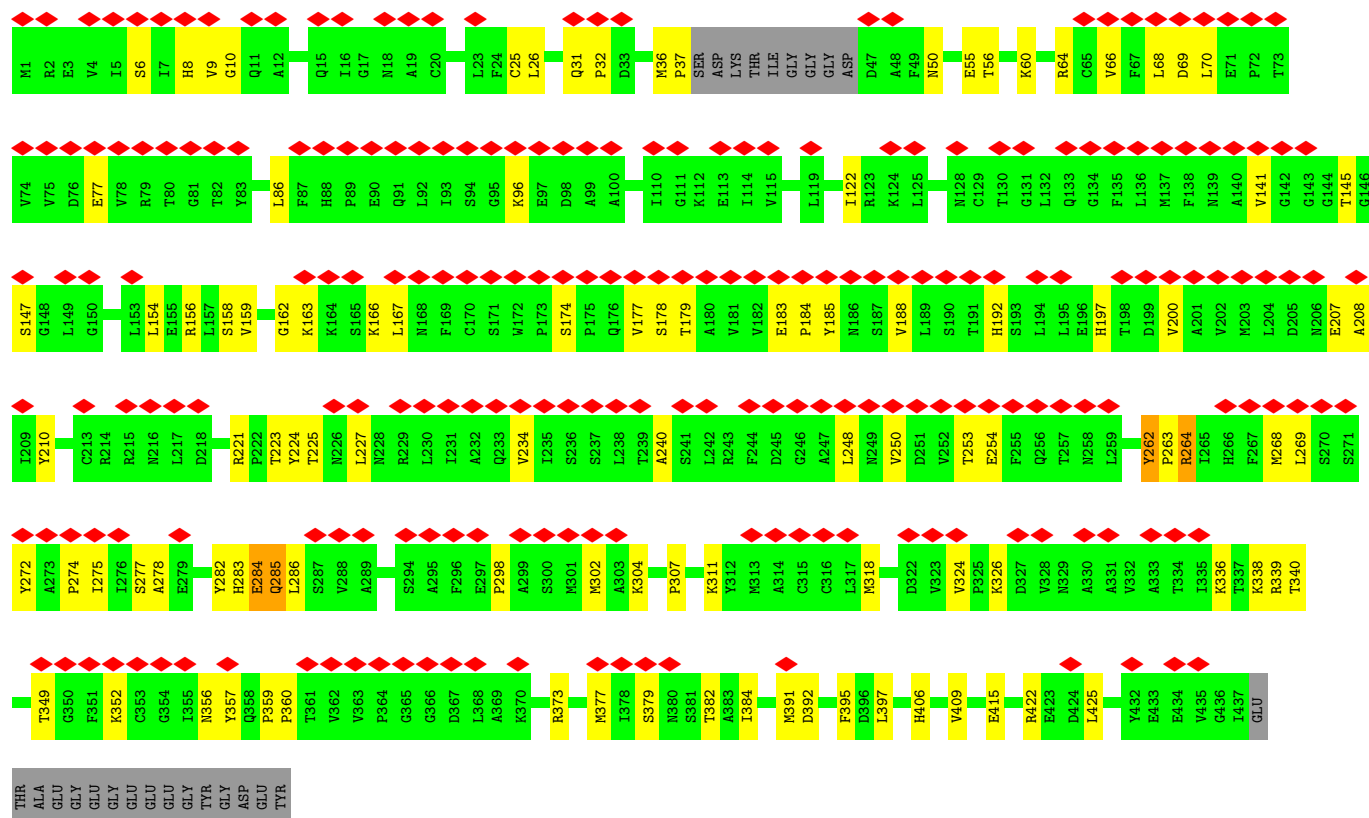
• Molecule 2: Tubulin alpha chain





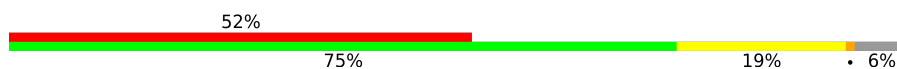
• Molecule 2: Tubulin alpha chain

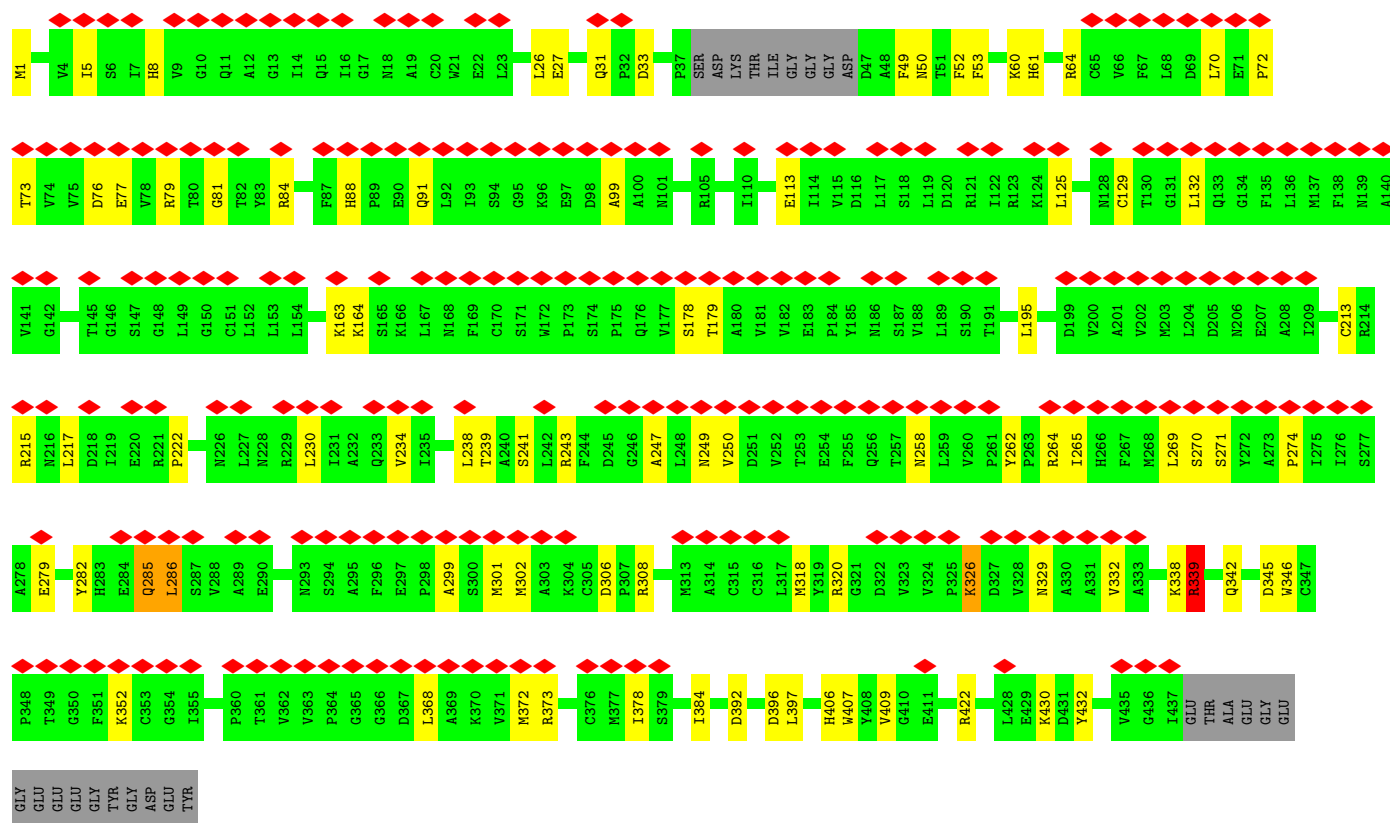
Chain B4:



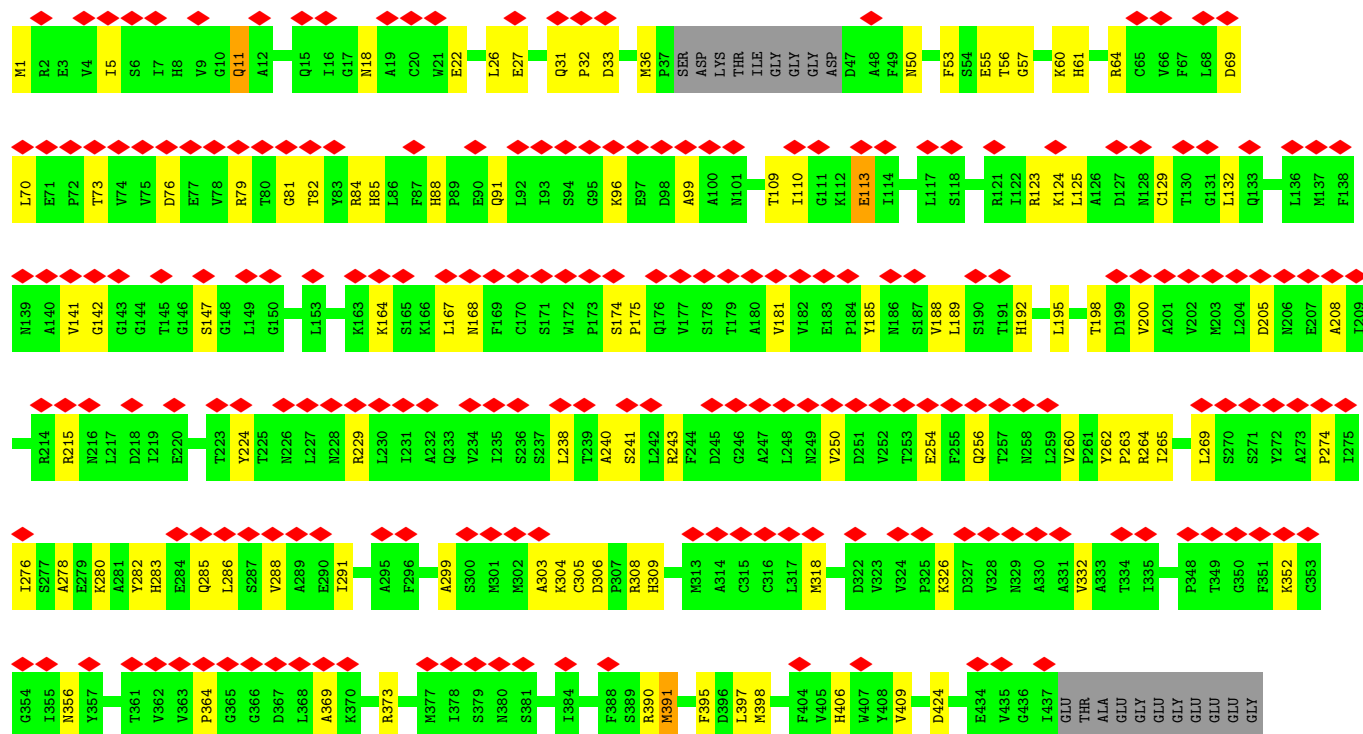
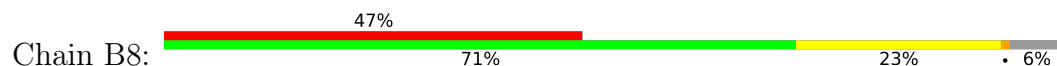
• Molecule 2: Tubulin alpha chain

Chain B6:





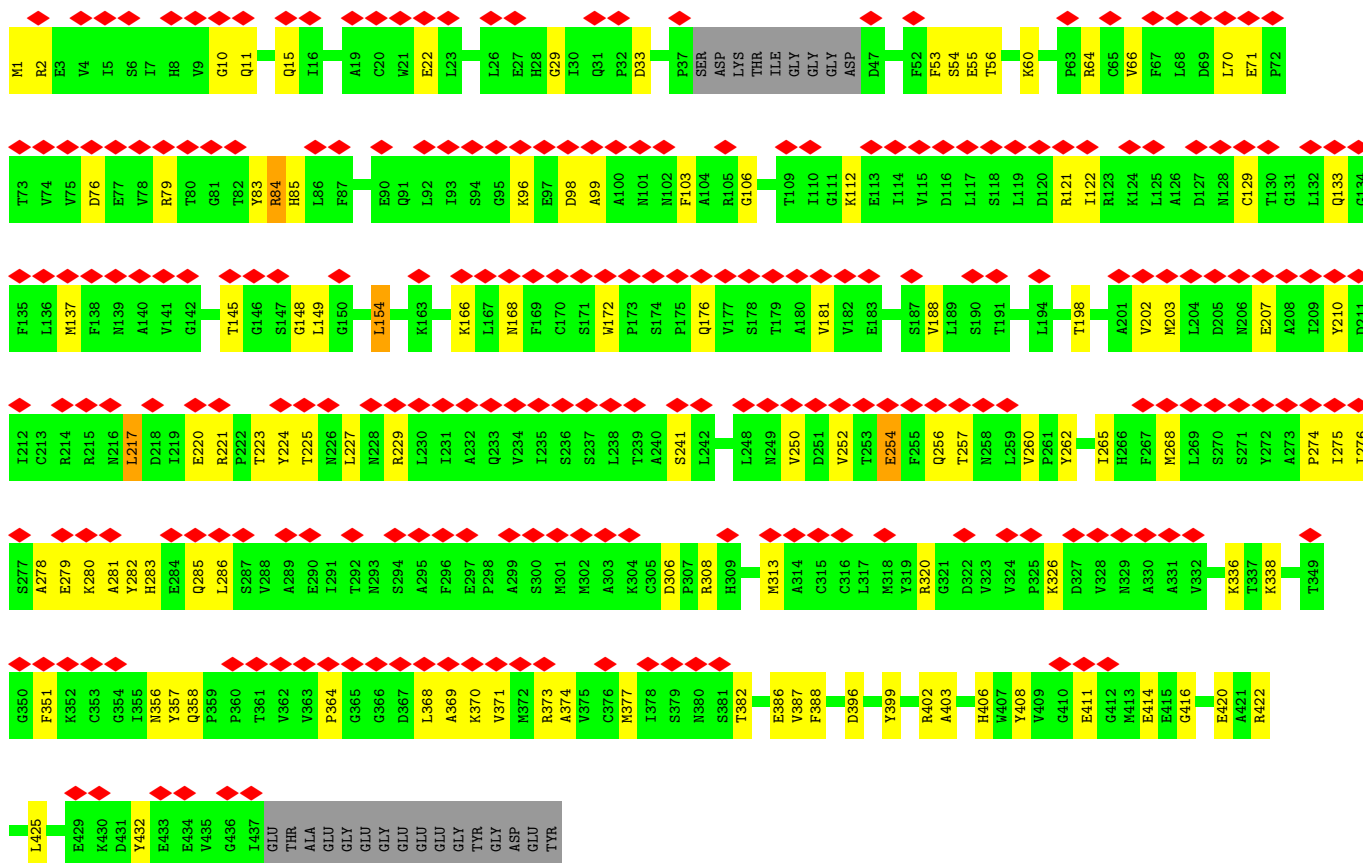
• Molecule 2: Tubulin alpha chain



TYR  
GLY  
ASP  
GLU  
TYR

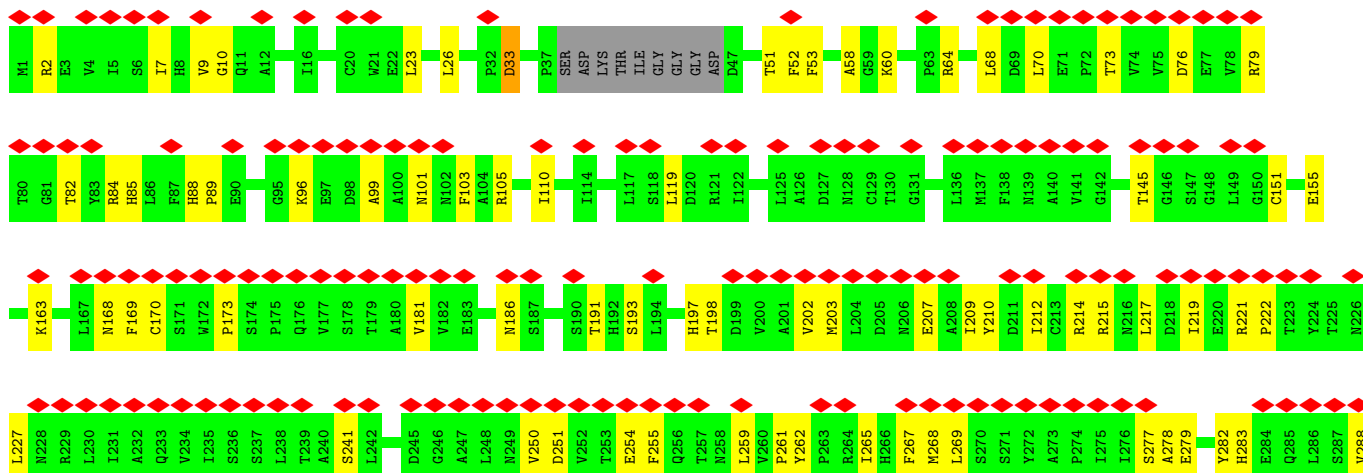
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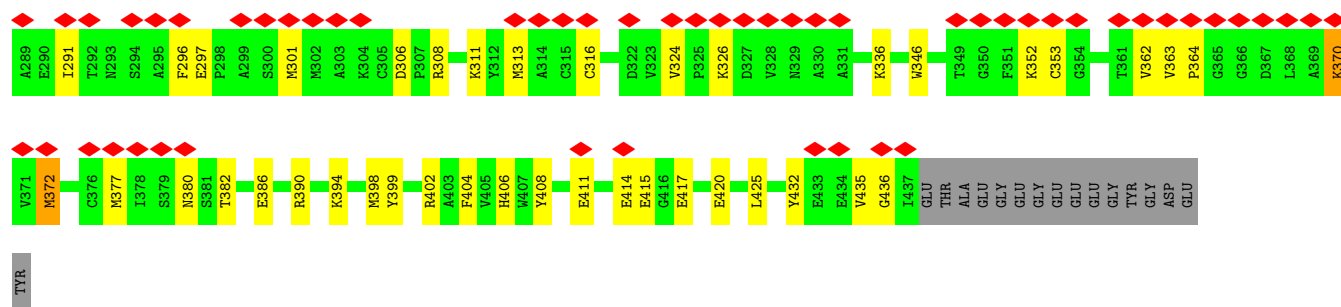
Chain C0: 53% 70% 24% 6%



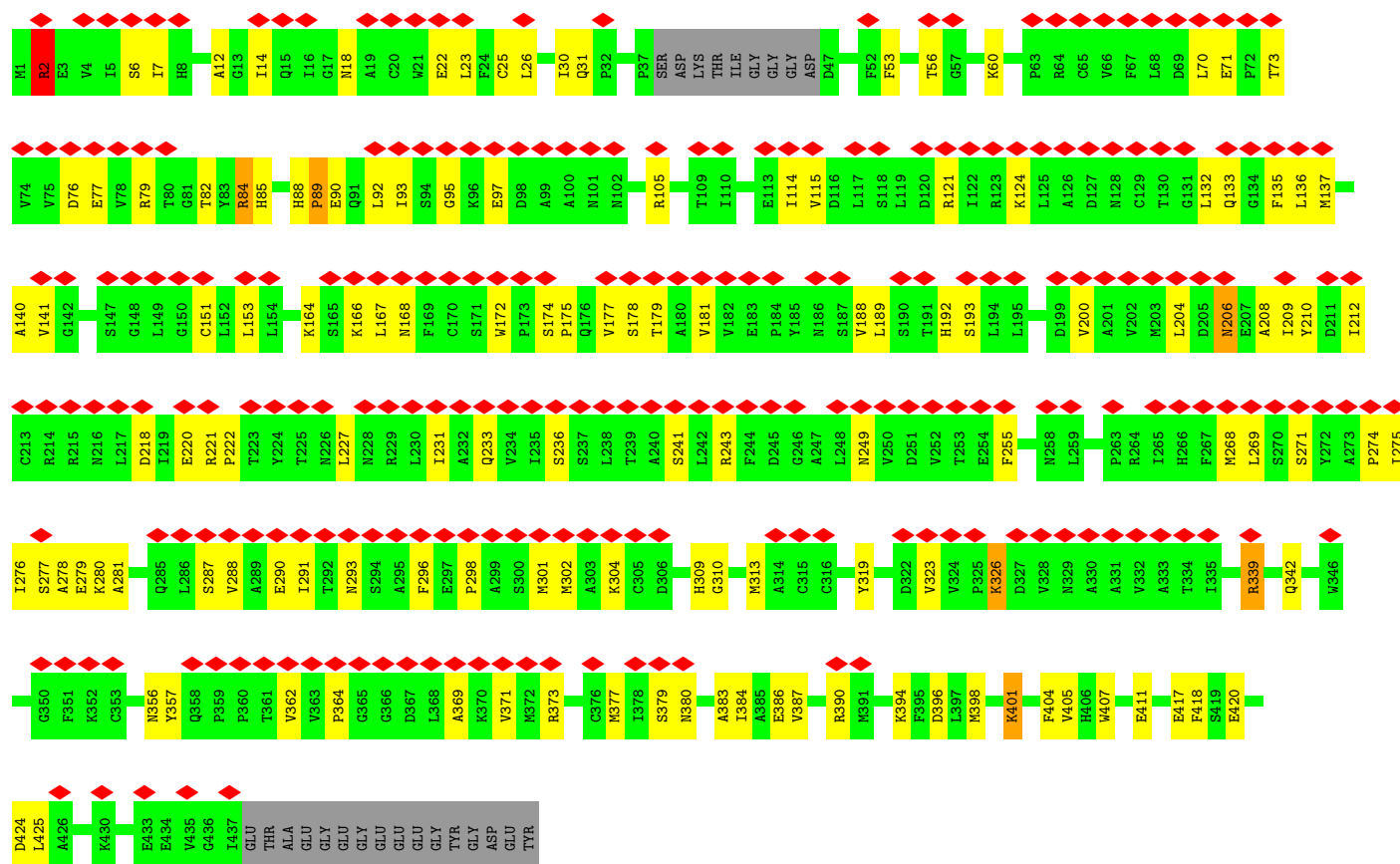
• Molecule 2: Tubulin alpha chain

Chain C2: 46% 69% 25% 6%

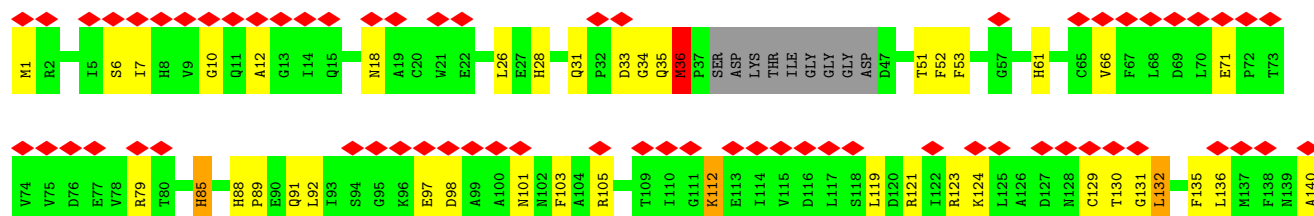


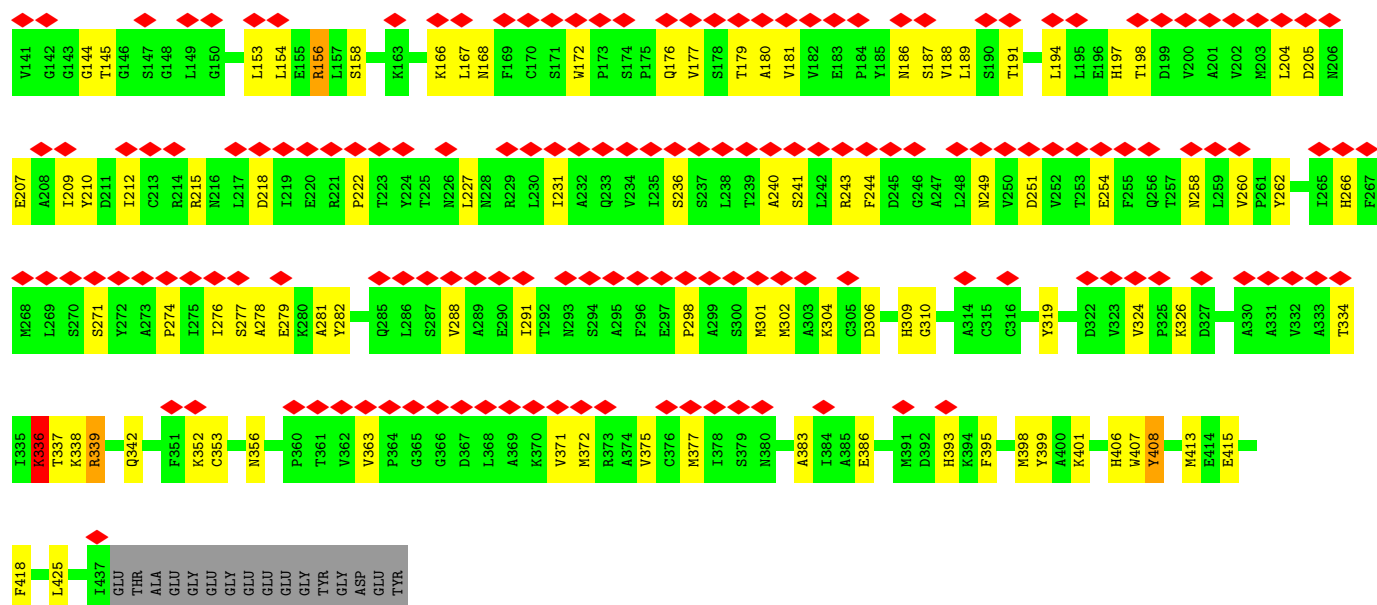


• Molecule 2: Tubulin alpha chain

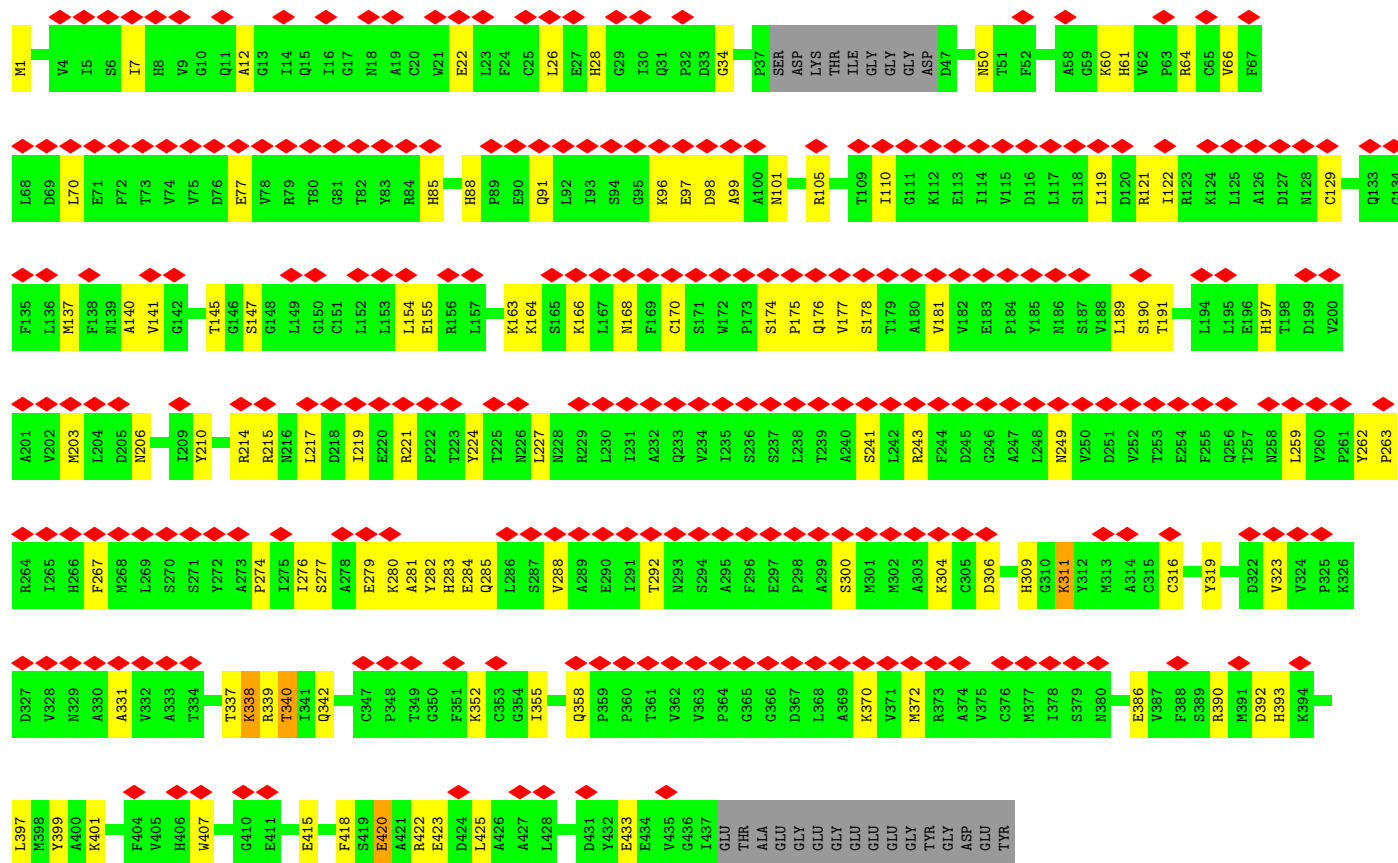


• Molecule 2: Tubulin alpha chain

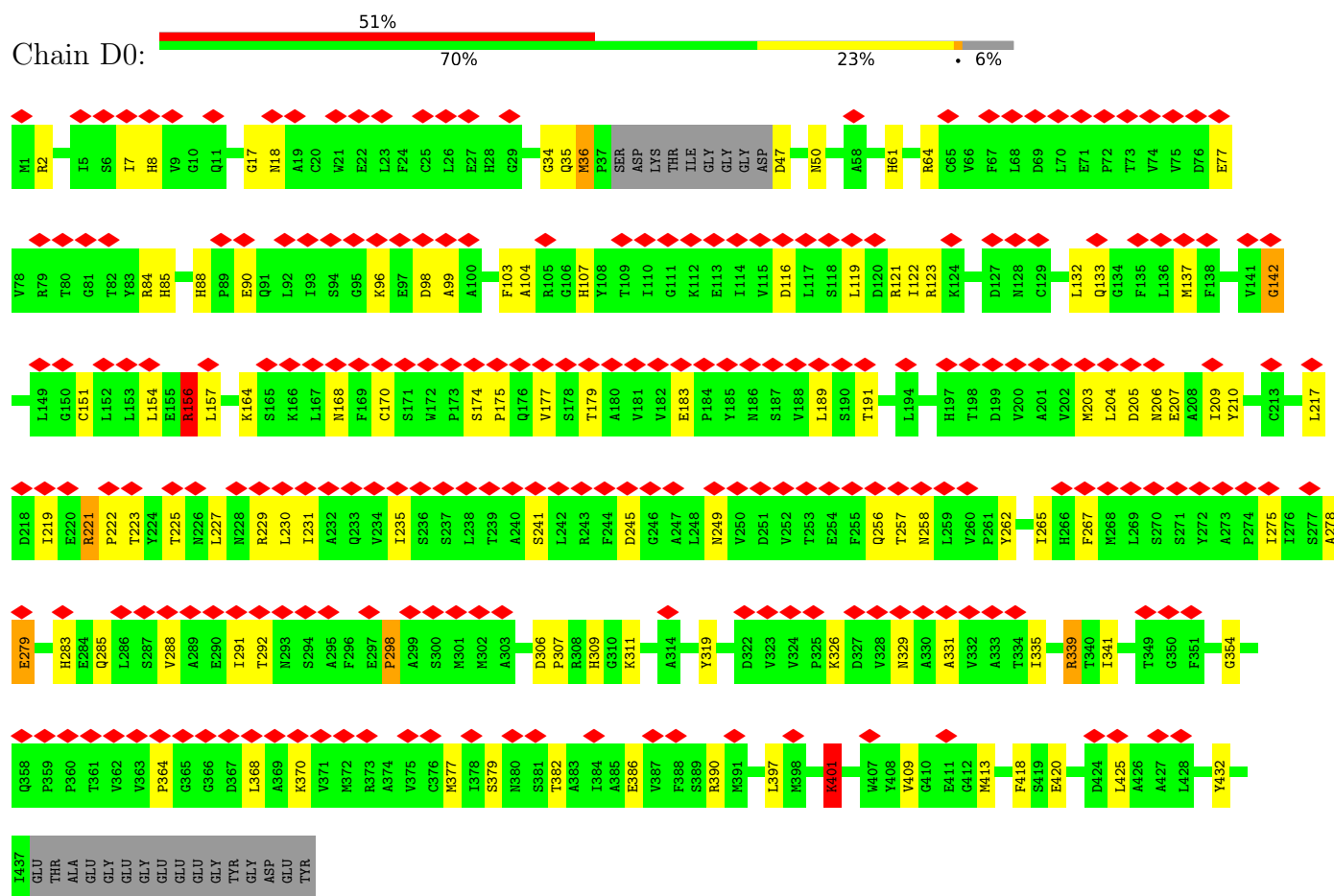




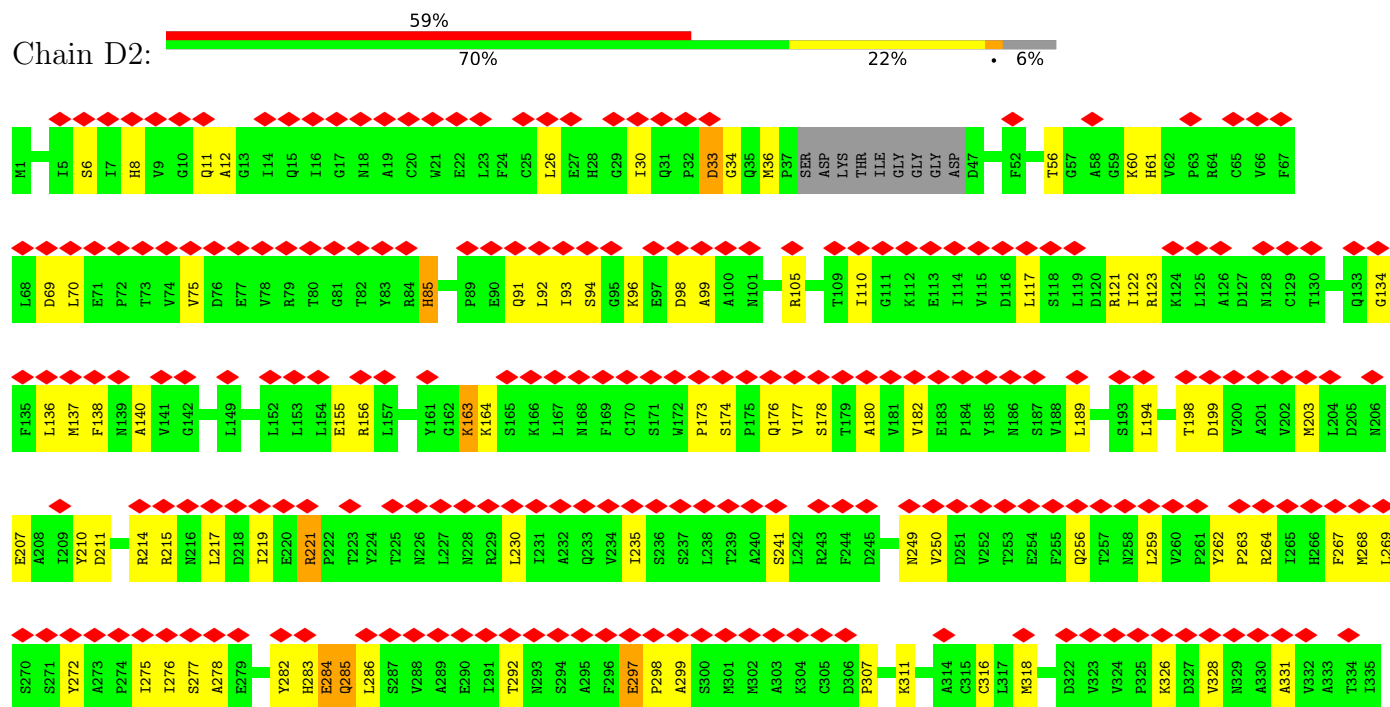
• Molecule 2: Tubulin alpha chain

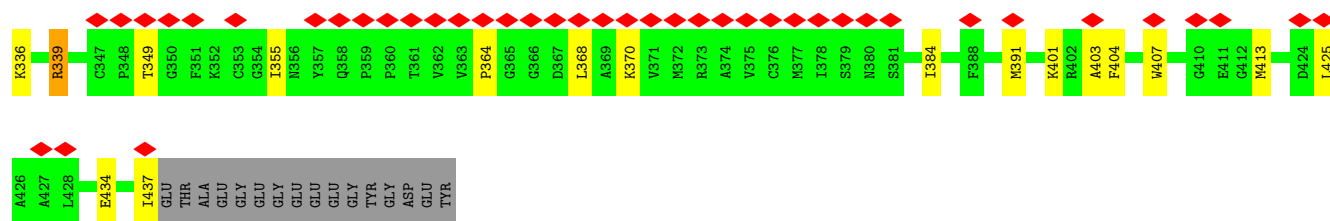


• Molecule 2: Tubulin alpha chain

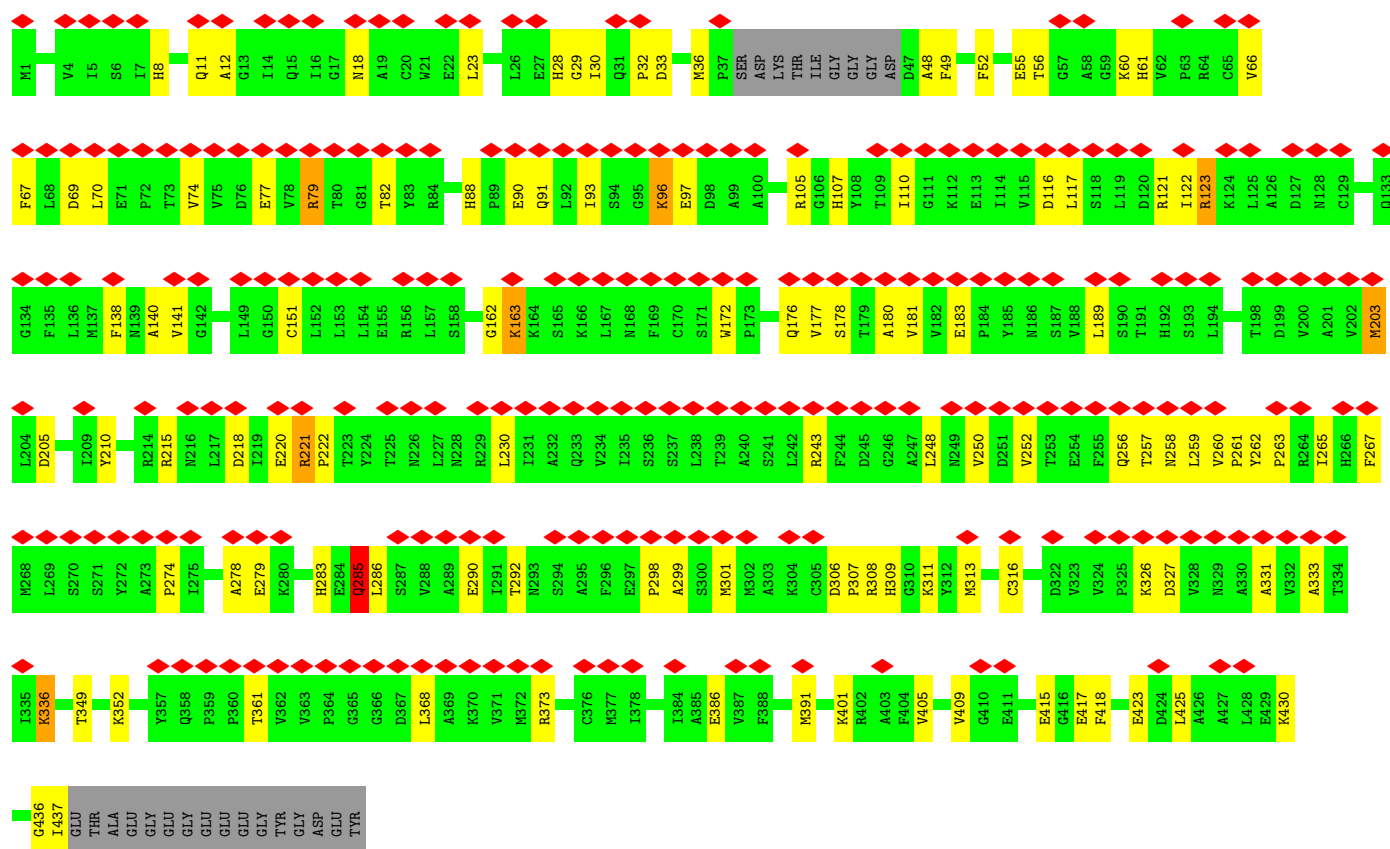


• Molecule 2: Tubulin alpha chain

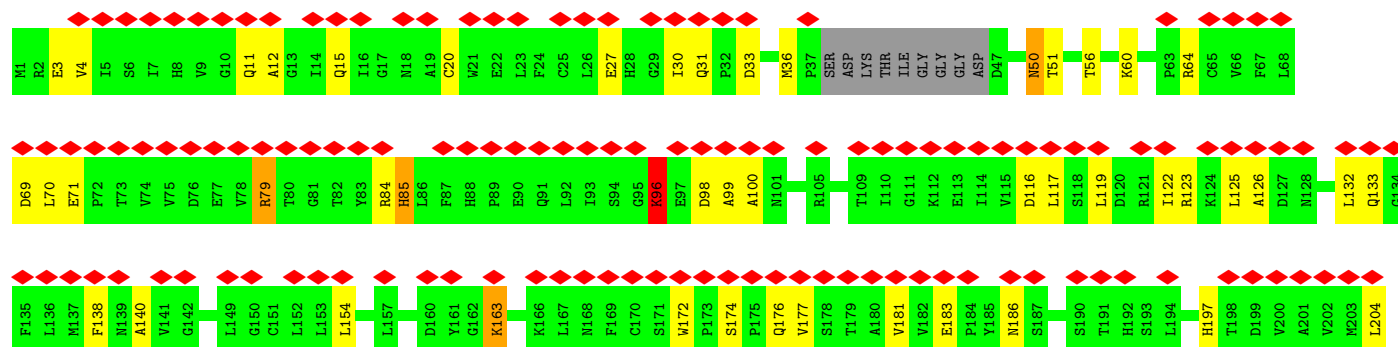
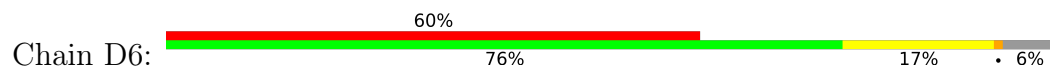


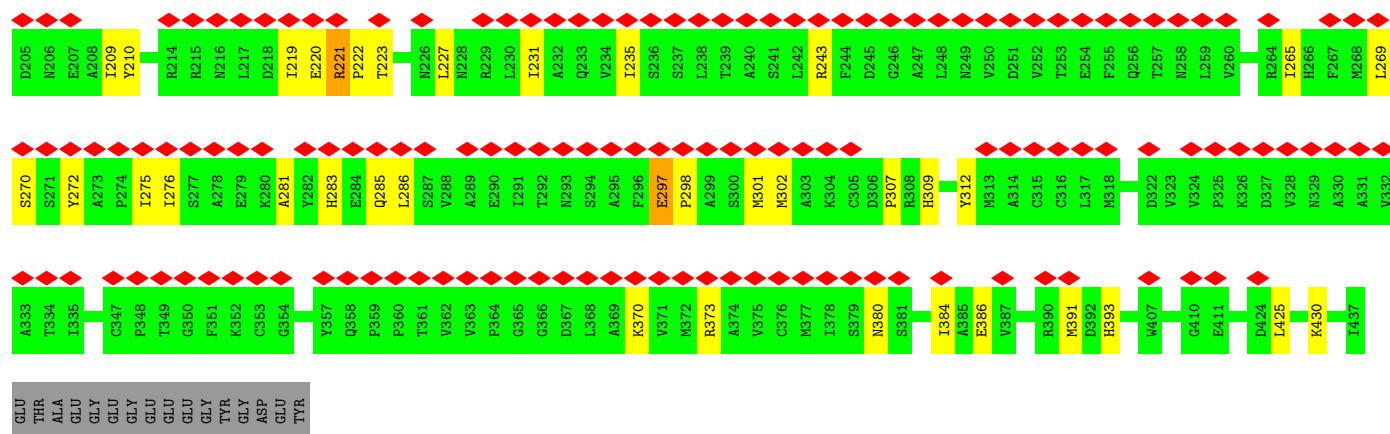


• Molecule 2: Tubulin alpha chain

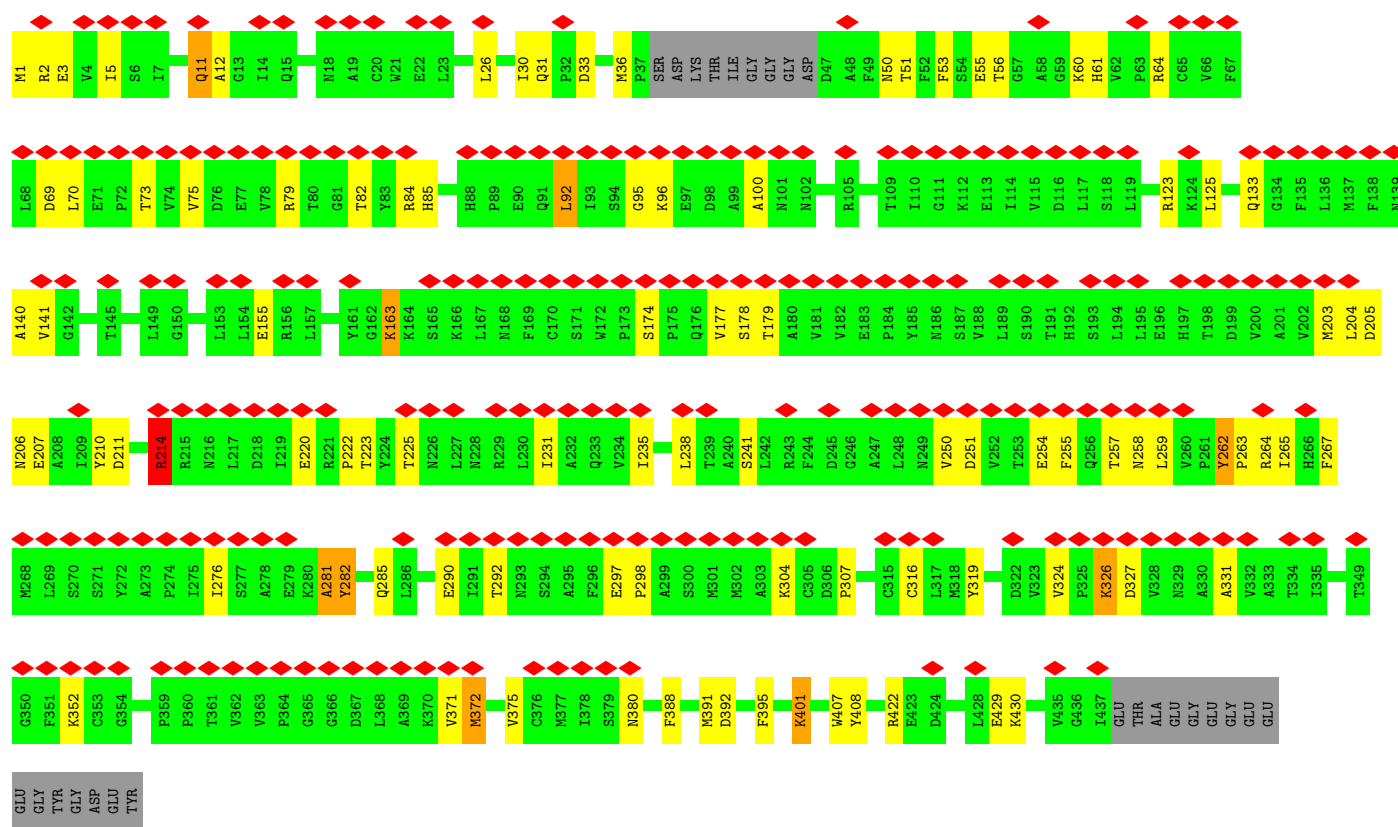
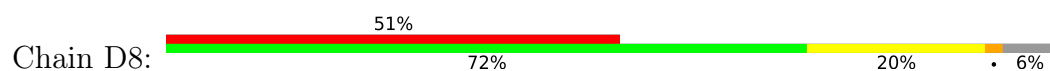


• Molecule 2: Tubulin alpha chain

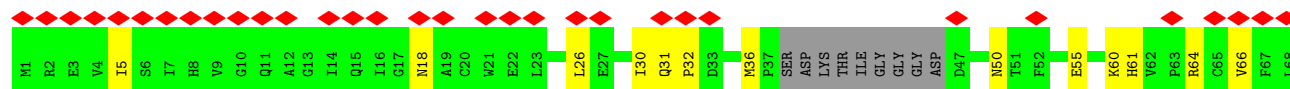
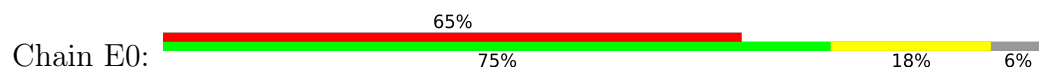


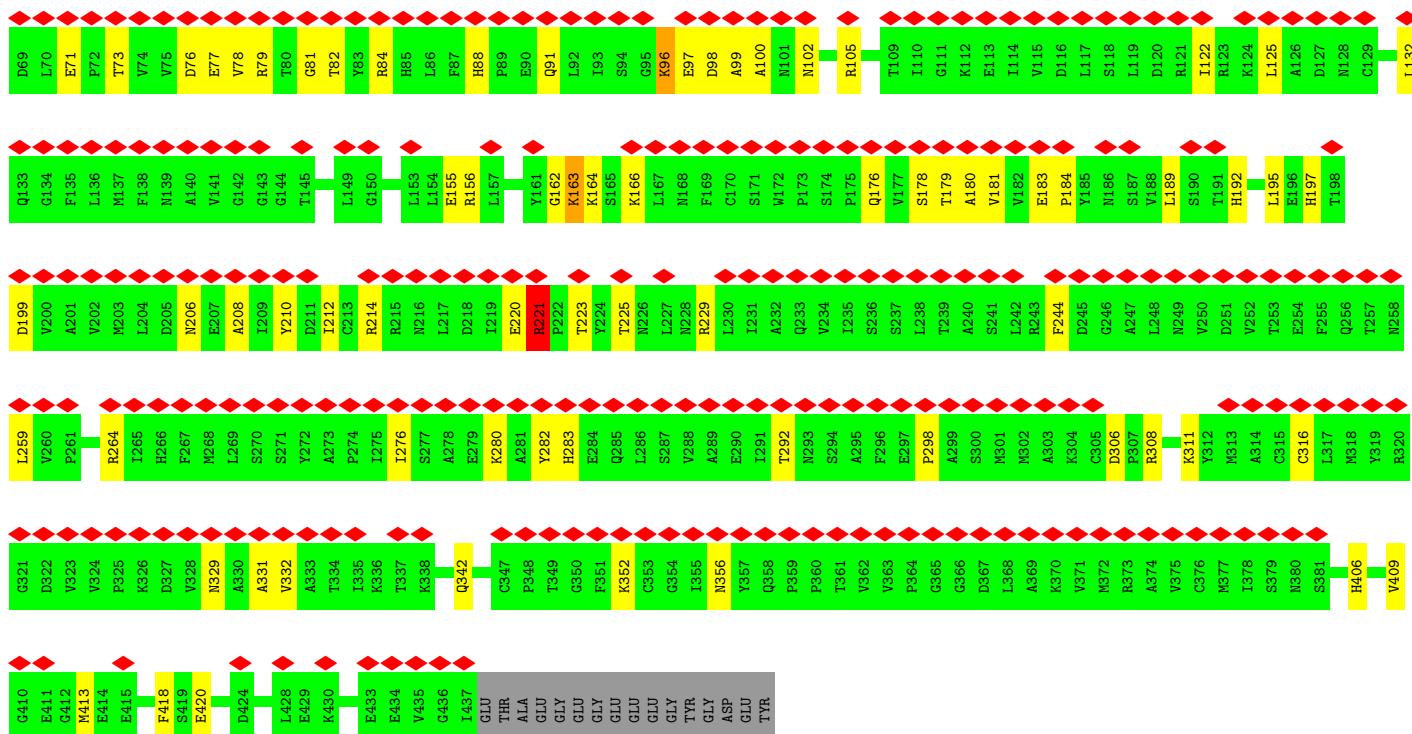


• Molecule 2: Tubulin alpha chain

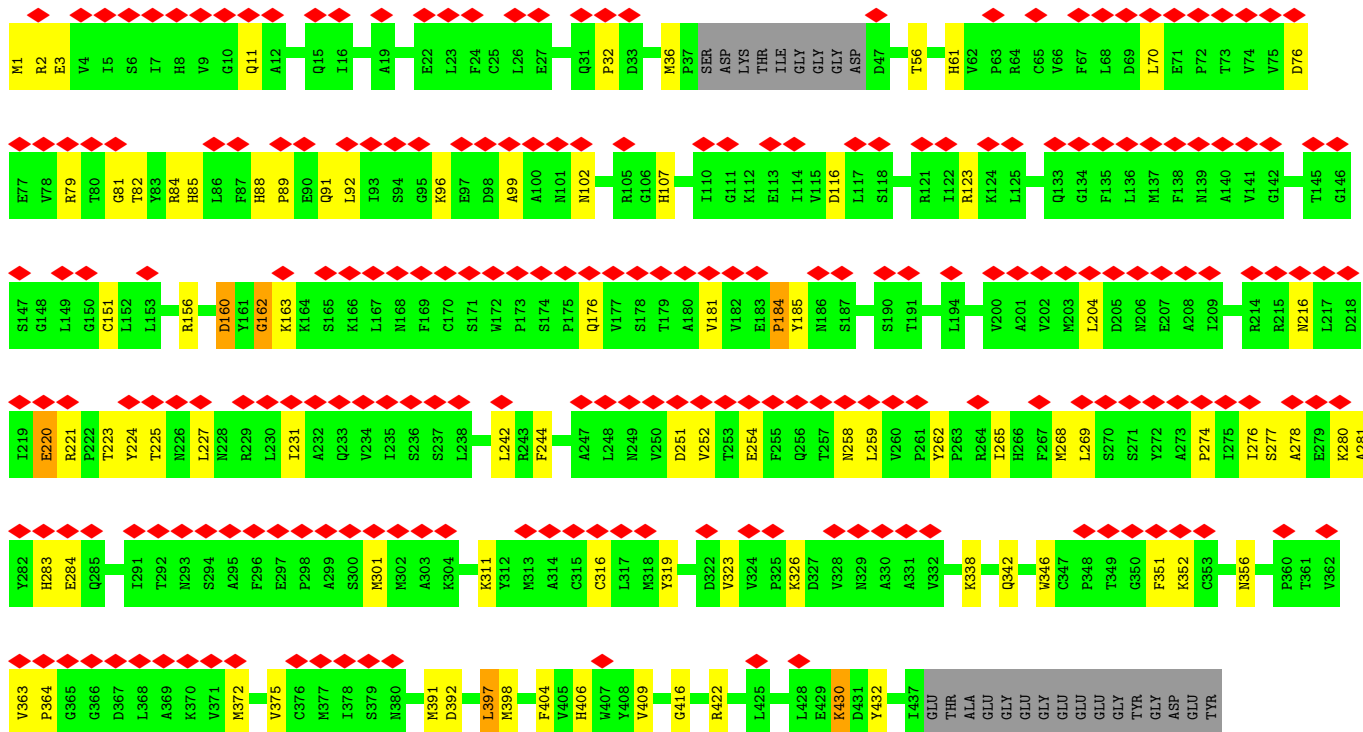
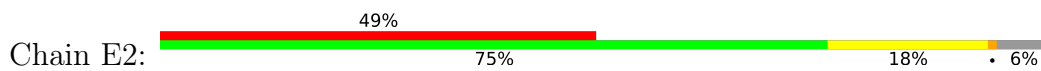


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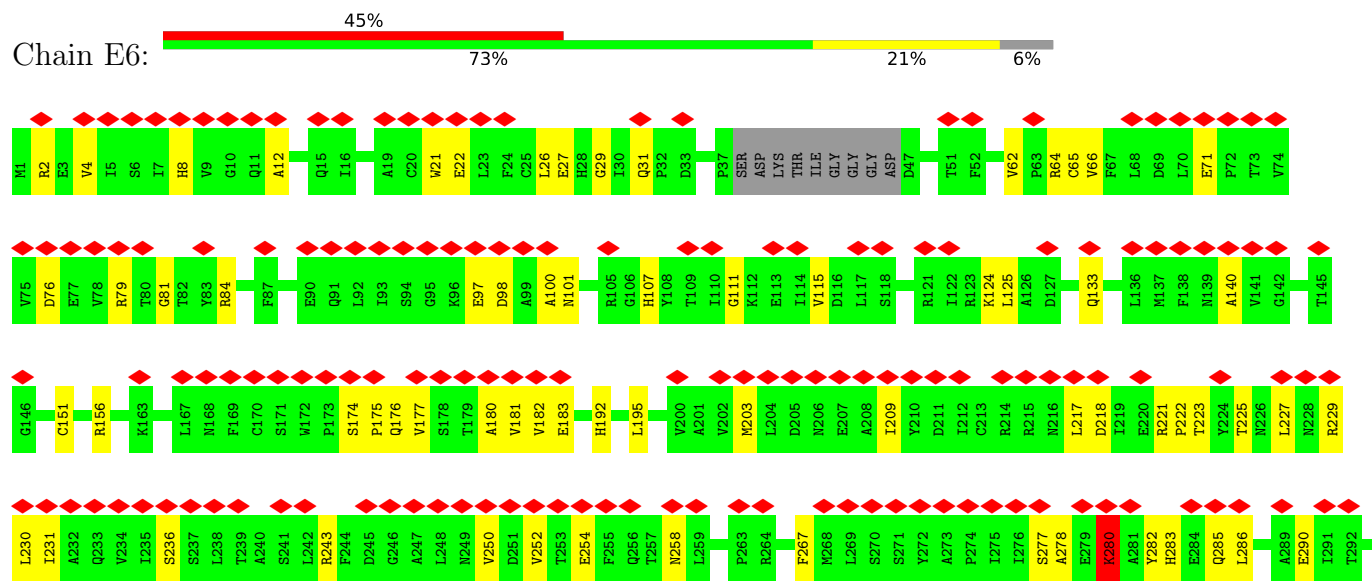
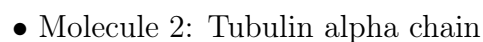


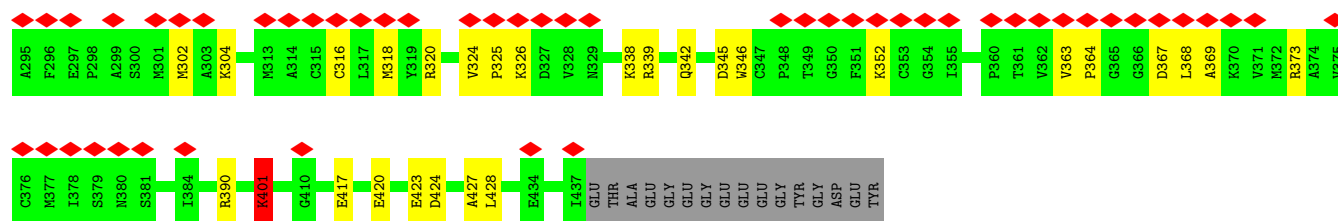


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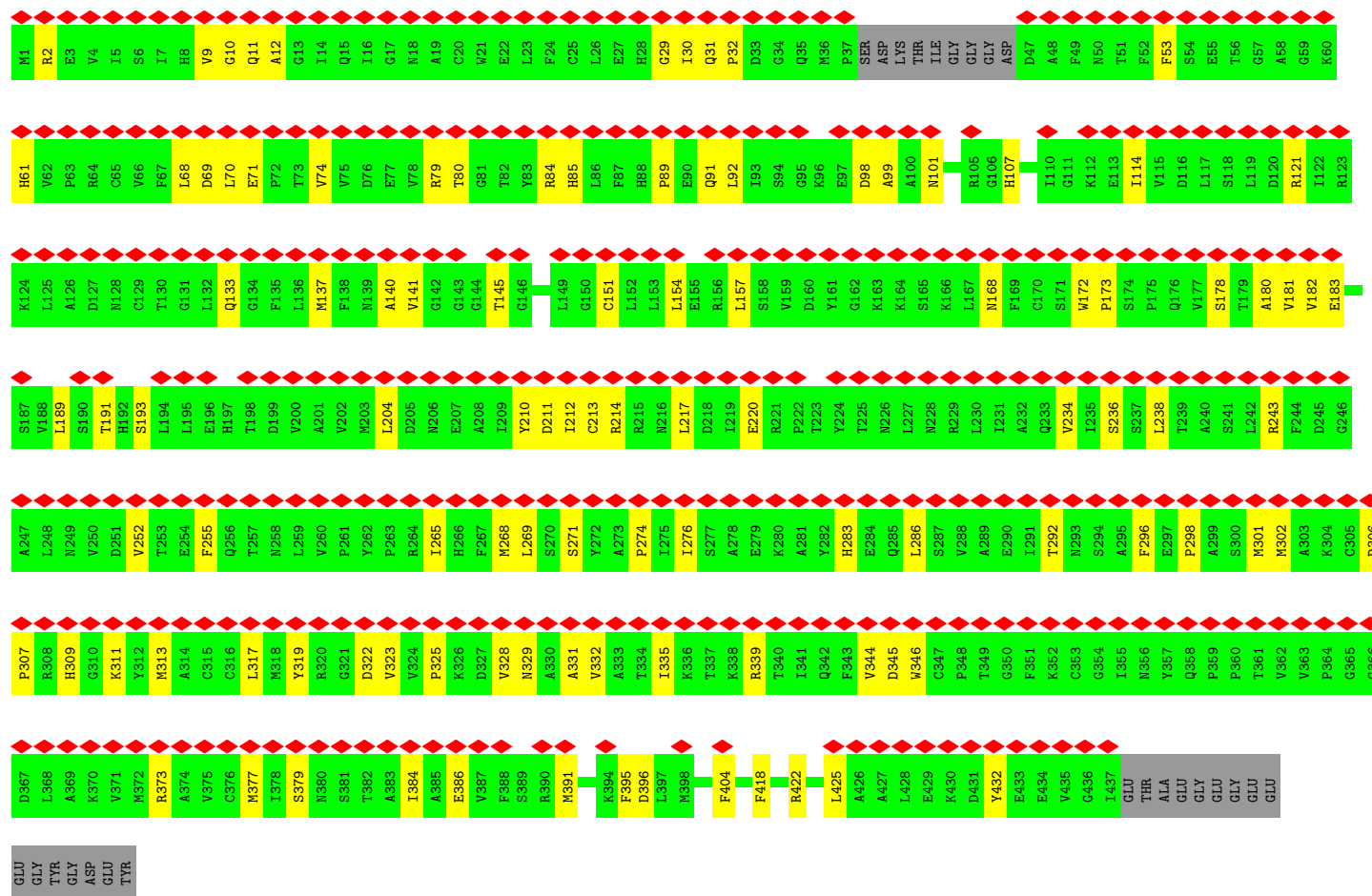
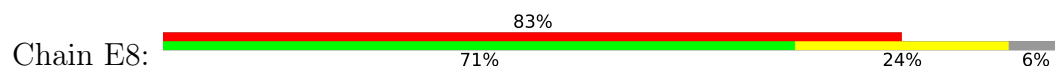


• Molecule 2: Tubulin alpha chain

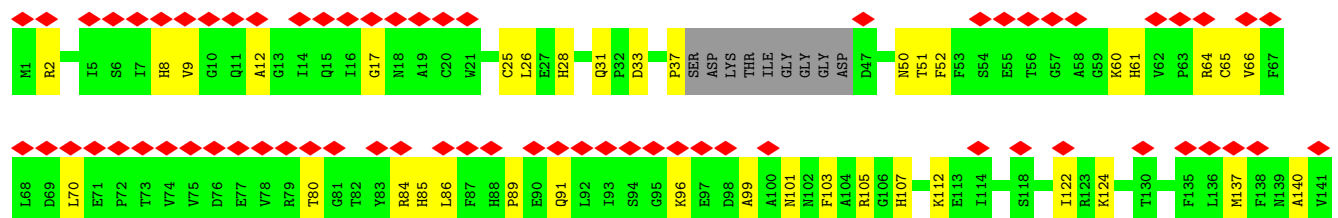


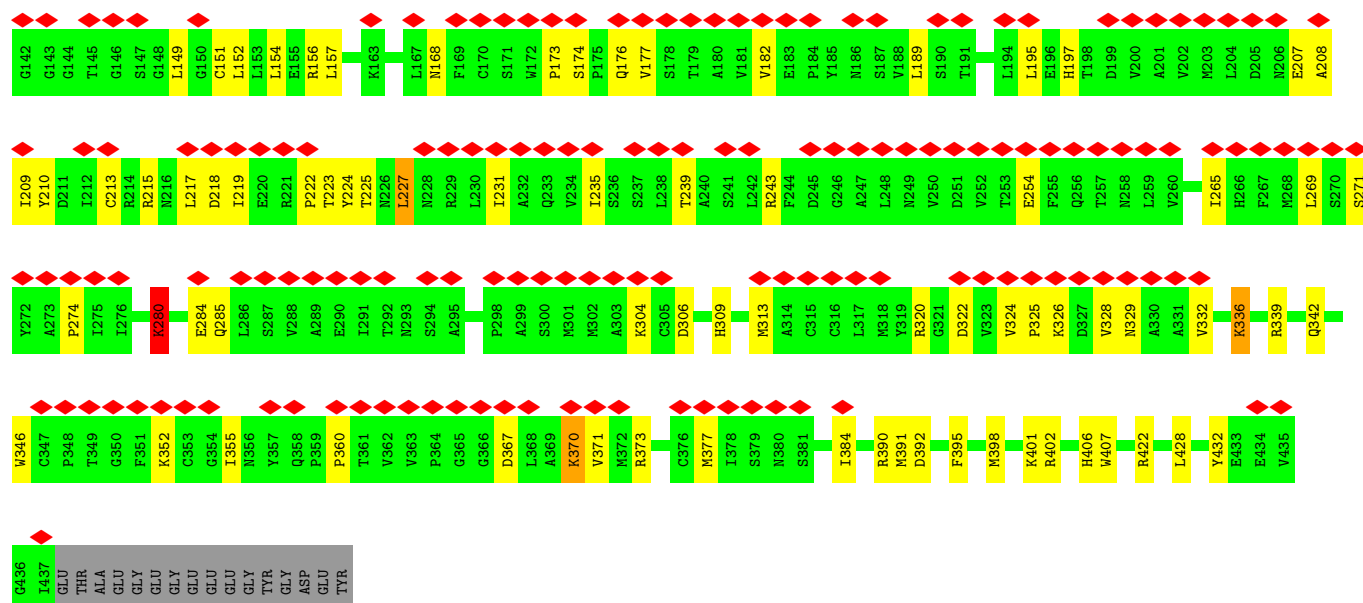


• Molecule 2: Tubulin alpha chain

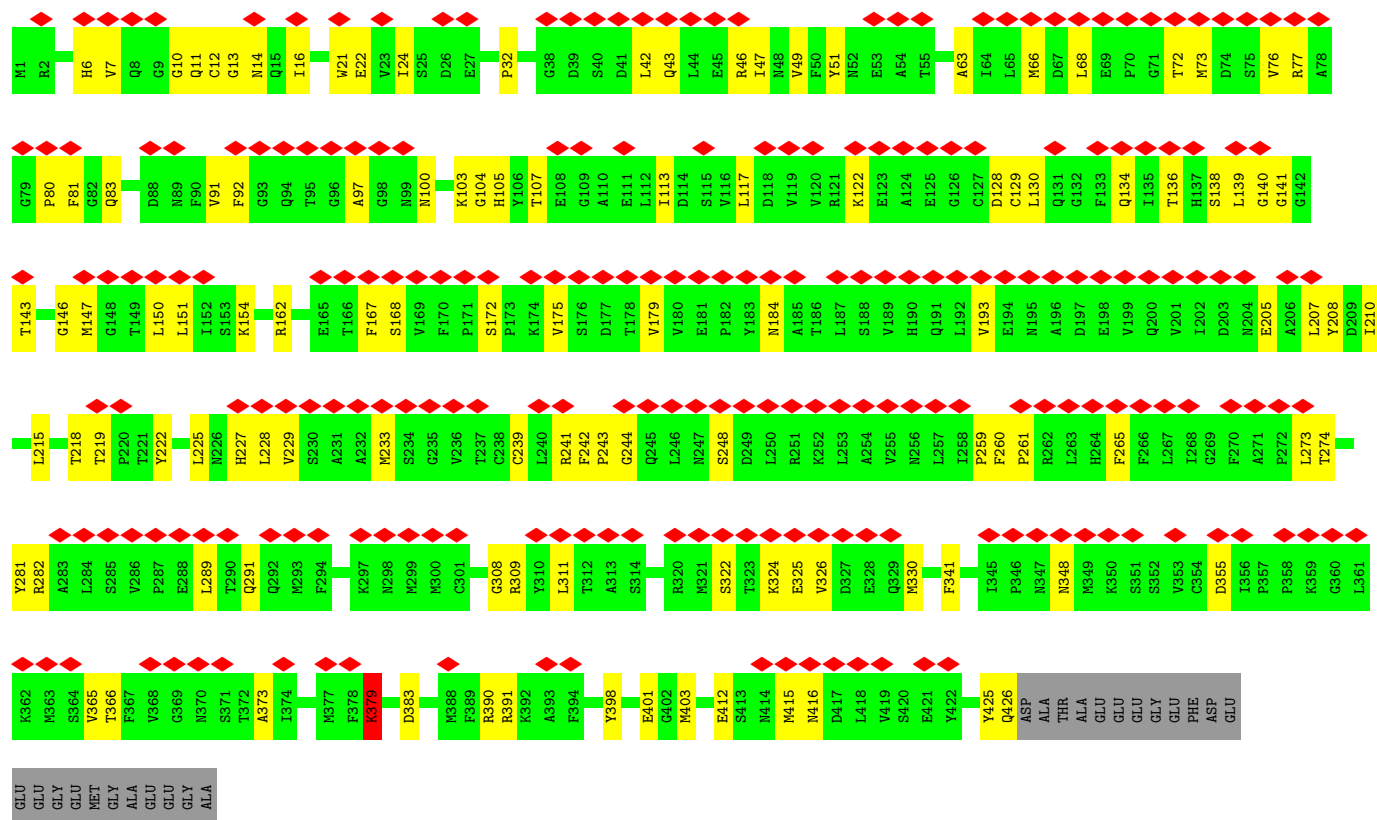


• Molecule 2: Tubulin alpha chain

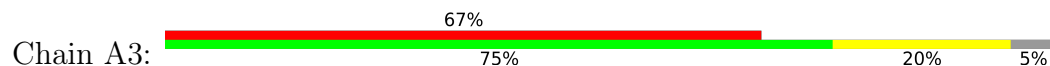


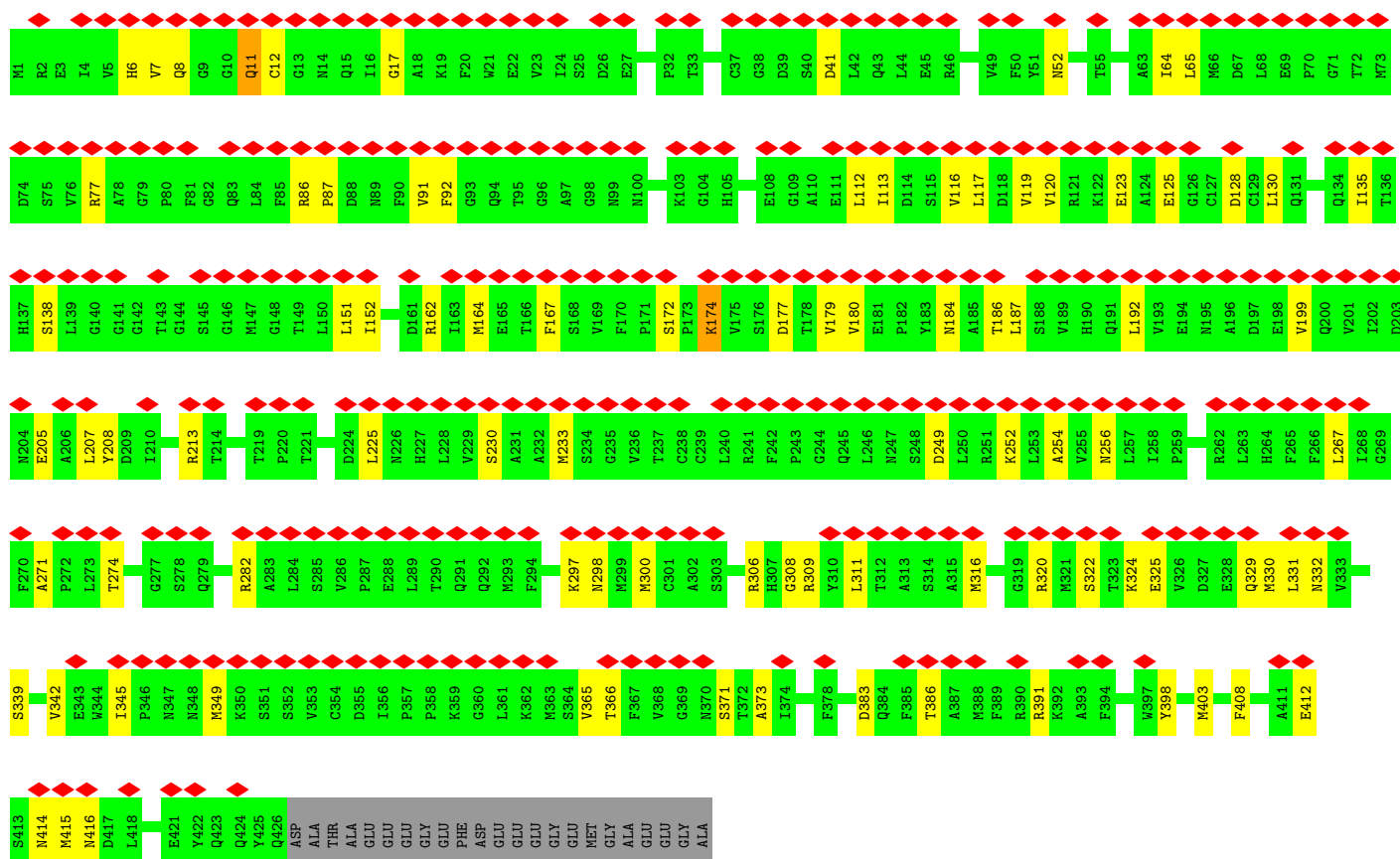


• Molecule 3: Tubulin beta chain

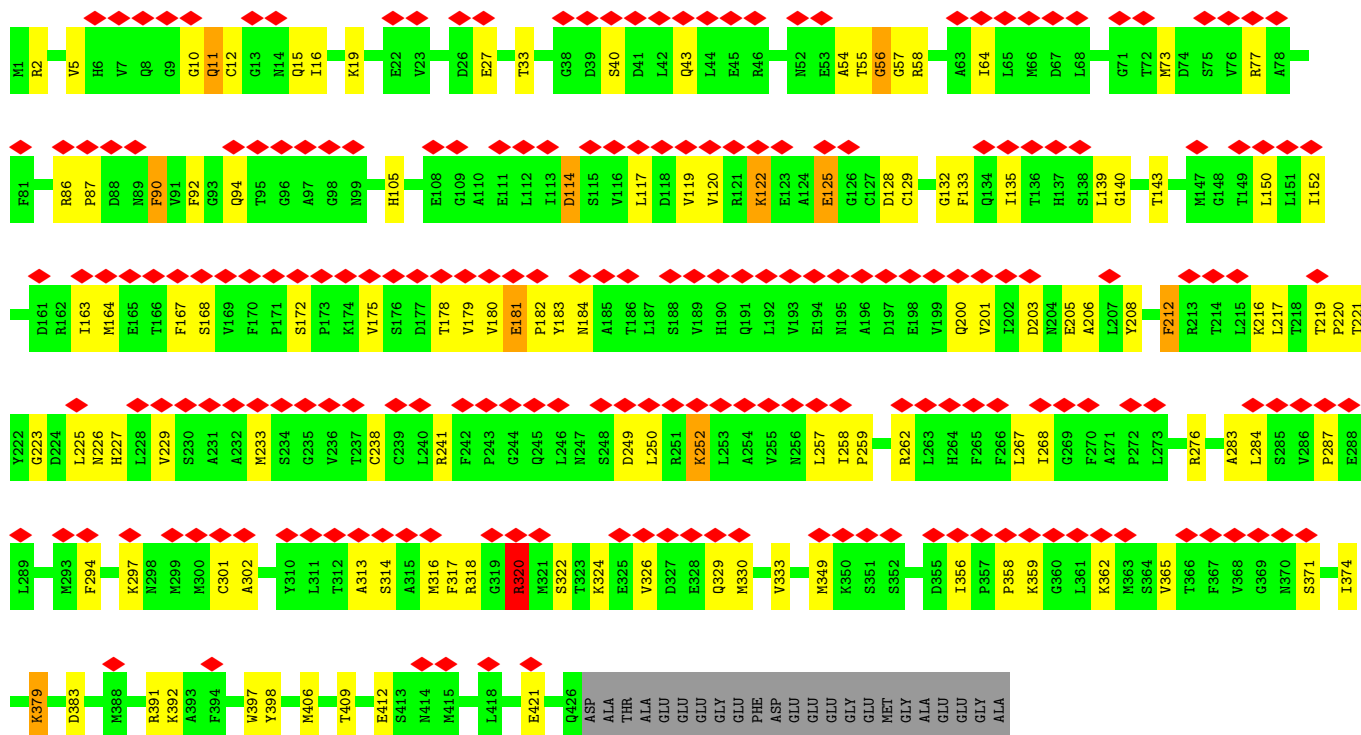


• Molecule 3: Tubulin beta chain





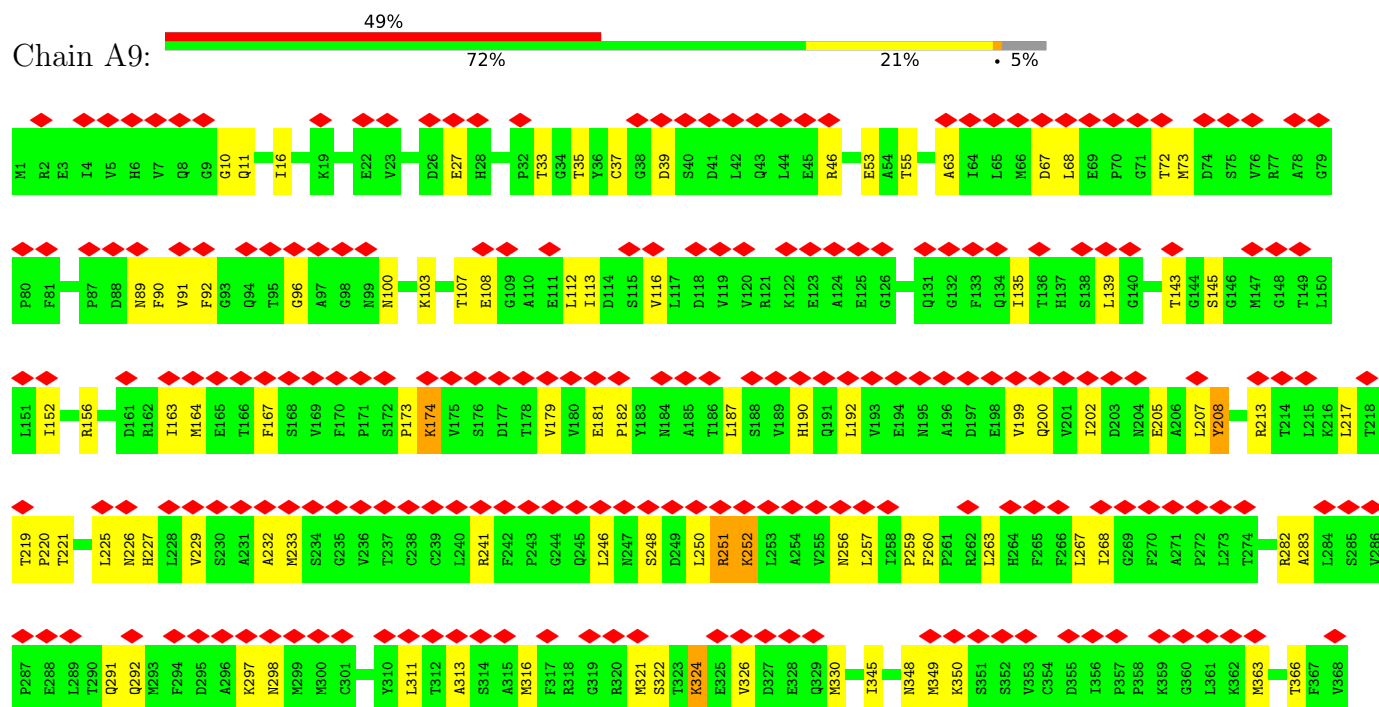
• Molecule 3: Tubulin beta chain

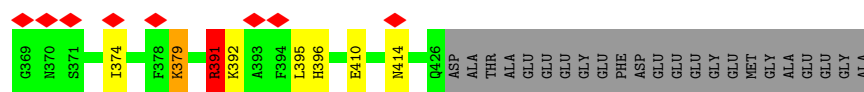


## Chain A7:

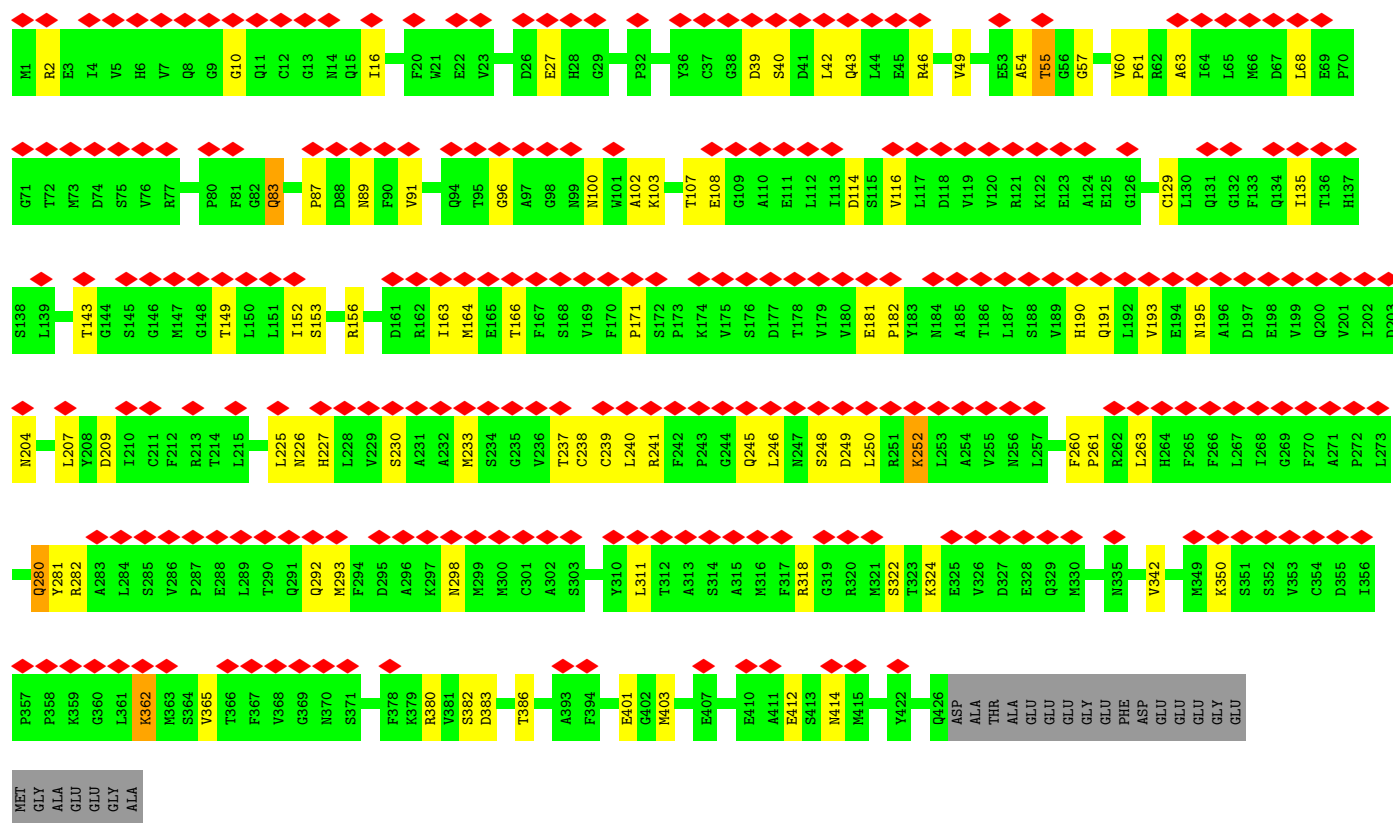
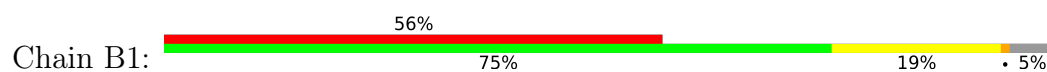


## Chain A9:

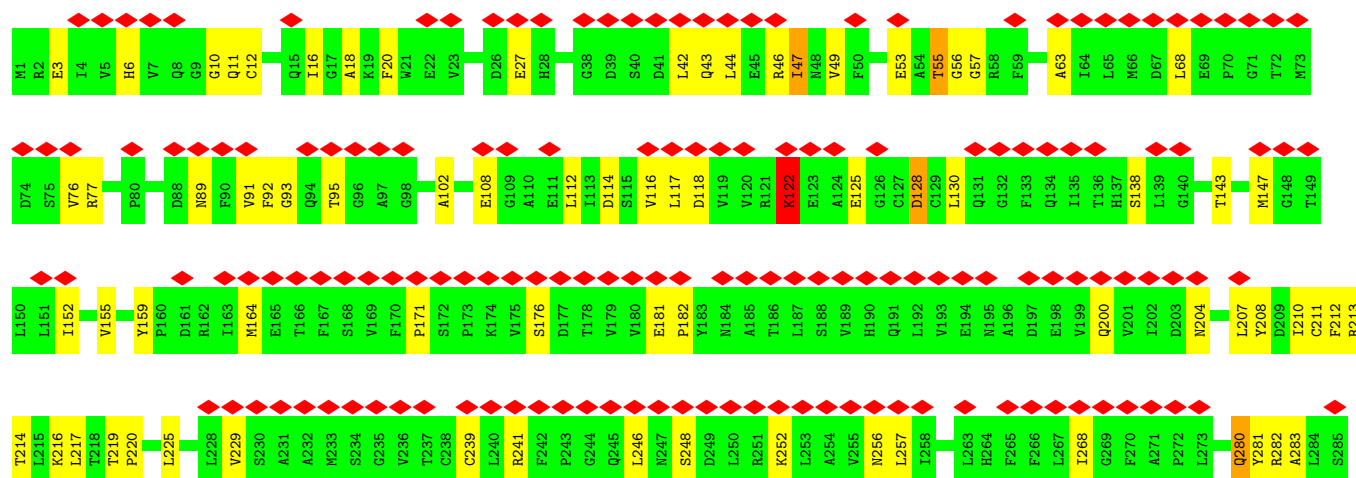
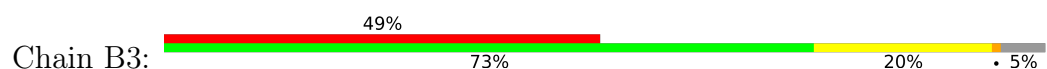


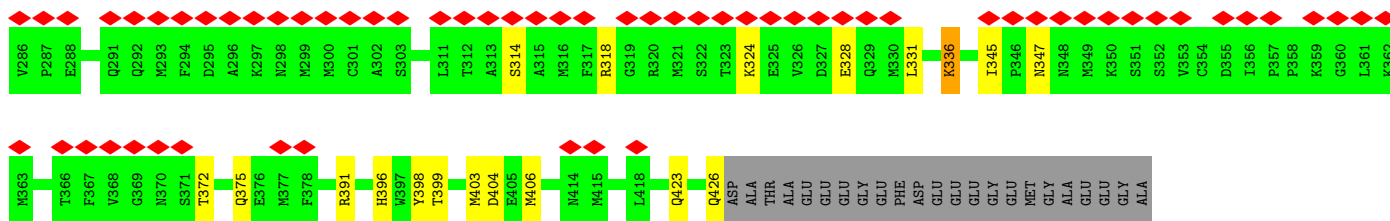


• Molecule 3: Tubulin beta chain

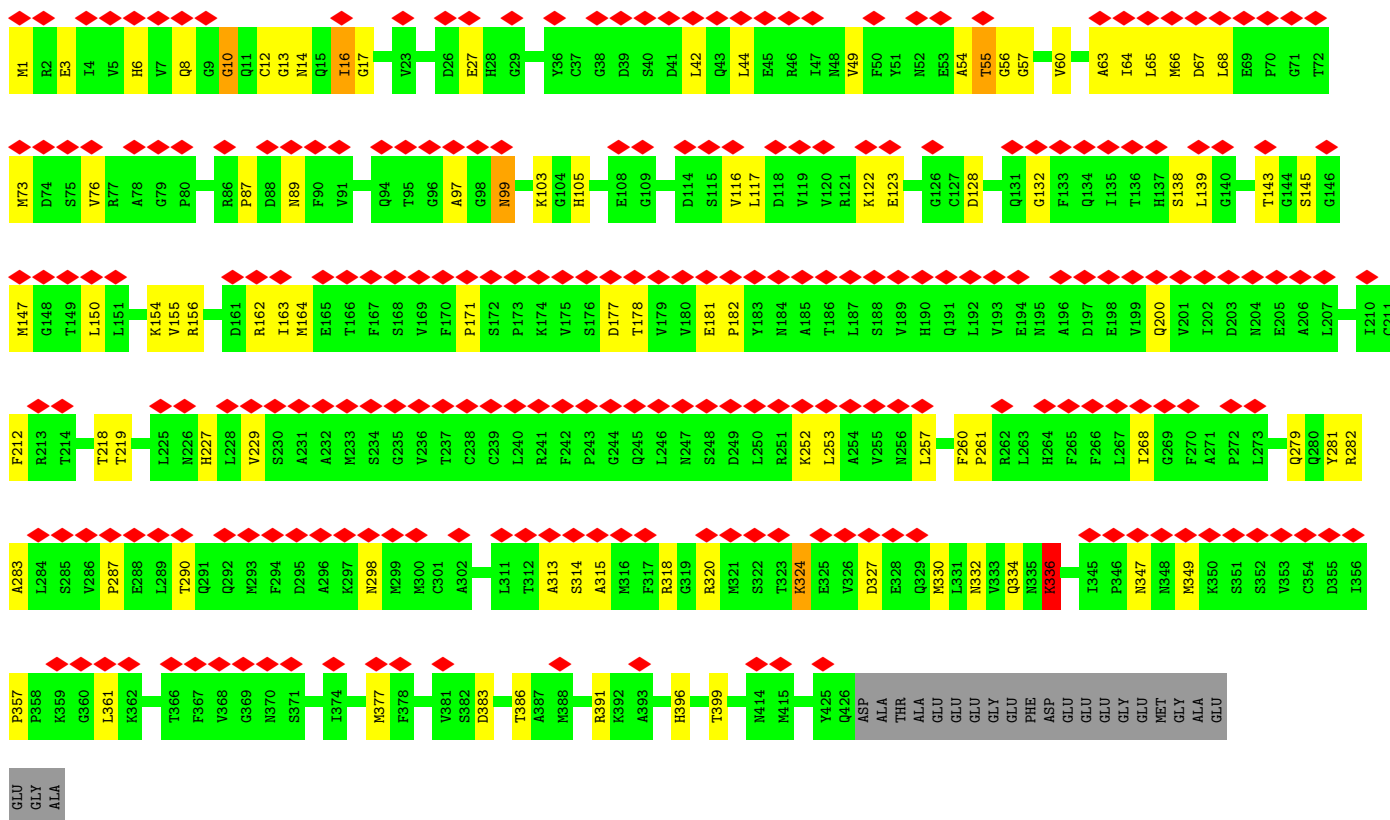
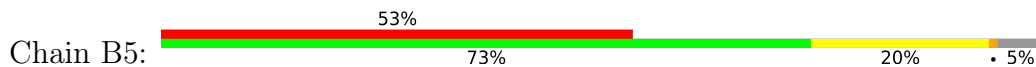


• Molecule 3: Tubulin beta chain

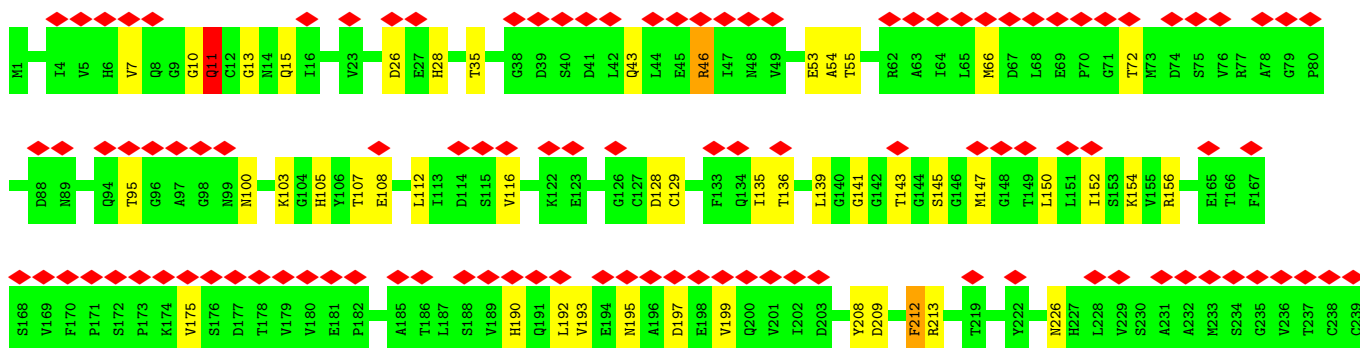
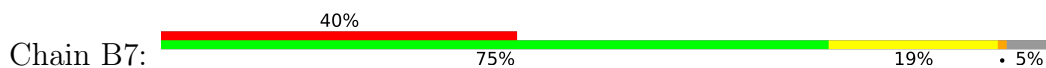


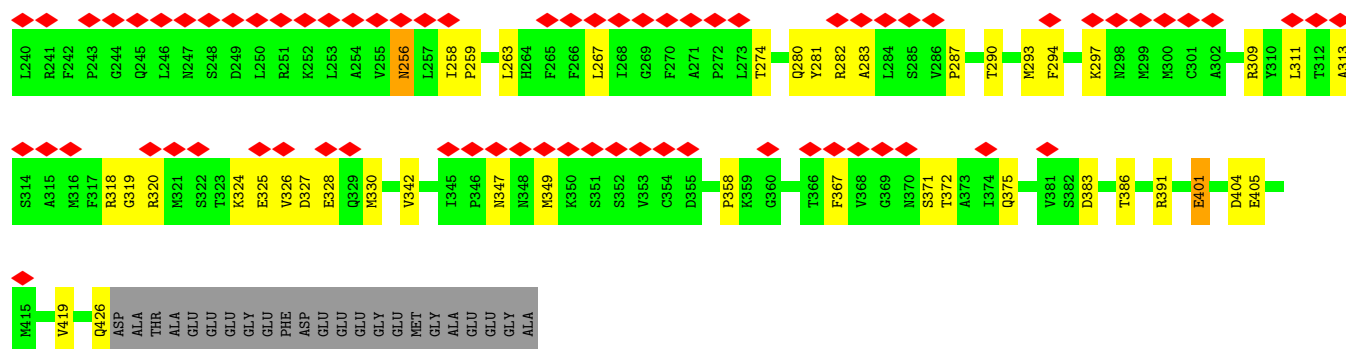


• Molecule 3: Tubulin beta chain

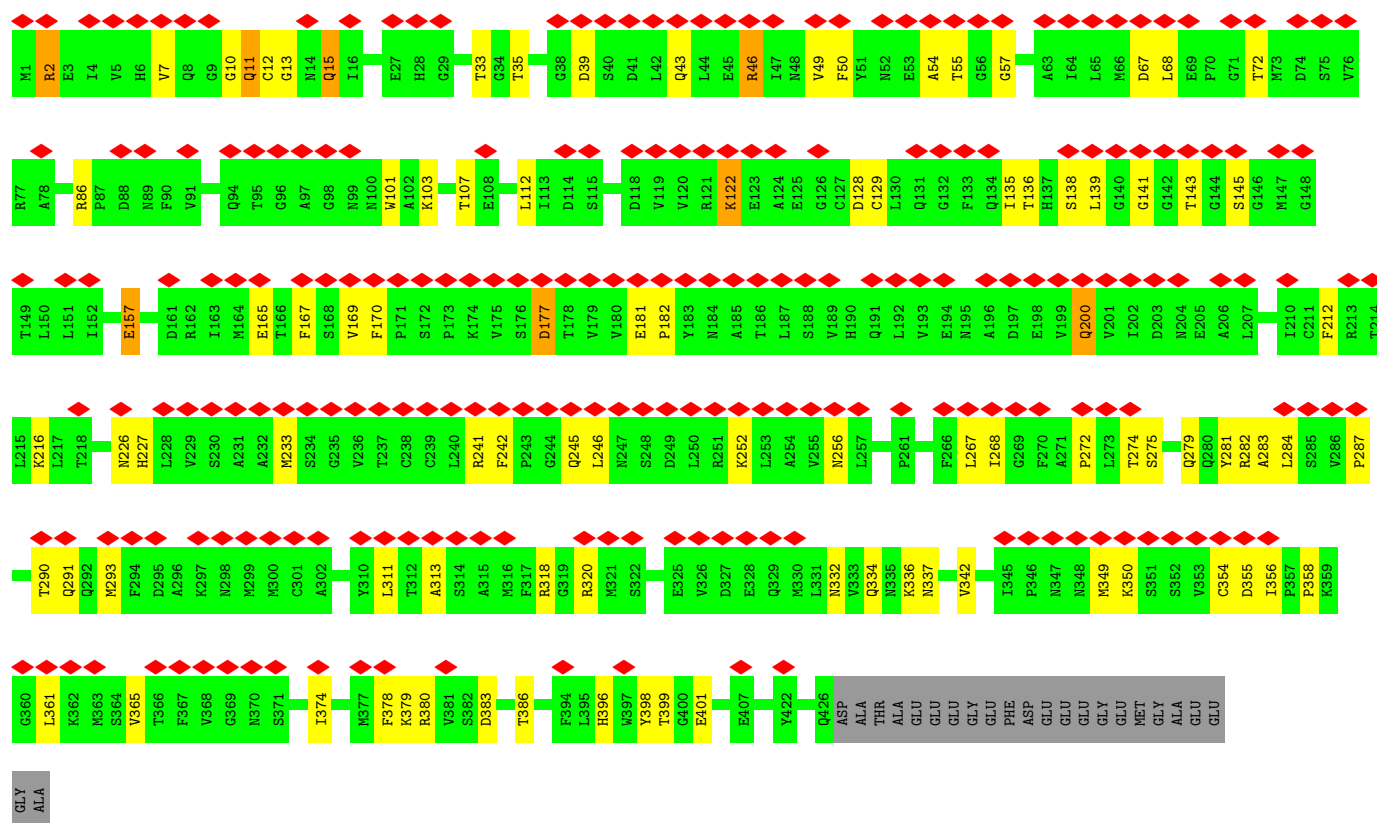
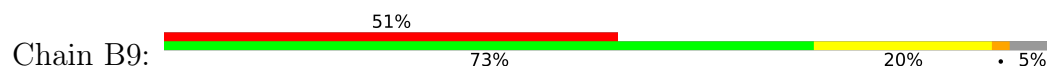


• Molecule 3: Tubulin beta chain

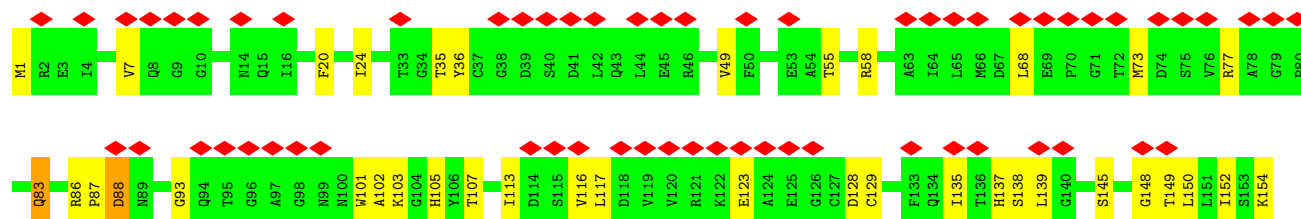
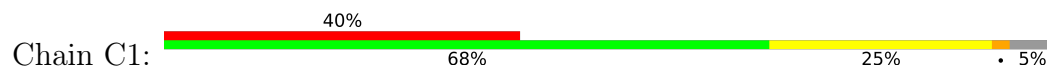


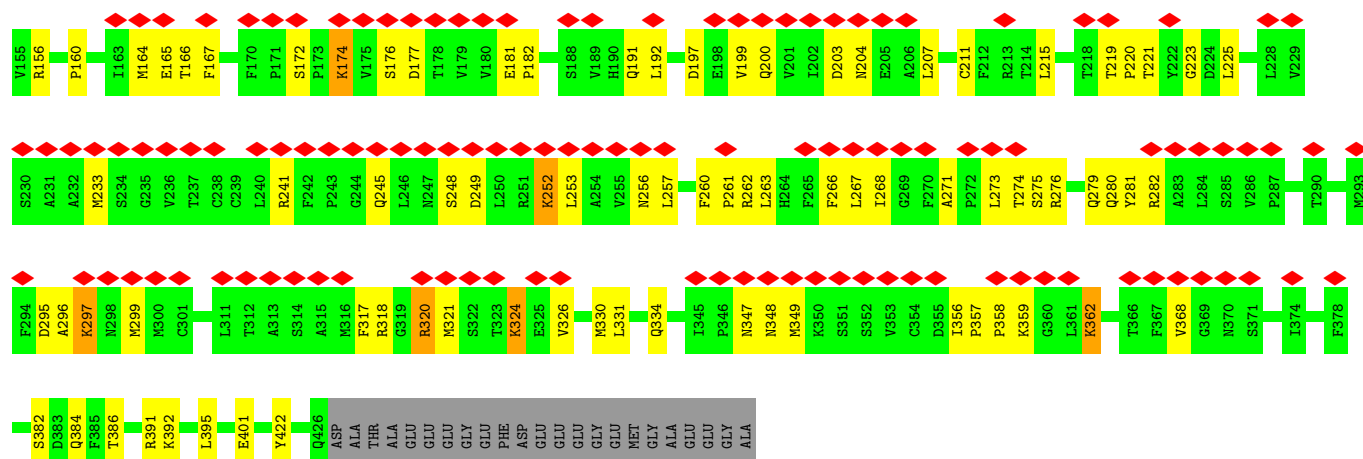


• Molecule 3: Tubulin beta chain

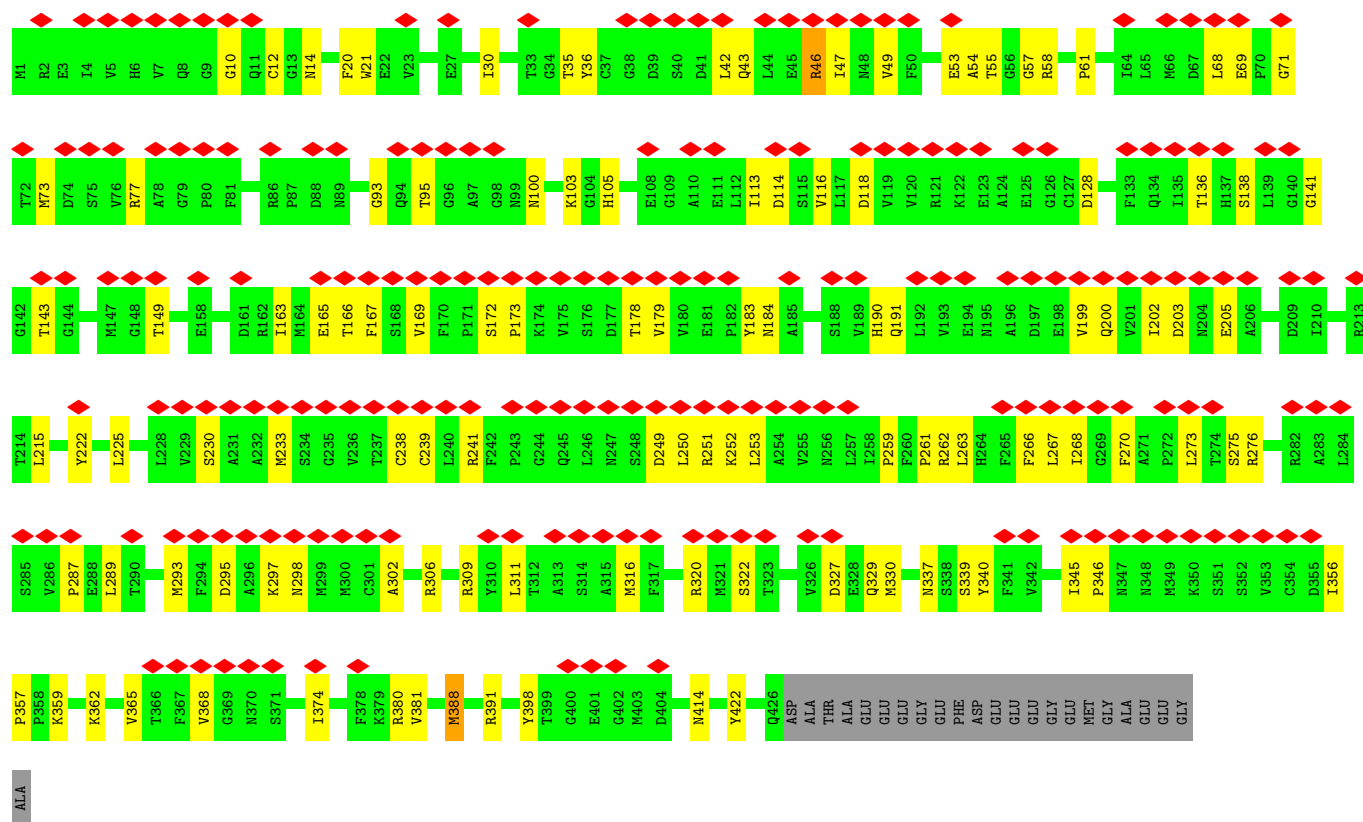
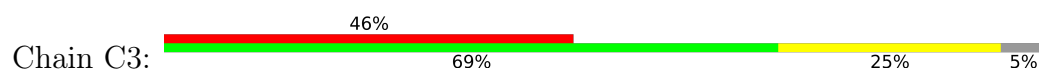


• Molecule 3: Tubulin beta chain

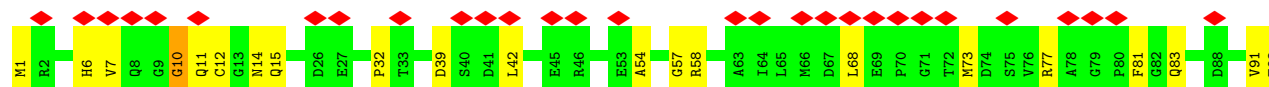
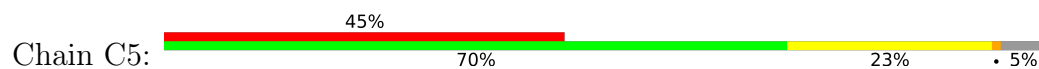


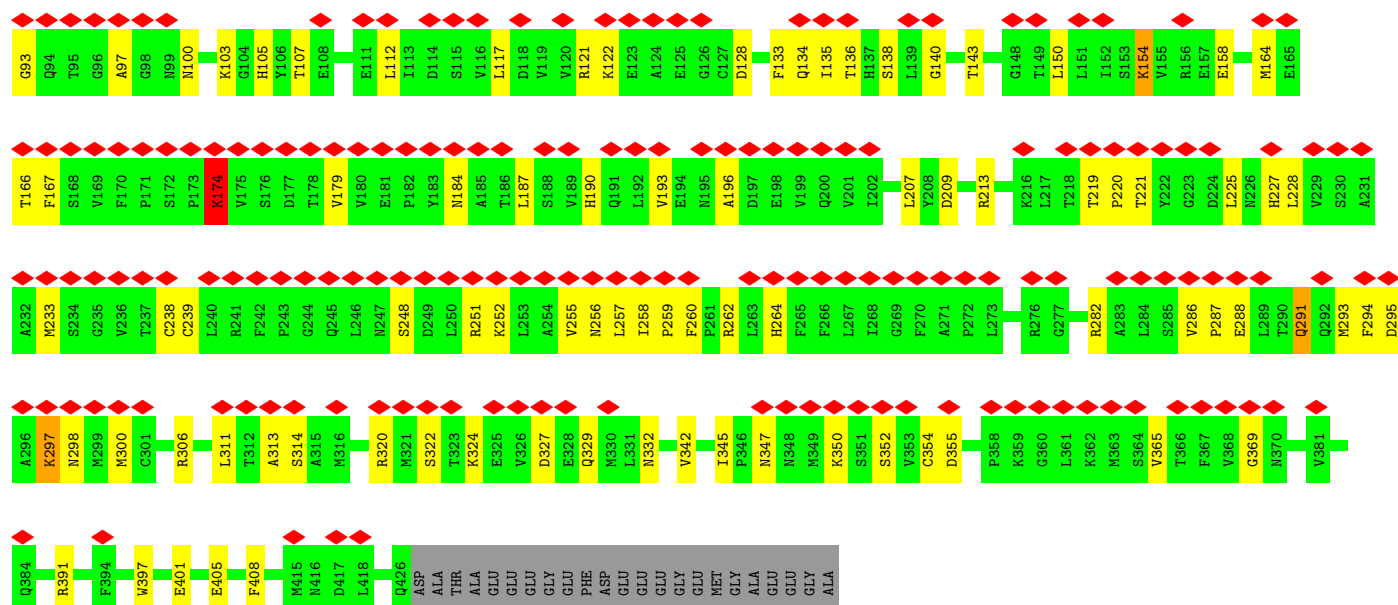


• Molecule 3: Tubulin beta chain

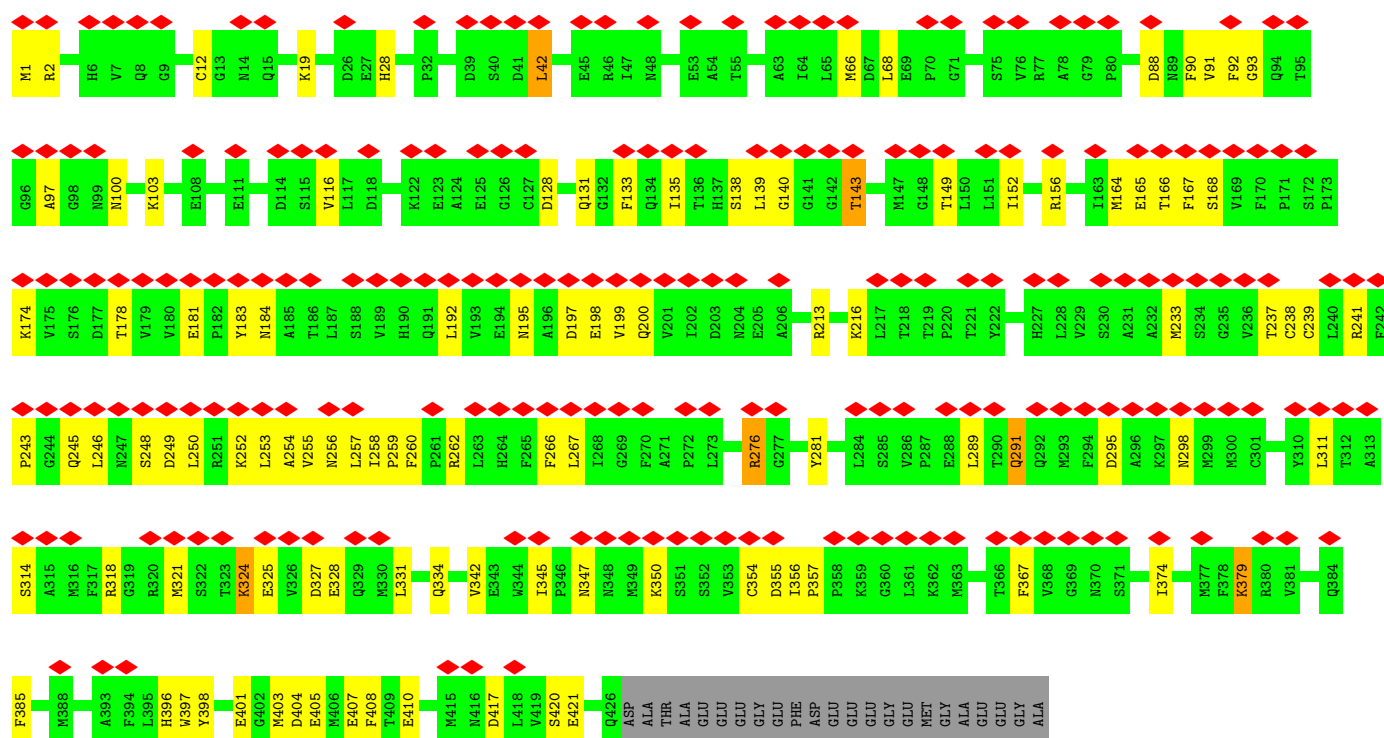
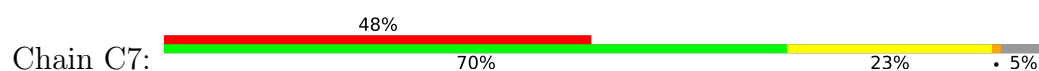


• Molecule 3: Tubulin beta chain

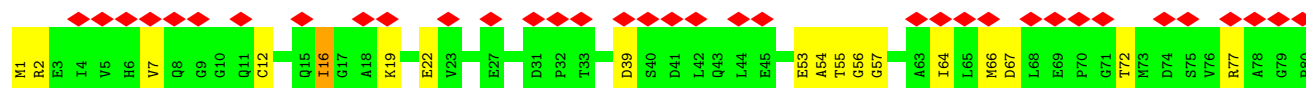


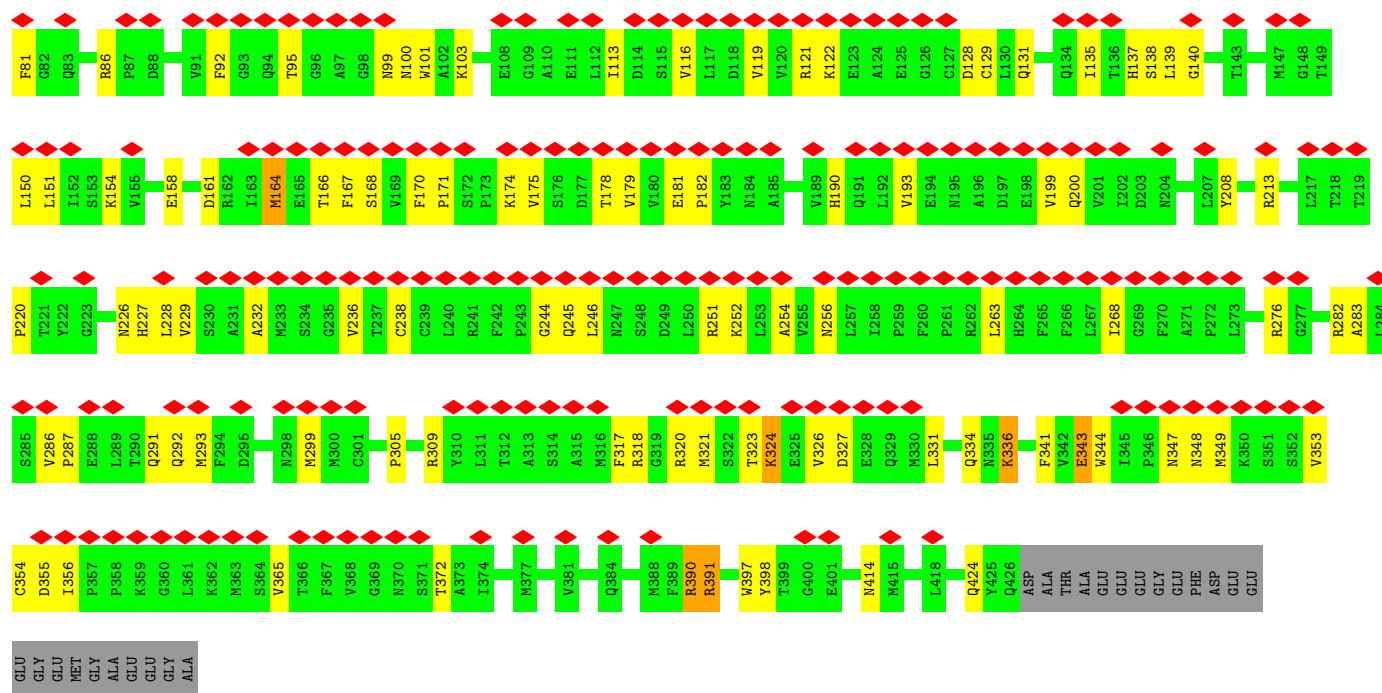


• Molecule 3: Tubulin beta chain

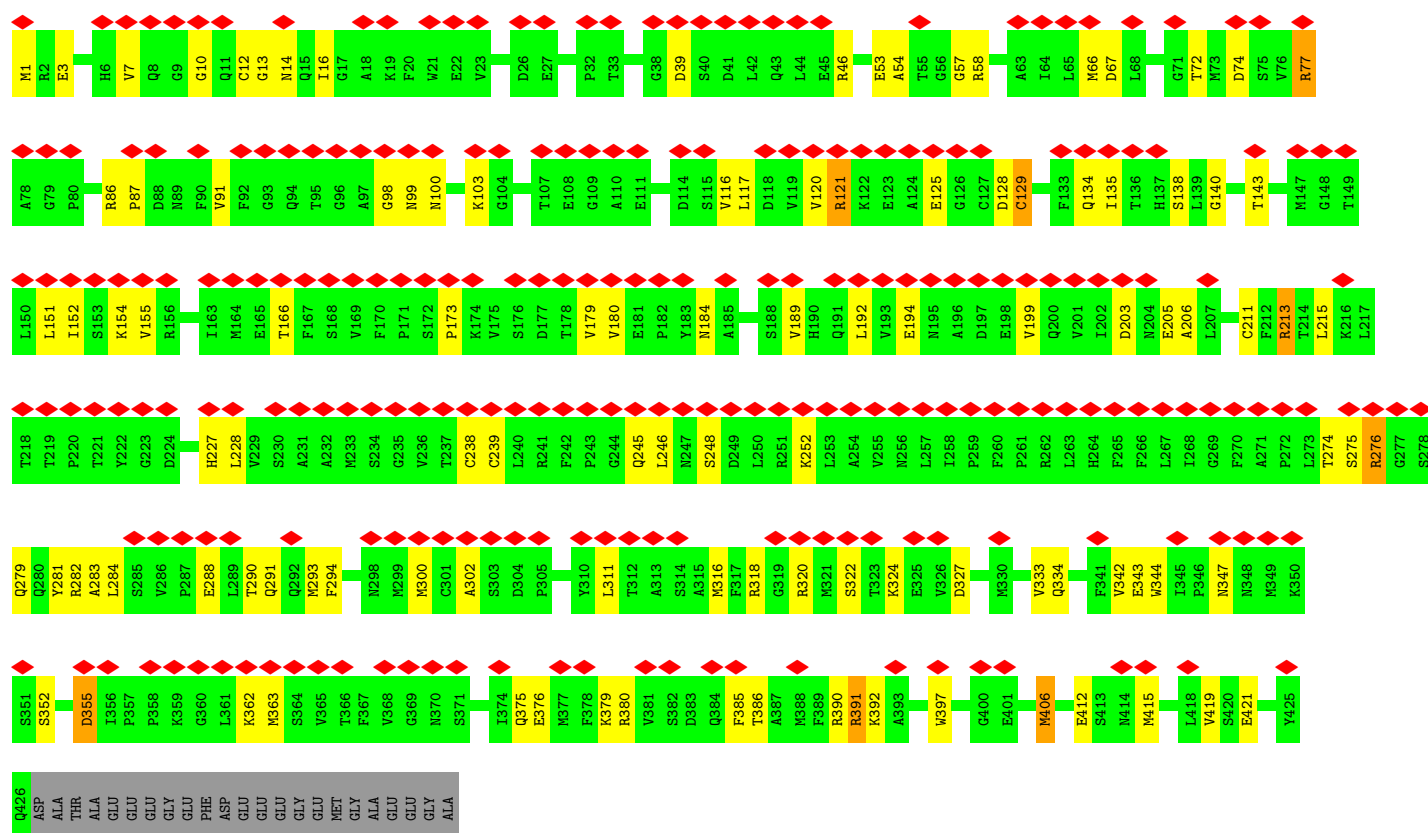
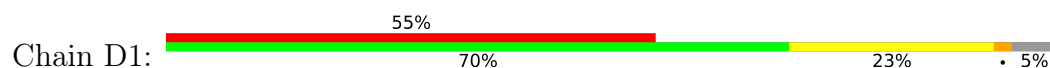


• Molecule 3: Tubulin beta chain

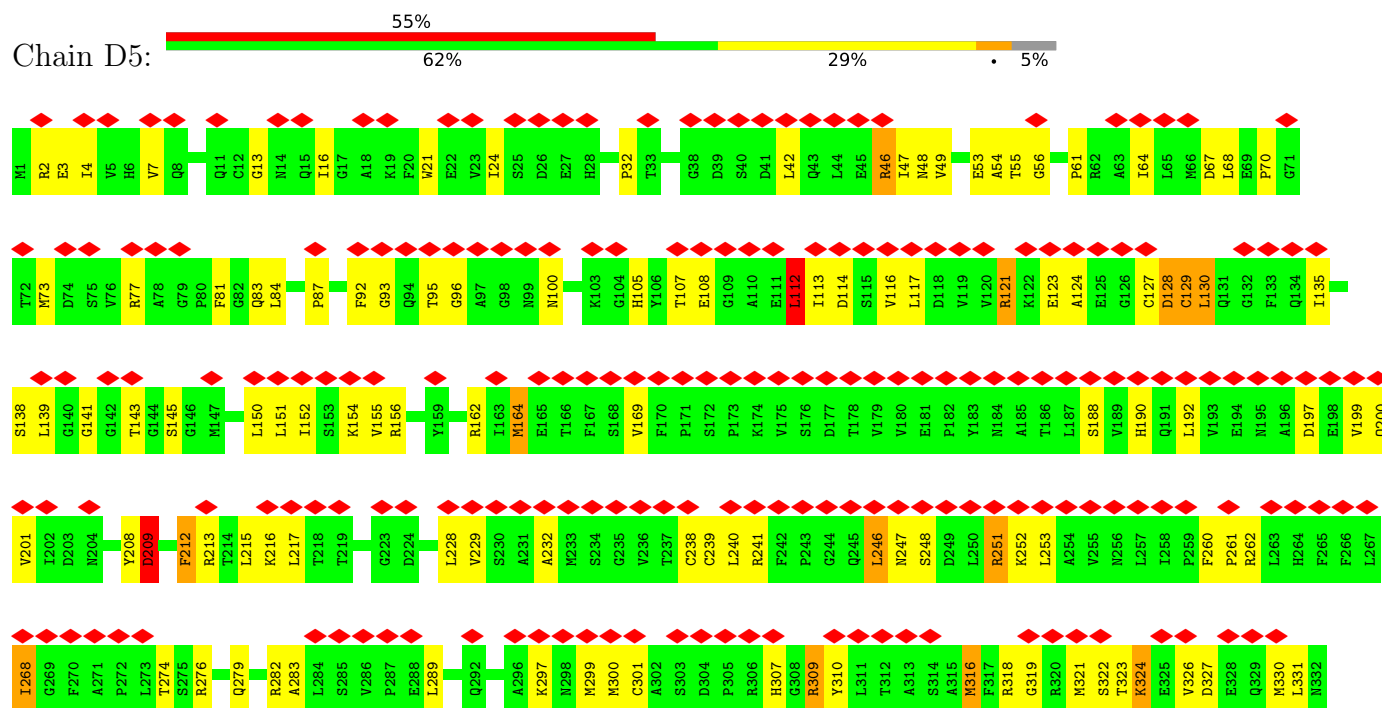


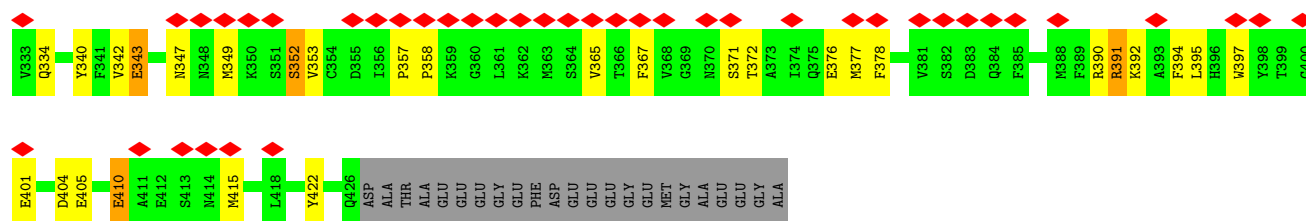


• Molecule 3: Tubulin beta chain

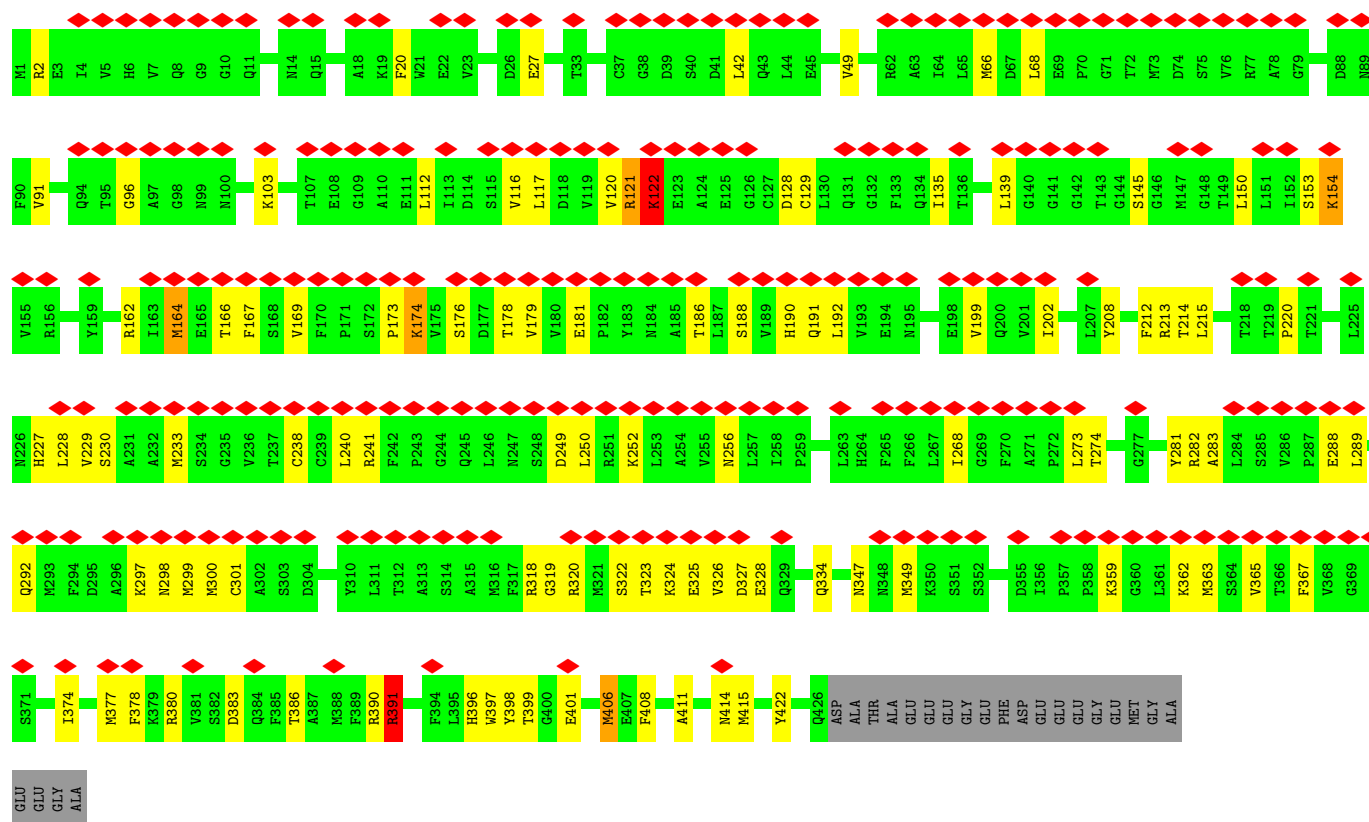
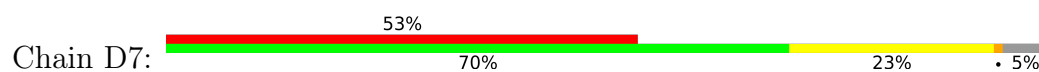


• Molecule 3: Tubulin beta chain

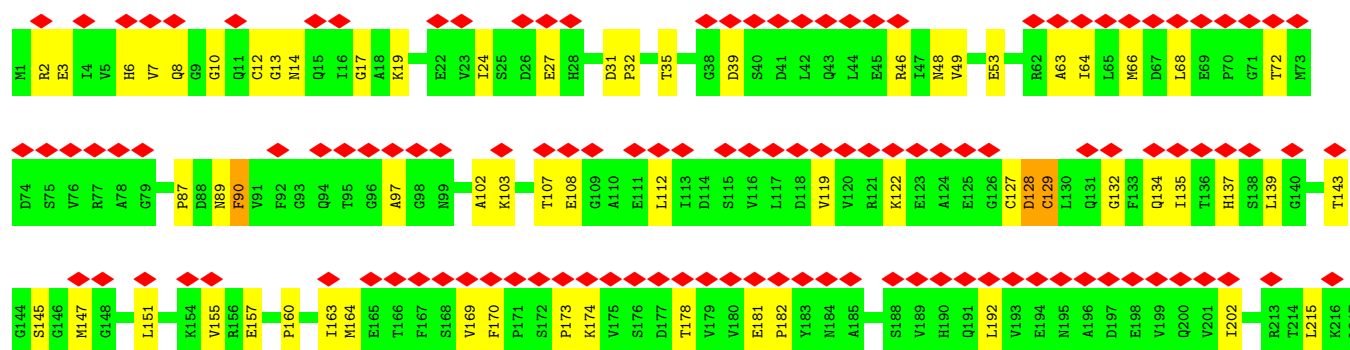
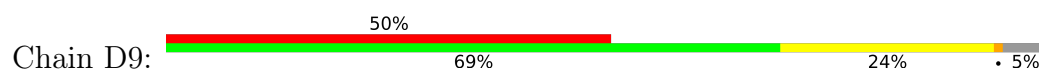


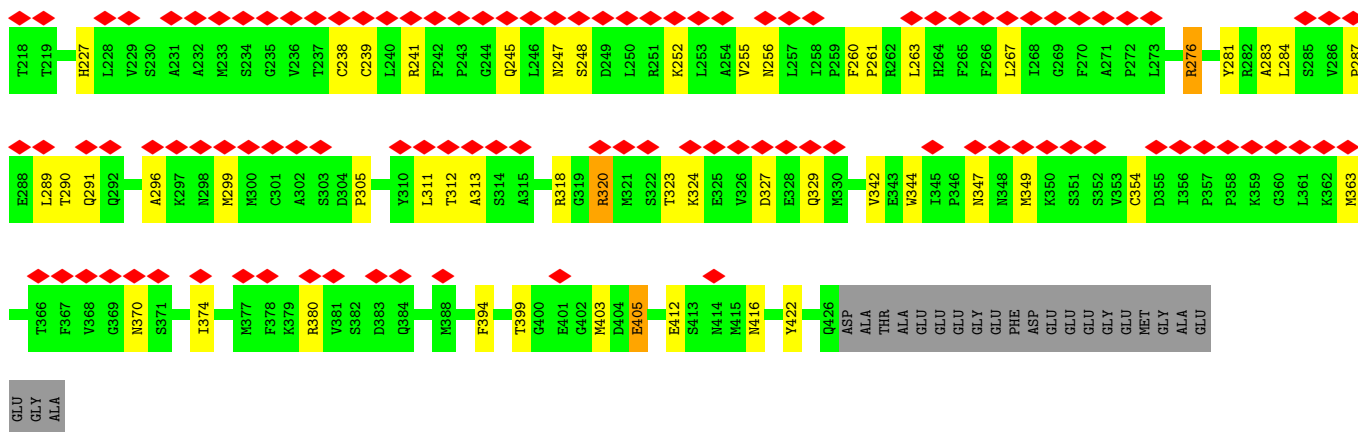


• Molecule 3: Tubulin beta chain



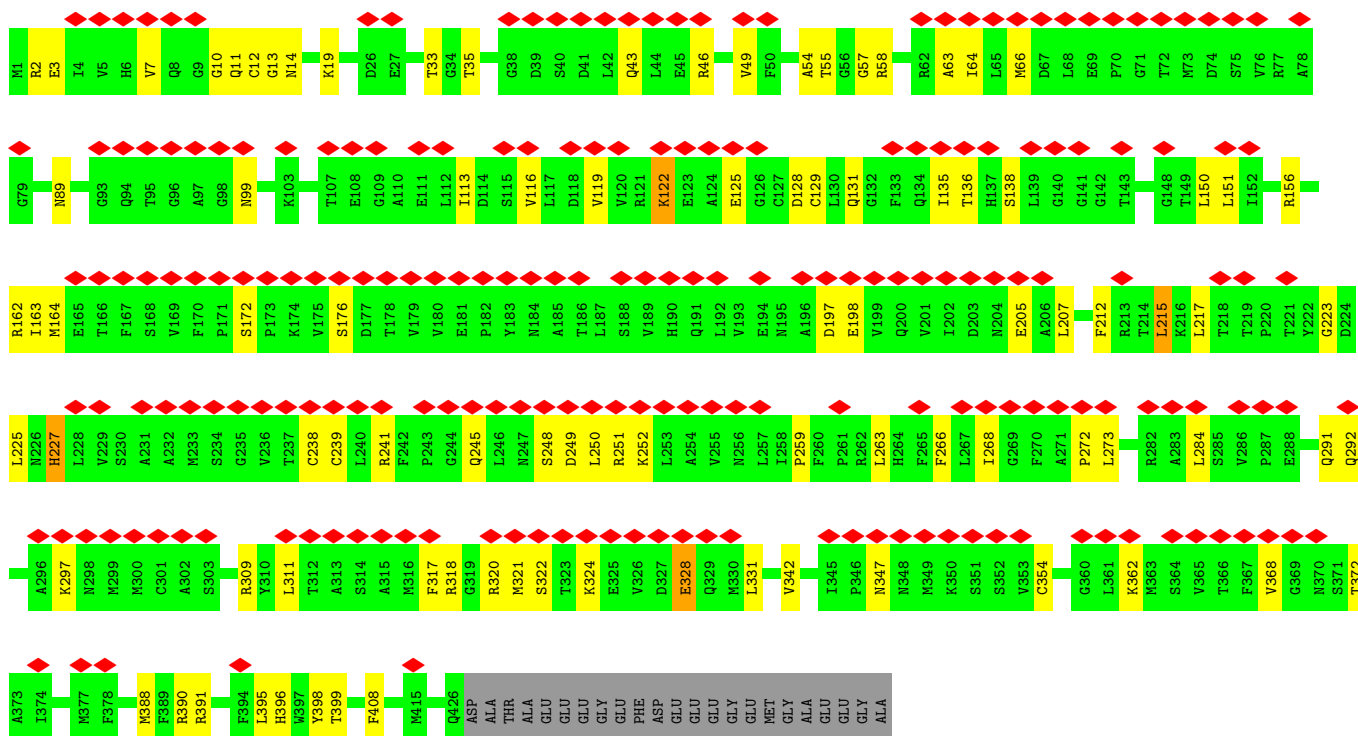
• Molecule 3: Tubulin beta chain





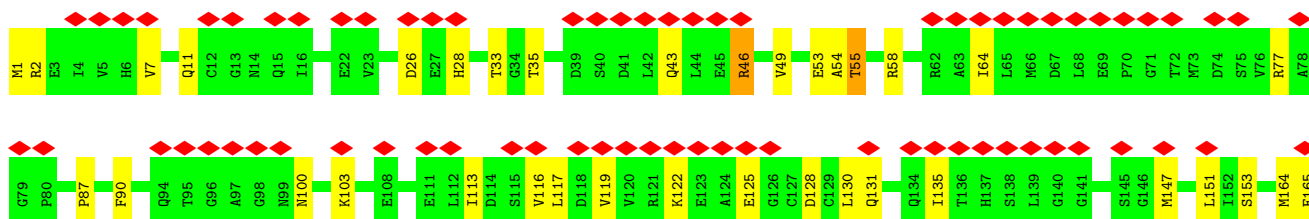
• Molecule 3: Tubulin beta chain

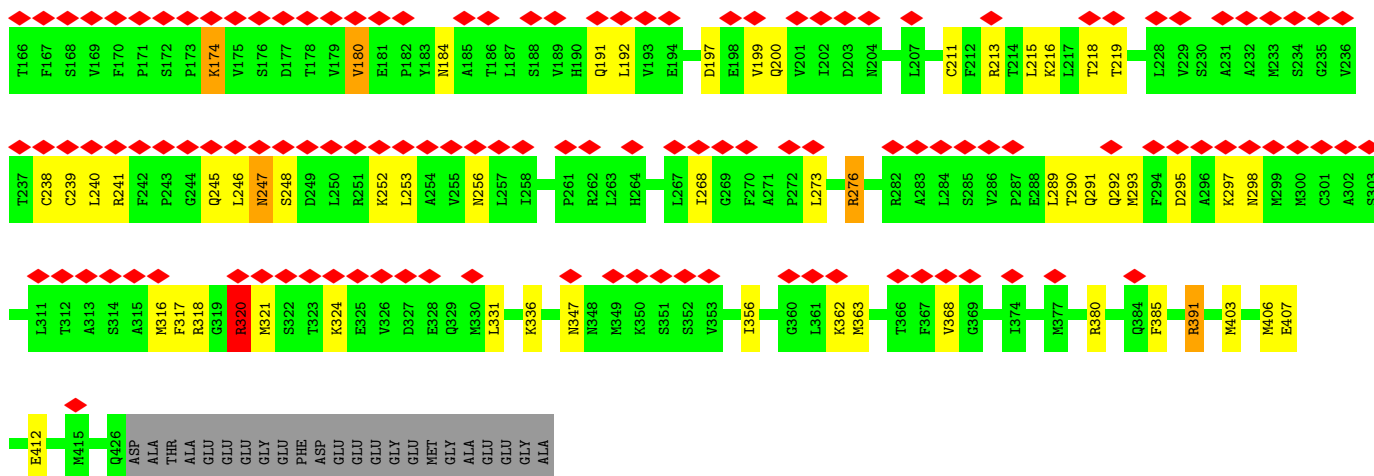
Chain E1: 46% 74% 20% 5%



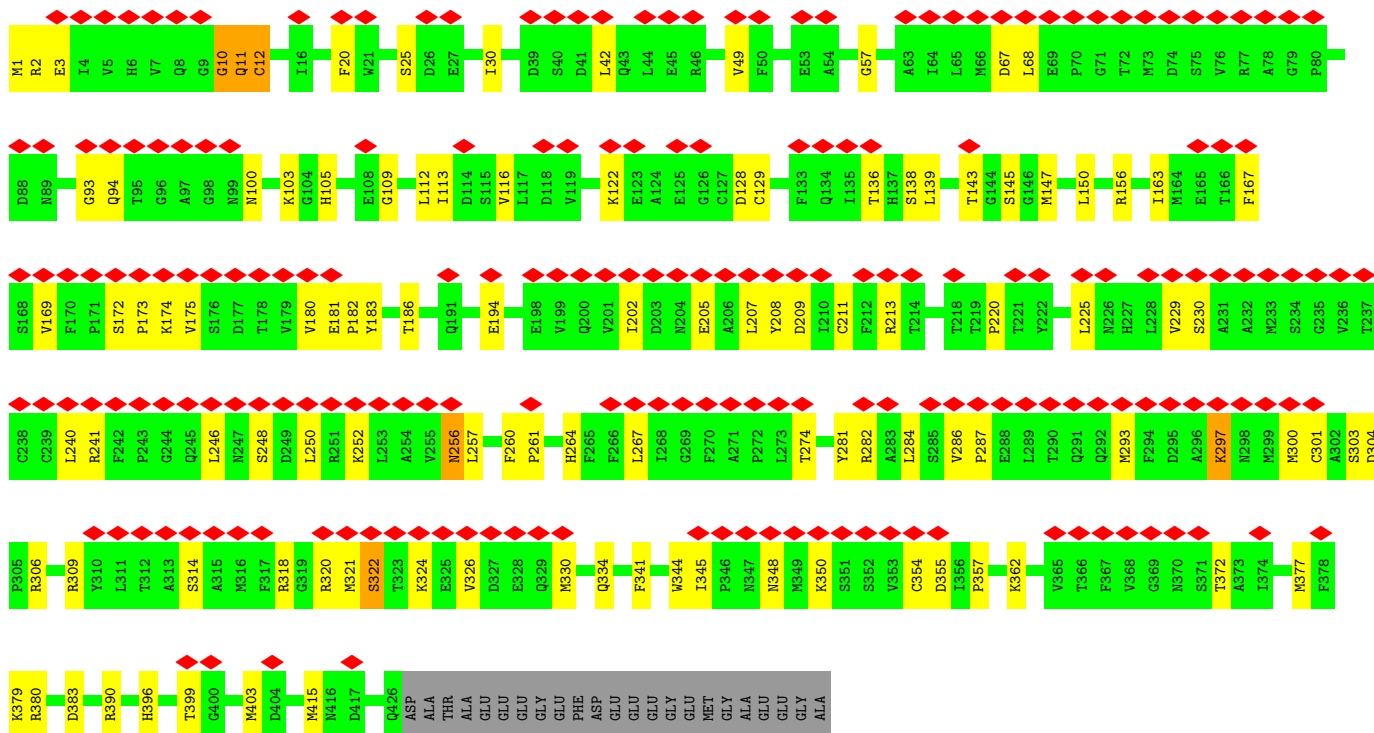
• Molecule 3: Tubulin beta chain

Chain E3: 43% 74% 19% 5%

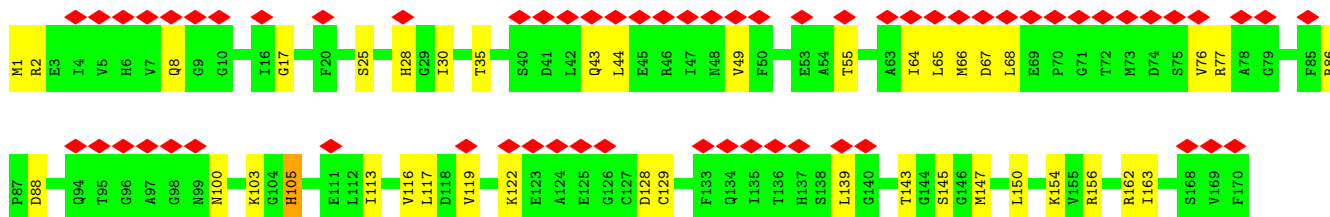
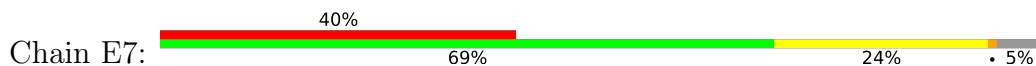


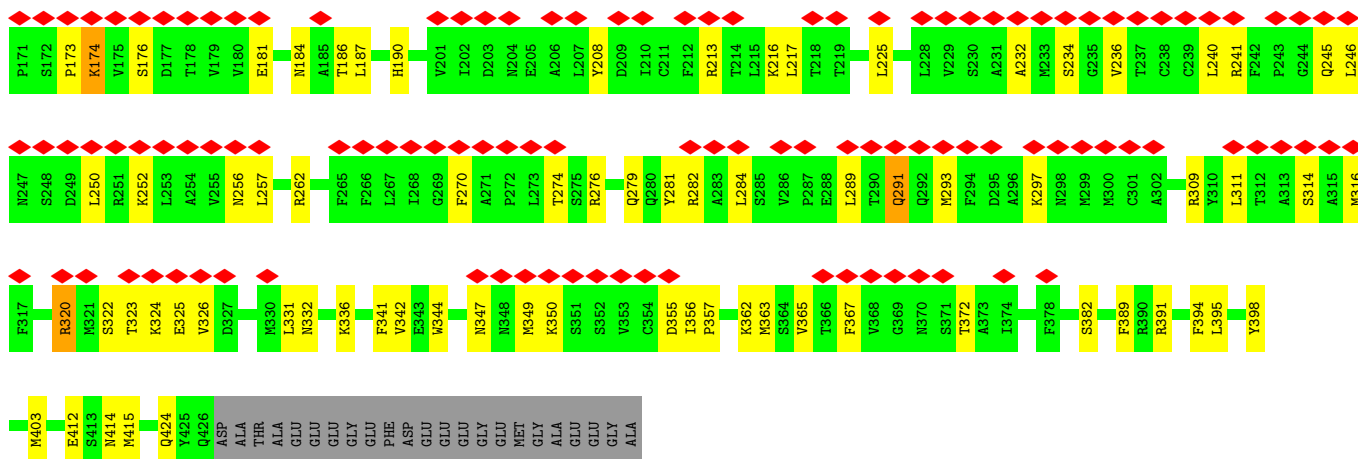


• Molecule 3: Tubulin beta chain

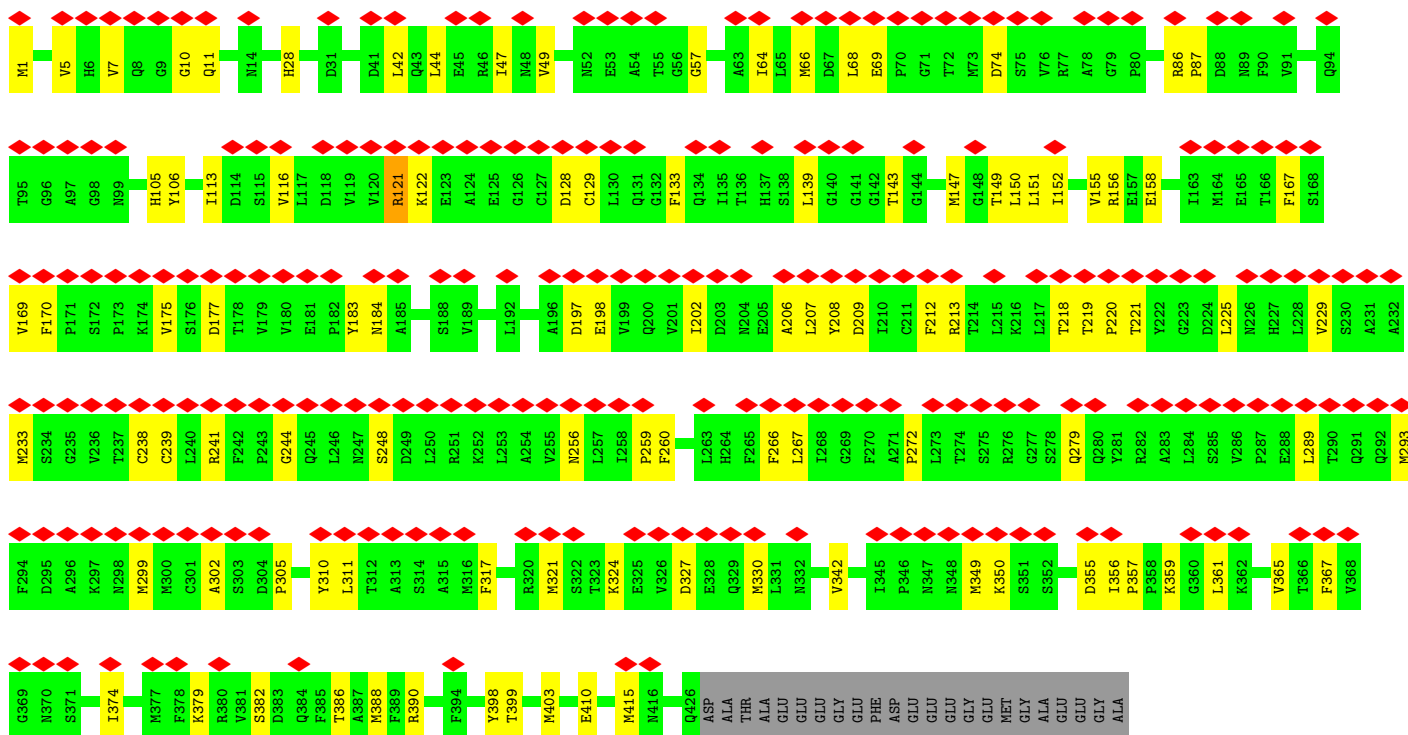
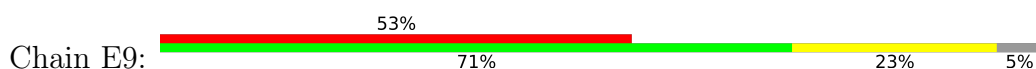


• Molecule 3: Tubulin beta chain

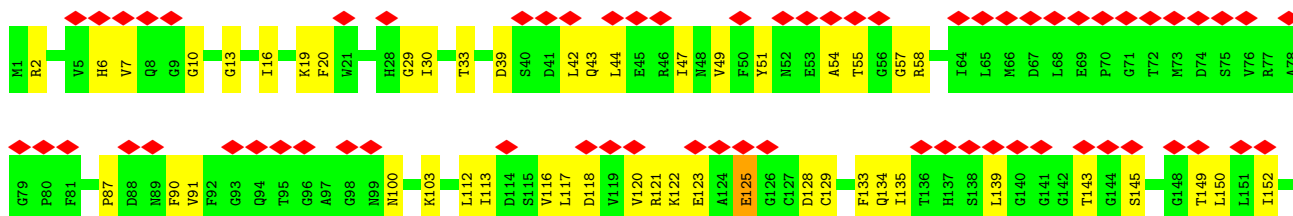
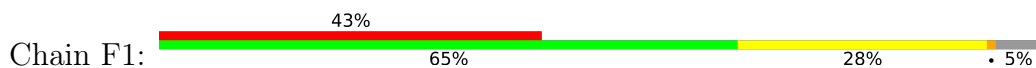


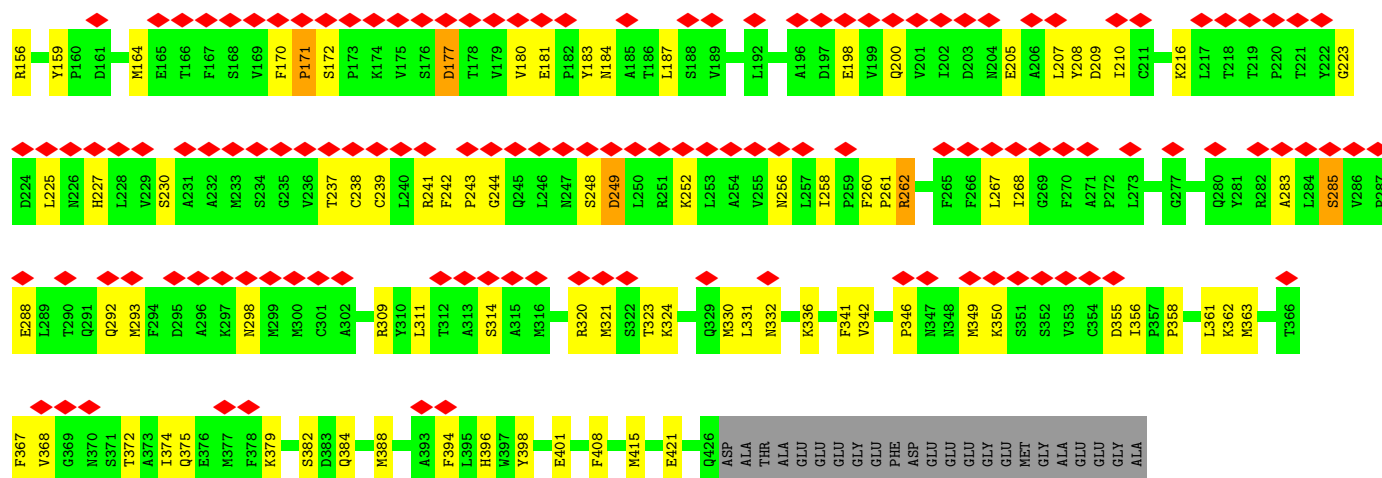


• Molecule 3: Tubulin beta chain

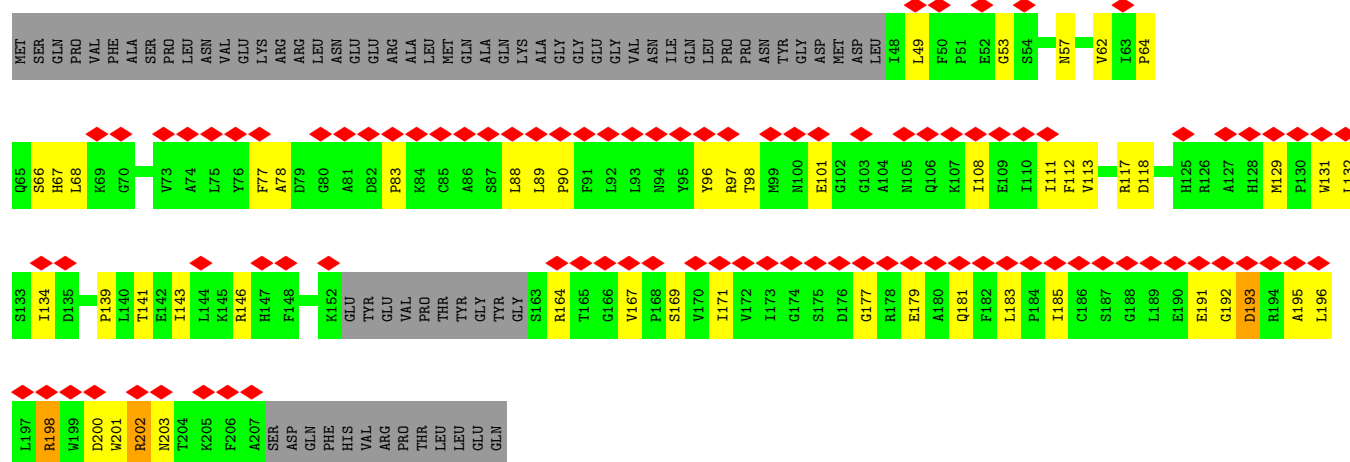
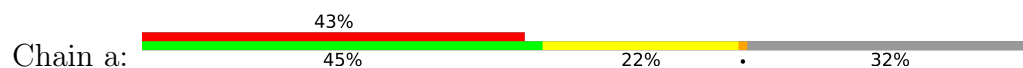


• Molecule 3: Tubulin beta chain

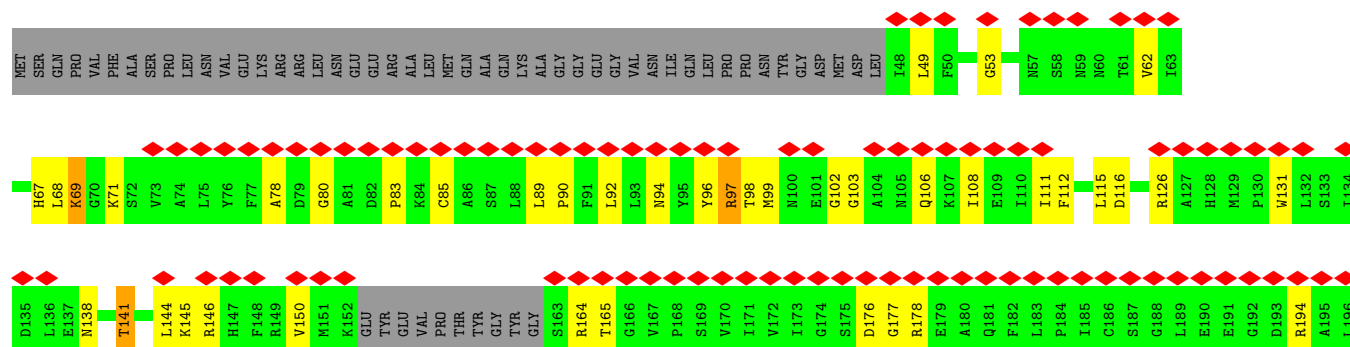


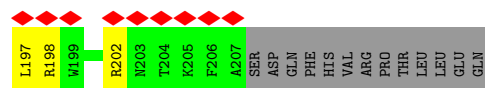


• Molecule 4: PDI family protein

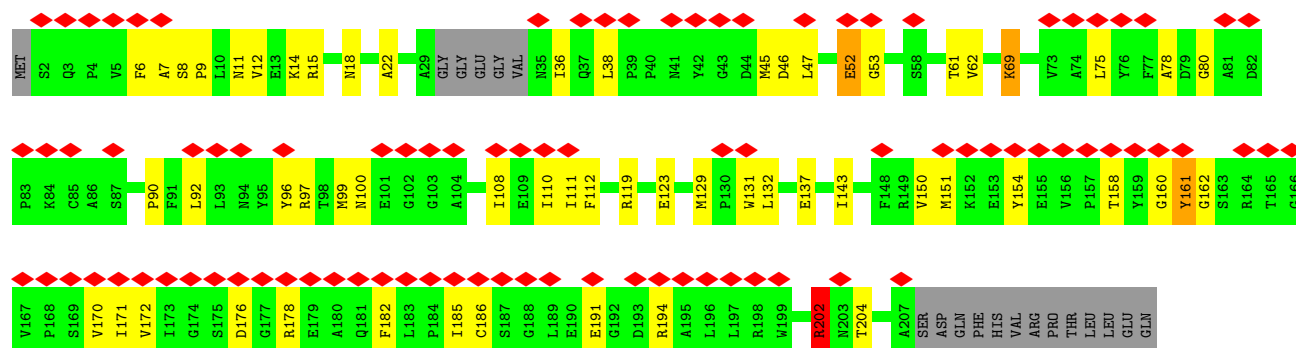
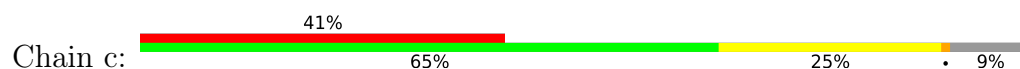


• Molecule 4: PDI family protein

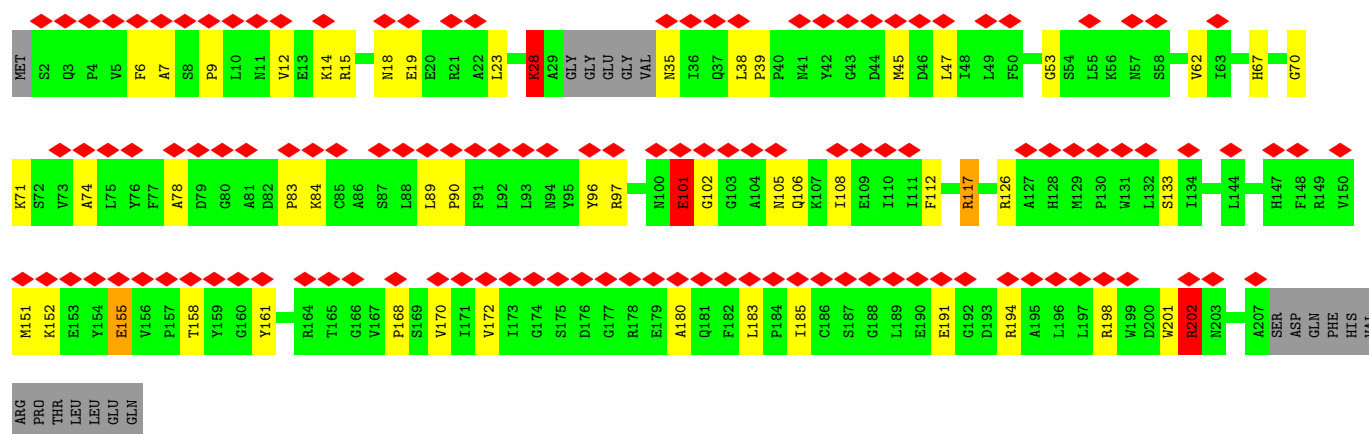




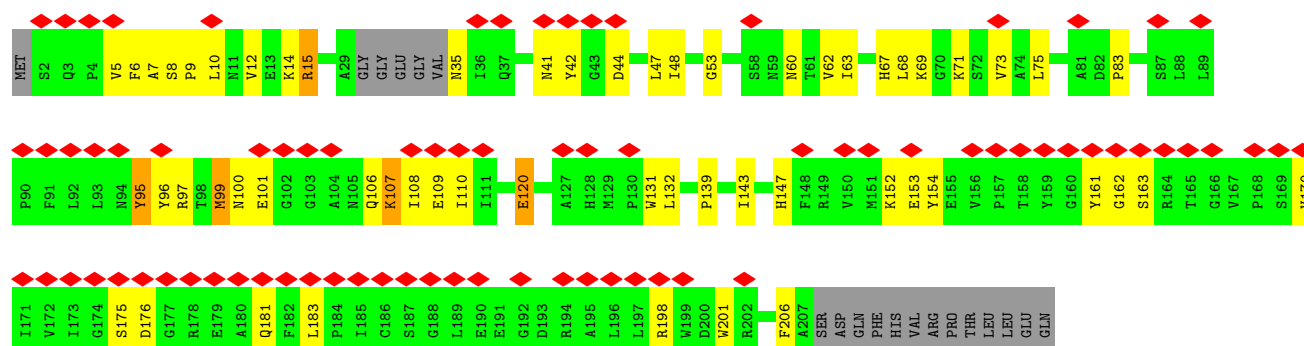
• Molecule 4: PDI family protein



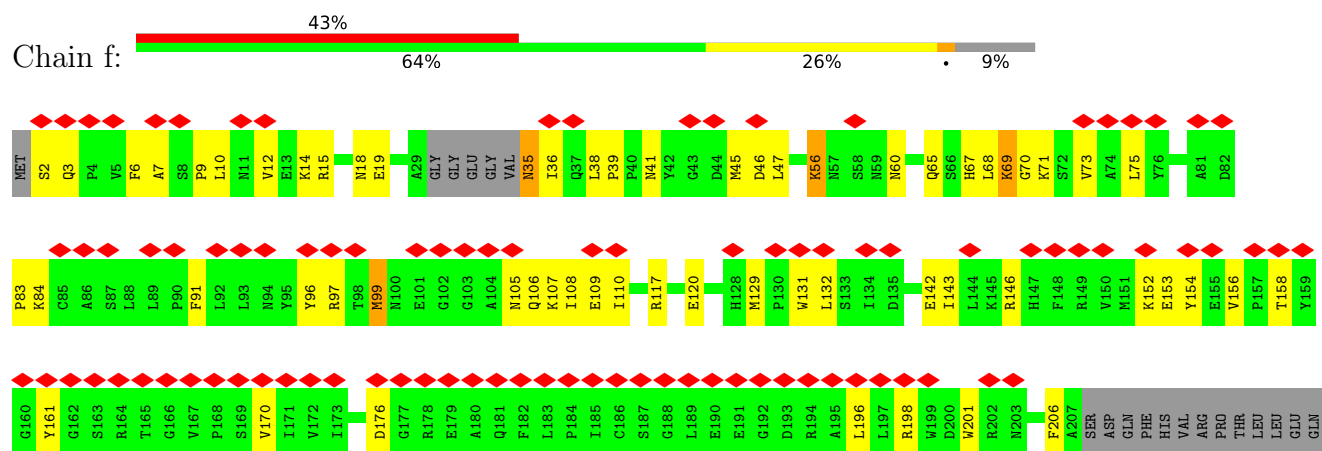
• Molecule 4: PDI family protein



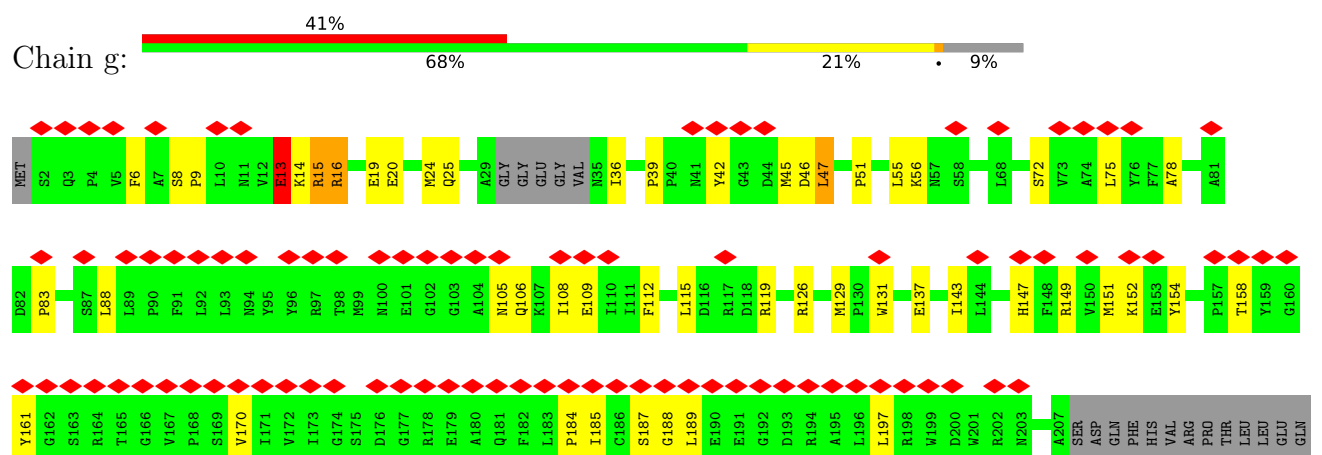
• Molecule 4: PDI family protein



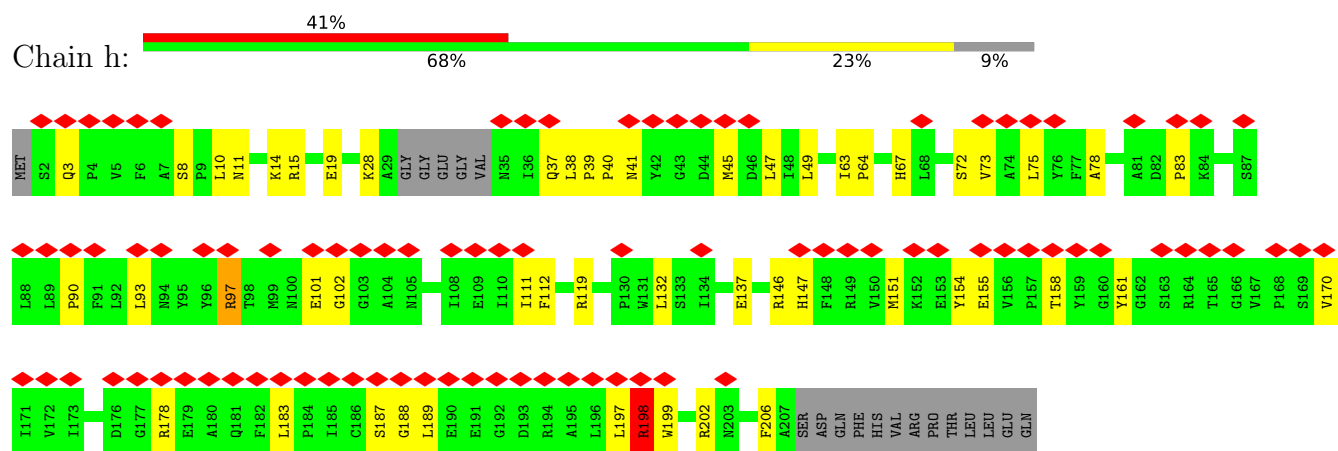
- Molecule 4: PDI family protein



- Molecule 4: PDI family protein

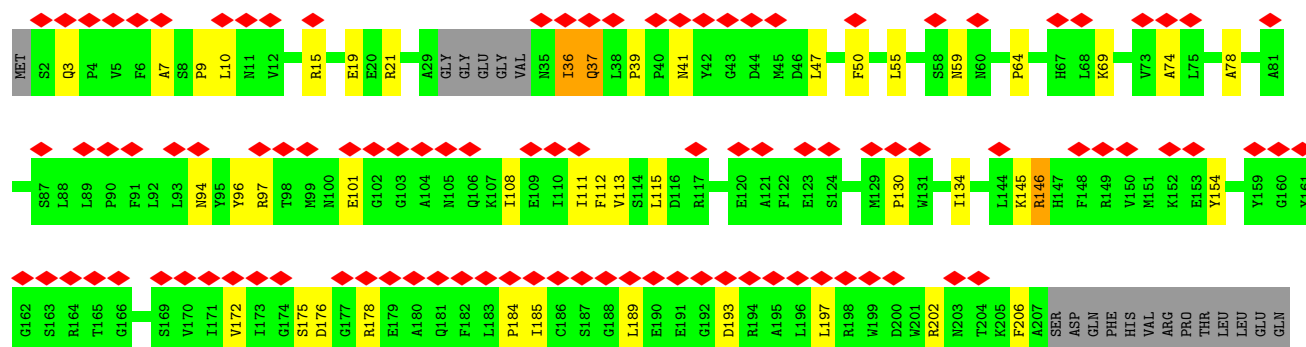


- Molecule 4: PDI family protein

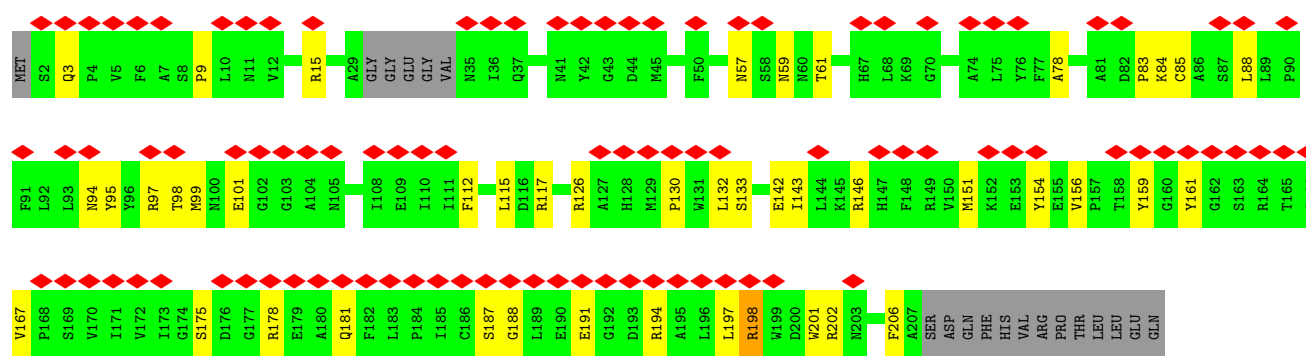
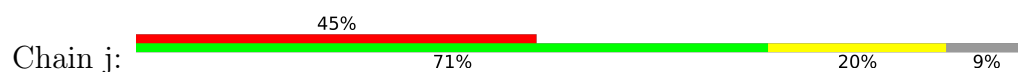


- Molecule 4: PDI family protein

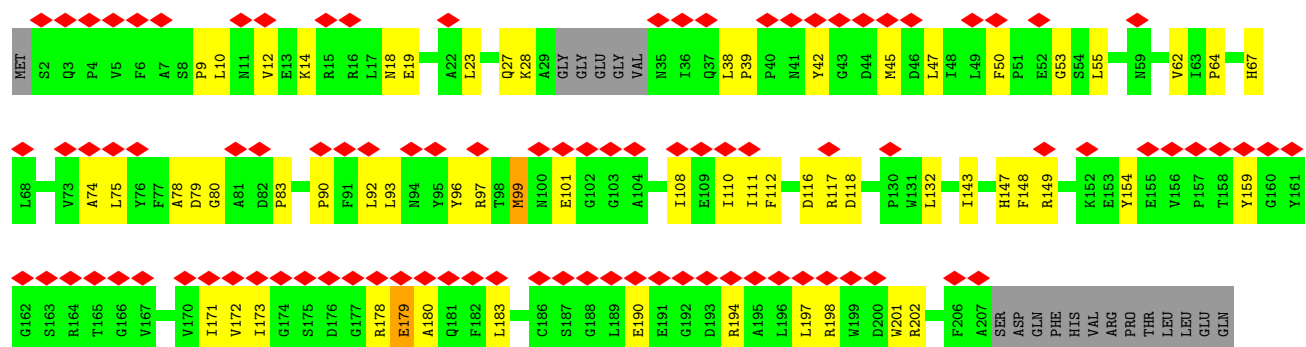
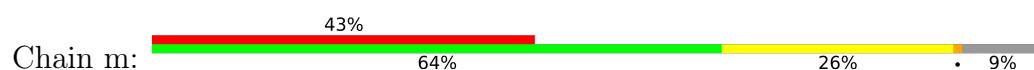




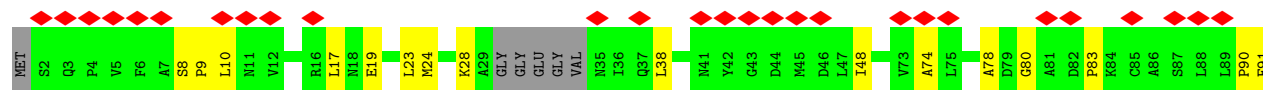
• Molecule 4: PDI family protein

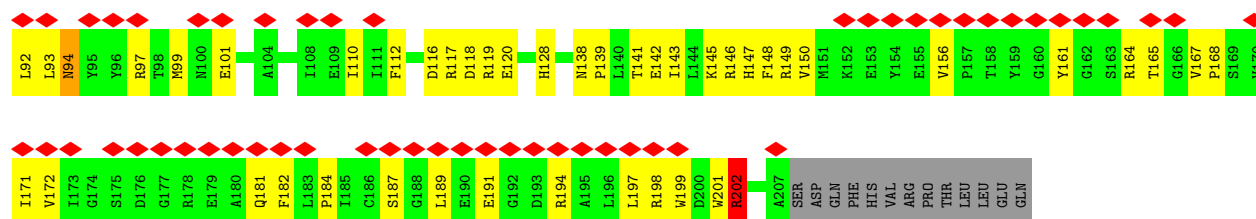


• Molecule 4: PDI family protein

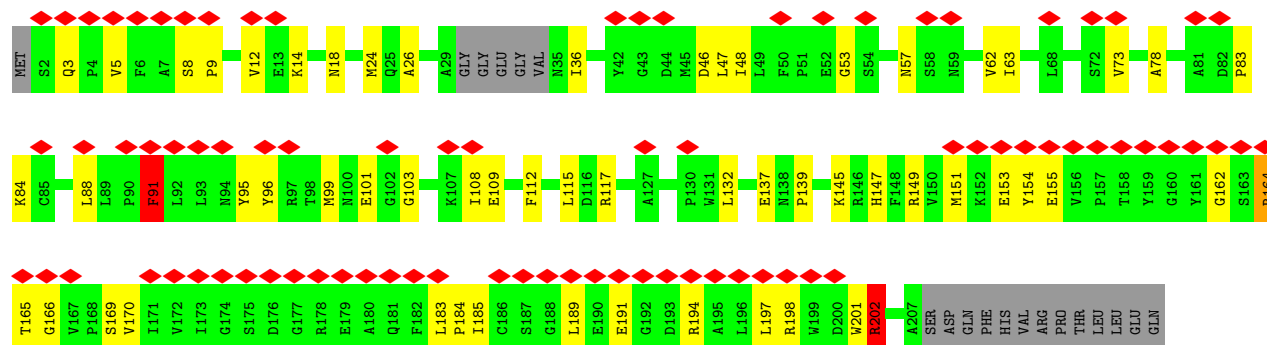


• Molecule 4: PDI family protein

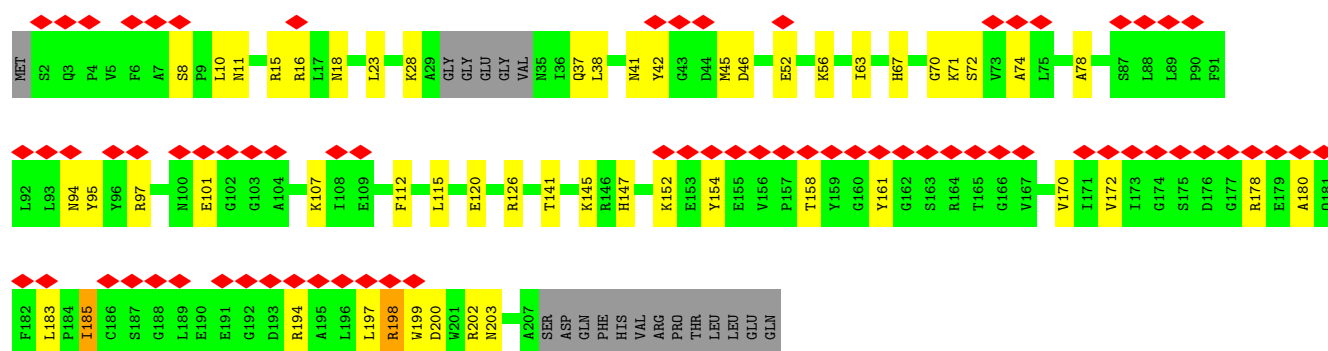




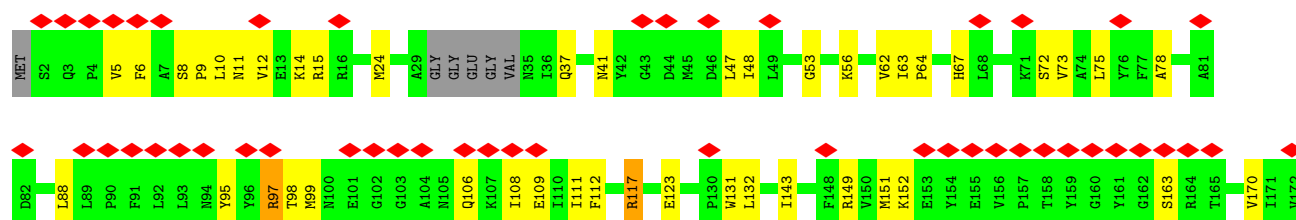
• Molecule 4: PDI family protein

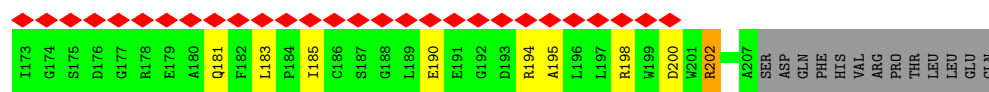


• Molecule 4: PDI family protein

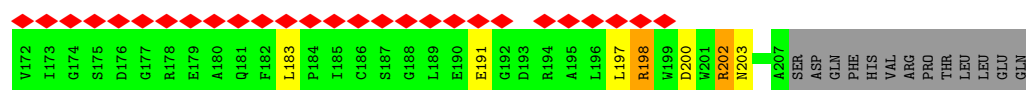
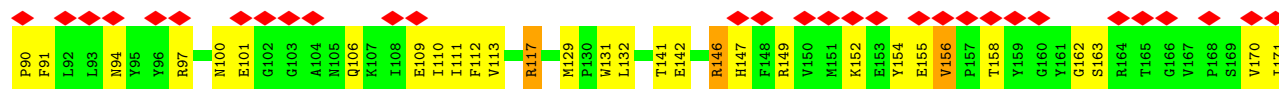
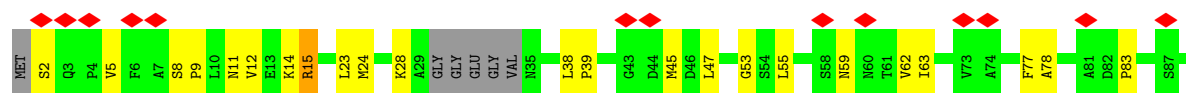


• Molecule 4: PDI family protein

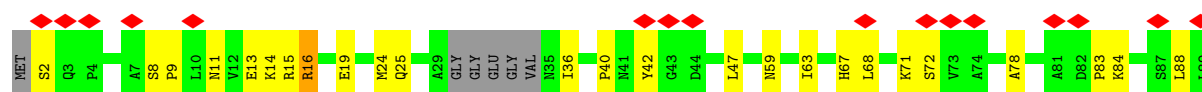




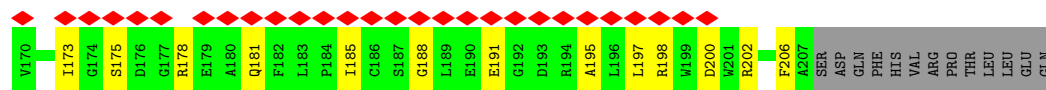
- Molecule 4: PDI family protein



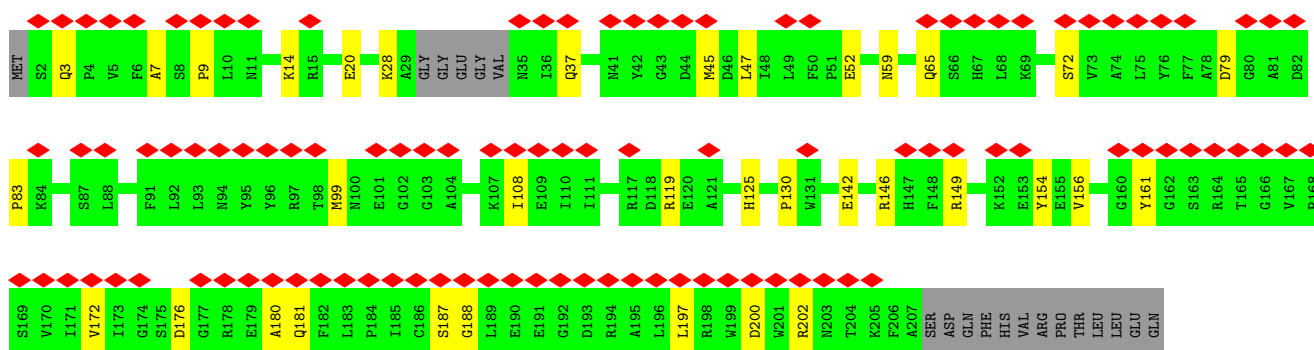
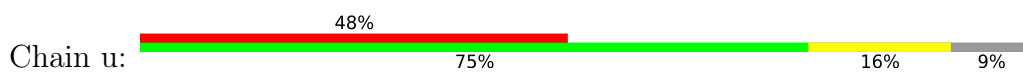
- Molecule 4: PDI family protein



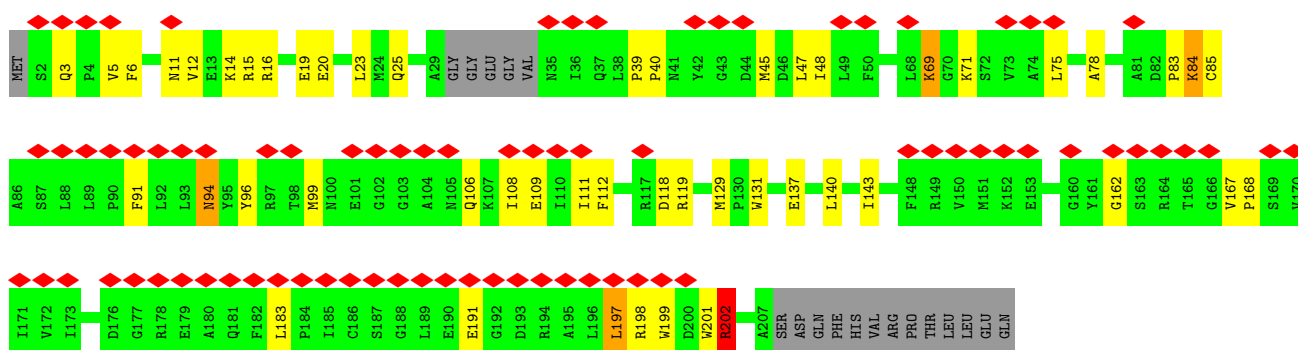
- Molecule 4: PDI family protein



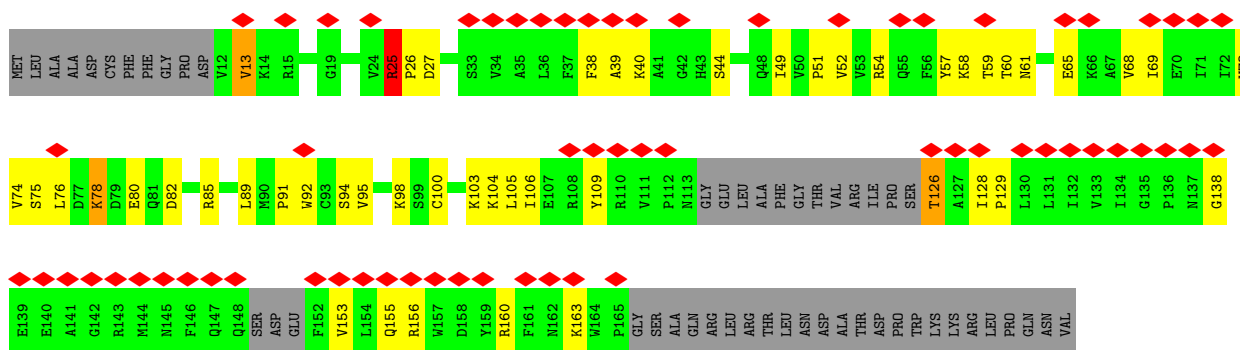
- Molecule 4: PDI family protein



• Molecule 4: PDI family protein

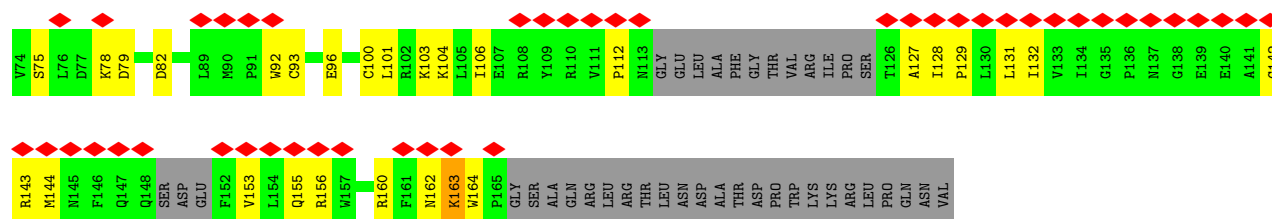


• Molecule 5: PDI family protein

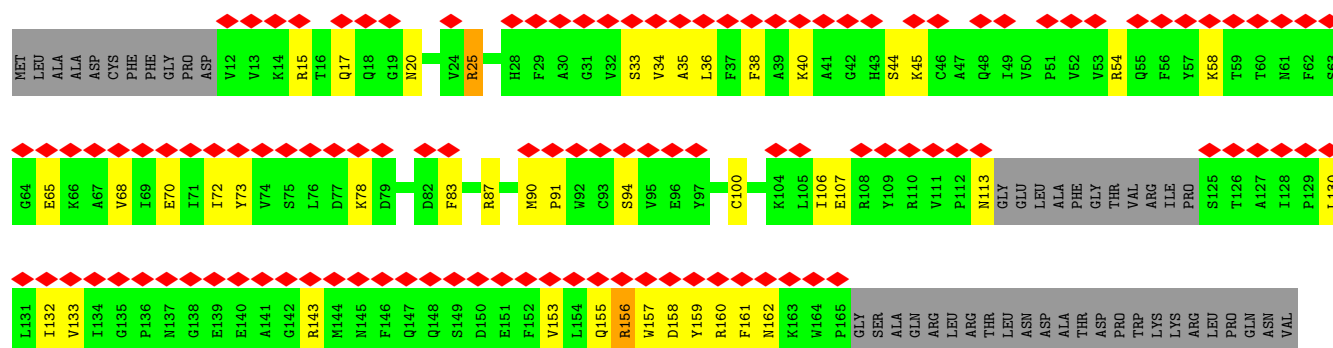


• Molecule 5: PDI family protein

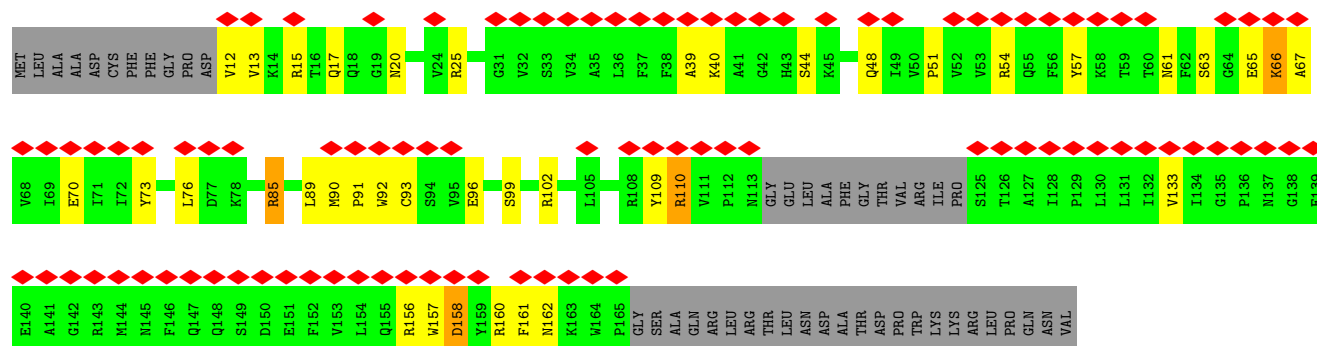




• Molecule 5: PDI family protein



• Molecule 5: PDI family protein



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING     | Depositor |
| Imposed symmetry                     | POINT, C1                 | Depositor |
| Number of subtomograms used          | 39122                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY       | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 132                       | Depositor |
| Minimum defocus (nm)                 | 1000                      | Depositor |
| Maximum defocus (nm)                 | 5000                      | Depositor |
| Magnification                        | 105000                    | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 10.004                    | Depositor |
| Minimum map value                    | -8.373                    | Depositor |
| Average map value                    | 0.015                     | Depositor |
| Map value standard deviation         | 0.892                     | Depositor |
| Recommended contour level            | 2                         | Depositor |
| Map size ( $\text{\AA}$ )            | 447.444, 447.444, 447.444 | wwPDB     |
| Map dimensions                       | 216, 216, 216             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.0715, 2.0715, 2.0715    | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | 0     | 0.72         | 0/181         | 1.40        | 1/248 (0.4%)   |
| 1   | 1     | 0.68         | 0/181         | 1.40        | 2/248 (0.8%)   |
| 1   | 10    | 0.60         | 0/181         | 1.25        | 0/248          |
| 1   | 11    | 0.73         | 0/181         | 1.53        | 2/248 (0.8%)   |
| 1   | 12    | 0.74         | 0/181         | 1.73        | 6/248 (2.4%)   |
| 1   | 13    | 0.74         | 0/181         | 1.43        | 1/248 (0.4%)   |
| 1   | 14    | 0.65         | 0/181         | 1.11        | 1/248 (0.4%)   |
| 1   | 15    | 0.78         | 0/181         | 1.64        | 3/248 (1.2%)   |
| 1   | 16    | 0.62         | 0/181         | 1.25        | 1/248 (0.4%)   |
| 1   | 17    | 0.75         | 0/181         | 1.60        | 3/248 (1.2%)   |
| 1   | 18    | 0.69         | 0/181         | 1.37        | 0/248          |
| 1   | 19    | 1.09         | 2/181 (1.1%)  | 1.42        | 3/248 (1.2%)   |
| 1   | 2     | 0.75         | 0/181         | 1.41        | 0/248          |
| 1   | 20    | 0.59         | 0/181         | 1.05        | 0/248          |
| 1   | 21    | 0.85         | 0/181         | 1.39        | 2/248 (0.8%)   |
| 1   | 22    | 0.81         | 0/166         | 1.61        | 1/227 (0.4%)   |
| 1   | 23    | 0.67         | 0/166         | 1.34        | 0/227          |
| 1   | 3     | 0.65         | 0/181         | 1.20        | 0/248          |
| 1   | 4     | 0.67         | 0/181         | 1.43        | 2/248 (0.8%)   |
| 1   | 5     | 0.63         | 0/181         | 1.44        | 2/248 (0.8%)   |
| 1   | 6     | 0.67         | 0/181         | 1.56        | 4/248 (1.6%)   |
| 1   | 7     | 0.69         | 0/181         | 1.40        | 0/248          |
| 1   | 8     | 0.71         | 0/181         | 1.40        | 1/248 (0.4%)   |
| 1   | 9     | 0.70         | 0/181         | 1.32        | 1/248 (0.4%)   |
| 2   | A0    | 0.71         | 0/3398        | 1.31        | 20/4606 (0.4%) |
| 2   | A2    | 0.66         | 1/3398 (0.0%) | 1.18        | 13/4606 (0.3%) |
| 2   | A4    | 0.85         | 6/3398 (0.2%) | 1.33        | 17/4606 (0.4%) |
| 2   | A6    | 0.67         | 1/3398 (0.0%) | 1.23        | 17/4606 (0.4%) |
| 2   | A8    | 0.83         | 4/3398 (0.1%) | 1.37        | 31/4606 (0.7%) |
| 2   | B0    | 0.67         | 1/3398 (0.0%) | 1.19        | 15/4606 (0.3%) |
| 2   | B2    | 0.74         | 4/3398 (0.1%) | 1.21        | 9/4606 (0.2%)  |
| 2   | B4    | 0.62         | 1/3398 (0.0%) | 1.09        | 6/4606 (0.1%)  |
| 2   | B6    | 0.66         | 3/3398 (0.1%) | 1.09        | 8/4606 (0.2%)  |
| 2   | B8    | 0.60         | 0/3398        | 1.07        | 7/4606 (0.2%)  |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 2   | C0    | 0.62         | 0/3398        | 1.09        | 3/4606 (0.1%)  |
| 2   | C2    | 0.61         | 0/3398        | 1.09        | 3/4606 (0.1%)  |
| 2   | C4    | 0.76         | 6/3398 (0.2%) | 1.14        | 10/4606 (0.2%) |
| 2   | C6    | 0.68         | 0/3398        | 1.20        | 13/4606 (0.3%) |
| 2   | C8    | 0.70         | 1/3398 (0.0%) | 1.18        | 8/4606 (0.2%)  |
| 2   | D0    | 0.72         | 1/3398 (0.0%) | 1.24        | 13/4606 (0.3%) |
| 2   | D2    | 0.64         | 0/3398        | 1.16        | 15/4606 (0.3%) |
| 2   | D4    | 0.79         | 2/3398 (0.1%) | 1.33        | 22/4606 (0.5%) |
| 2   | D6    | 0.66         | 2/3398 (0.1%) | 1.09        | 10/4606 (0.2%) |
| 2   | D8    | 0.70         | 1/3398 (0.0%) | 1.23        | 20/4606 (0.4%) |
| 2   | E0    | 0.53         | 0/3398        | 0.96        | 6/4606 (0.1%)  |
| 2   | E2    | 0.65         | 2/3398 (0.1%) | 1.13        | 12/4606 (0.3%) |
| 2   | E4    | 0.53         | 0/3398        | 0.93        | 4/4606 (0.1%)  |
| 2   | E6    | 0.60         | 0/3398        | 1.06        | 3/4606 (0.1%)  |
| 2   | E8    | 0.50         | 0/3398        | 0.88        | 0/4606         |
| 2   | F0    | 0.65         | 2/3398 (0.1%) | 1.07        | 6/4606 (0.1%)  |
| 3   | A1    | 0.69         | 4/3404 (0.1%) | 1.19        | 12/4606 (0.3%) |
| 3   | A3    | 0.57         | 0/3404        | 1.08        | 7/4606 (0.2%)  |
| 3   | A5    | 0.77         | 4/3404 (0.1%) | 1.32        | 22/4606 (0.5%) |
| 3   | A7    | 0.58         | 0/3404        | 1.07        | 9/4606 (0.2%)  |
| 3   | A9    | 0.72         | 3/3404 (0.1%) | 1.20        | 8/4606 (0.2%)  |
| 3   | B1    | 0.63         | 0/3404        | 1.13        | 7/4606 (0.2%)  |
| 3   | B3    | 0.65         | 0/3404        | 1.21        | 10/4606 (0.2%) |
| 3   | B5    | 0.64         | 1/3404 (0.0%) | 1.16        | 9/4606 (0.2%)  |
| 3   | B7    | 0.60         | 0/3404        | 1.13        | 11/4606 (0.2%) |
| 3   | B9    | 0.58         | 2/3404 (0.1%) | 1.09        | 11/4606 (0.2%) |
| 3   | C1    | 0.61         | 0/3404        | 1.12        | 14/4606 (0.3%) |
| 3   | C3    | 0.62         | 0/3404        | 1.14        | 10/4606 (0.2%) |
| 3   | C5    | 0.64         | 2/3404 (0.1%) | 1.13        | 11/4606 (0.2%) |
| 3   | C7    | 0.68         | 2/3404 (0.1%) | 1.18        | 11/4606 (0.2%) |
| 3   | C9    | 0.67         | 2/3404 (0.1%) | 1.21        | 16/4606 (0.3%) |
| 3   | D1    | 0.83         | 7/3404 (0.2%) | 1.39        | 27/4606 (0.6%) |
| 3   | D3    | 0.73         | 3/3404 (0.1%) | 1.32        | 31/4606 (0.7%) |
| 3   | D5    | 0.81         | 3/3404 (0.1%) | 1.42        | 33/4606 (0.7%) |
| 3   | D7    | 0.68         | 4/3404 (0.1%) | 1.16        | 12/4606 (0.3%) |
| 3   | D9    | 0.72         | 3/3404 (0.1%) | 1.24        | 12/4606 (0.3%) |
| 3   | E1    | 0.57         | 1/3404 (0.0%) | 1.01        | 4/4606 (0.1%)  |
| 3   | E3    | 0.64         | 1/3404 (0.0%) | 1.14        | 16/4606 (0.3%) |
| 3   | E5    | 0.57         | 0/3404        | 1.07        | 9/4606 (0.2%)  |
| 3   | E7    | 0.66         | 1/3404 (0.0%) | 1.16        | 13/4606 (0.3%) |
| 3   | E9    | 0.58         | 0/3404        | 1.06        | 8/4606 (0.2%)  |
| 3   | F1    | 0.68         | 1/3404 (0.0%) | 1.25        | 19/4606 (0.4%) |
| 4   | a     | 0.78         | 3/1225 (0.2%) | 1.28        | 8/1654 (0.5%)  |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 4   | b     | 0.73         | 2/1225 (0.2%)     | 1.18        | 8/1654 (0.5%)     |
| 4   | c     | 1.11         | 3/1645 (0.2%)     | 1.53        | 14/2225 (0.6%)    |
| 4   | d     | 0.81         | 2/1645 (0.1%)     | 1.27        | 9/2225 (0.4%)     |
| 4   | e     | 0.69         | 0/1645            | 1.25        | 9/2225 (0.4%)     |
| 4   | f     | 0.67         | 0/1645            | 1.20        | 5/2225 (0.2%)     |
| 4   | g     | 0.68         | 1/1645 (0.1%)     | 1.24        | 8/2225 (0.4%)     |
| 4   | h     | 0.70         | 3/1645 (0.2%)     | 1.24        | 6/2225 (0.3%)     |
| 4   | i     | 0.79         | 2/1645 (0.1%)     | 1.26        | 14/2225 (0.6%)    |
| 4   | j     | 0.83         | 2/1645 (0.1%)     | 1.19        | 7/2225 (0.3%)     |
| 4   | m     | 0.66         | 0/1645            | 1.19        | 10/2225 (0.4%)    |
| 4   | n     | 0.82         | 3/1645 (0.2%)     | 1.28        | 15/2225 (0.7%)    |
| 4   | o     | 0.66         | 0/1645            | 1.26        | 13/2225 (0.6%)    |
| 4   | p     | 1.01         | 2/1645 (0.1%)     | 1.36        | 14/2225 (0.6%)    |
| 4   | q     | 0.80         | 2/1645 (0.1%)     | 1.24        | 7/2225 (0.3%)     |
| 4   | r     | 0.72         | 1/1645 (0.1%)     | 1.24        | 10/2225 (0.4%)    |
| 4   | s     | 0.63         | 0/1645            | 1.19        | 9/2225 (0.4%)     |
| 4   | t     | 0.83         | 2/1645 (0.1%)     | 1.25        | 6/2225 (0.3%)     |
| 4   | u     | 0.65         | 0/1645            | 1.19        | 5/2225 (0.2%)     |
| 4   | v     | 0.81         | 2/1645 (0.1%)     | 1.32        | 6/2225 (0.3%)     |
| 5   | k     | 0.69         | 0/1168            | 1.31        | 10/1578 (0.6%)    |
| 5   | l     | 0.68         | 1/1168 (0.1%)     | 1.23        | 5/1578 (0.3%)     |
| 5   | w     | 0.63         | 1/1201 (0.1%)     | 1.08        | 1/1623 (0.1%)     |
| 5   | x     | 0.75         | 0/1201            | 1.34        | 9/1623 (0.6%)     |
| All | All   | 0.69         | 116/217964 (0.1%) | 1.19        | 887/295182 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 13    | 0                   | 1                   |
| 1   | 15    | 0                   | 2                   |
| 1   | 18    | 0                   | 1                   |
| 1   | 23    | 0                   | 2                   |
| 1   | 4     | 0                   | 1                   |
| 1   | 7     | 0                   | 1                   |
| 2   | A0    | 0                   | 1                   |
| 2   | A2    | 0                   | 2                   |
| 2   | A4    | 0                   | 2                   |
| 2   | A8    | 0                   | 3                   |
| 2   | B0    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B4    | 0                   | 1                   |
| 2   | B6    | 0                   | 1                   |
| 2   | C4    | 0                   | 1                   |
| 2   | C8    | 0                   | 1                   |
| 2   | D0    | 0                   | 2                   |
| 2   | D2    | 0                   | 1                   |
| 2   | E2    | 0                   | 1                   |
| 3   | B3    | 0                   | 1                   |
| 3   | B9    | 0                   | 1                   |
| 3   | E5    | 0                   | 2                   |
| 4   | c     | 0                   | 1                   |
| 4   | e     | 0                   | 1                   |
| 4   | o     | 0                   | 1                   |
| 4   | t     | 0                   | 1                   |
| 5   | k     | 0                   | 1                   |
| 5   | l     | 0                   | 1                   |
| All | All   | 0                   | 35                  |

All (116) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | c     | 178 | ARG  | NE-CZ   | 28.66 | 1.64        | 1.33     |
| 4   | p     | 97  | ARG  | NE-CZ   | 26.48 | 1.62        | 1.33     |
| 4   | j     | 97  | ARG  | NE-CZ   | 18.65 | 1.53        | 1.33     |
| 4   | t     | 97  | ARG  | NE-CZ   | 17.93 | 1.52        | 1.33     |
| 2   | C4    | 2   | ARG  | CD-NE   | 17.05 | 1.70        | 1.46     |
| 4   | i     | 202 | ARG  | NE-CZ   | 16.62 | 1.51        | 1.33     |
| 4   | q     | 97  | ARG  | NE-CZ   | 16.44 | 1.51        | 1.33     |
| 4   | c     | 178 | ARG  | CZ-NH1  | 16.41 | 1.55        | 1.32     |
| 4   | v     | 202 | ARG  | CD-NE   | 15.32 | 1.67        | 1.46     |
| 4   | d     | 202 | ARG  | NE-CZ   | 14.65 | 1.49        | 1.33     |
| 2   | A8    | 192 | HIS  | CE1-NE2 | 11.46 | 1.44        | 1.32     |
| 2   | C4    | 2   | ARG  | CZ-NH2  | 11.31 | 1.48        | 1.33     |
| 3   | A9    | 252 | LYS  | CG-CD   | 10.56 | 1.84        | 1.52     |
| 2   | B6    | 285 | GLN  | CD-NE2  | 10.47 | 1.55        | 1.33     |
| 3   | D1    | 397 | TRP  | NE1-CE2 | 10.21 | 1.48        | 1.37     |
| 4   | n     | 202 | ARG  | CD-NE   | 10.11 | 1.60        | 1.46     |
| 4   | t     | 97  | ARG  | CD-NE   | 9.91  | 1.60        | 1.46     |
| 2   | A4    | 254 | GLU  | CG-CD   | 9.87  | 1.76        | 1.52     |
| 3   | D5    | 3   | GLU  | CD-OE1  | 9.67  | 1.43        | 1.25     |
| 3   | D3    | 227 | HIS  | CE1-NE2 | 9.27  | 1.41        | 1.32     |
| 4   | n     | 202 | ARG  | CZ-NH2  | 9.02  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | A5    | 252 | LYS  | CD-CE   | 8.60 | 1.78        | 1.52     |
| 2   | A4    | 254 | GLU  | CD-OE2  | 8.49 | 1.41        | 1.25     |
| 4   | c     | 178 | ARG  | CD-NE   | 8.40 | 1.58        | 1.46     |
| 2   | C4    | 2   | ARG  | NE-CZ   | 8.39 | 1.42        | 1.33     |
| 2   | F0    | 284 | GLU  | CD-OE1  | 8.38 | 1.41        | 1.25     |
| 4   | q     | 97  | ARG  | CD-NE   | 8.29 | 1.57        | 1.46     |
| 1   | 19    | 248 | ARG  | CD-NE   | 8.28 | 1.57        | 1.46     |
| 4   | n     | 202 | ARG  | NE-CZ   | 8.20 | 1.42        | 1.33     |
| 4   | p     | 97  | ARG  | CD-NE   | 8.16 | 1.57        | 1.46     |
| 2   | C4    | 2   | ARG  | CG-CD   | 8.01 | 1.76        | 1.52     |
| 3   | F1    | 396 | HIS  | CE1-NE2 | 7.92 | 1.40        | 1.32     |
| 2   | B2    | 192 | HIS  | CE1-NE2 | 7.87 | 1.40        | 1.32     |
| 2   | C4    | 2   | ARG  | CZ-NH1  | 7.72 | 1.43        | 1.32     |
| 5   | w     | 25  | ARG  | NE-CZ   | 7.67 | 1.41        | 1.33     |
| 2   | A8    | 424 | ASP  | CG-OD1  | 7.59 | 1.39        | 1.25     |
| 3   | D9    | 227 | HIS  | CE1-NE2 | 7.56 | 1.40        | 1.32     |
| 4   | r     | 147 | HIS  | CE1-NE2 | 7.52 | 1.40        | 1.32     |
| 2   | D4    | 123 | ARG  | CD-NE   | 7.49 | 1.56        | 1.46     |
| 4   | b     | 178 | ARG  | NE-CZ   | 7.44 | 1.41        | 1.33     |
| 4   | b     | 178 | ARG  | CD-NE   | 7.43 | 1.56        | 1.46     |
| 3   | A5    | 252 | LYS  | CE-NZ   | 7.39 | 1.71        | 1.49     |
| 3   | D1    | 397 | TRP  | CG-CD2  | 7.35 | 1.56        | 1.43     |
| 2   | A8    | 197 | HIS  | CE1-NE2 | 7.25 | 1.39        | 1.32     |
| 2   | D4    | 123 | ARG  | NE-CZ   | 7.21 | 1.41        | 1.33     |
| 2   | A6    | 326 | LYS  | CG-CD   | 7.18 | 1.74        | 1.52     |
| 2   | A4    | 2   | ARG  | NE-CZ   | 7.12 | 1.40        | 1.33     |
| 2   | D8    | 155 | GLU  | CD-OE1  | 7.10 | 1.38        | 1.25     |
| 4   | a     | 164 | ARG  | NE-CZ   | 6.95 | 1.40        | 1.33     |
| 4   | a     | 146 | ARG  | NE-CZ   | 6.94 | 1.40        | 1.33     |
| 2   | A8    | 264 | ARG  | NE-CZ   | 6.92 | 1.40        | 1.33     |
| 3   | D3    | 227 | HIS  | CG-ND1  | 6.89 | 1.45        | 1.38     |
| 4   | a     | 164 | ARG  | CD-NE   | 6.84 | 1.55        | 1.46     |
| 1   | 19    | 248 | ARG  | NE-CZ   | 6.83 | 1.40        | 1.33     |
| 3   | A9    | 227 | HIS  | CE1-NE2 | 6.79 | 1.39        | 1.32     |
| 2   | B2    | 61  | HIS  | CE1-NE2 | 6.74 | 1.39        | 1.32     |
| 3   | C9    | 276 | ARG  | NE-CZ   | 6.71 | 1.40        | 1.33     |
| 2   | F0    | 280 | LYS  | CG-CD   | 6.58 | 1.72        | 1.52     |
| 4   | j     | 97  | ARG  | CD-NE   | 6.58 | 1.55        | 1.46     |
| 4   | v     | 202 | ARG  | NE-CZ   | 6.57 | 1.40        | 1.33     |
| 3   | A1    | 227 | HIS  | CE1-NE2 | 6.51 | 1.39        | 1.32     |
| 2   | A4    | 254 | GLU  | CD-OE1  | 6.50 | 1.37        | 1.25     |
| 3   | C9    | 276 | ARG  | CD-NE   | 6.46 | 1.55        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | i     | 97  | ARG  | NE-CZ   | 6.38  | 1.40        | 1.33     |
| 2   | B6    | 285 | GLN  | CD-OE1  | 6.36  | 1.35        | 1.23     |
| 4   | d     | 202 | ARG  | CD-NE   | 6.34  | 1.55        | 1.46     |
| 3   | D7    | 122 | LYS  | CG-CD   | 6.29  | 1.71        | 1.52     |
| 4   | h     | 202 | ARG  | NE-CZ   | 6.27  | 1.40        | 1.33     |
| 2   | A4    | 28  | HIS  | CE1-NE2 | 6.25  | 1.38        | 1.32     |
| 3   | D7    | 227 | HIS  | CE1-NE2 | 6.22  | 1.38        | 1.32     |
| 2   | B4    | 192 | HIS  | CE1-NE2 | 6.16  | 1.38        | 1.32     |
| 3   | A5    | 379 | LYS  | CG-CD   | 6.16  | 1.71        | 1.52     |
| 3   | A5    | 227 | HIS  | CE1-NE2 | 6.14  | 1.38        | 1.32     |
| 2   | E2    | 221 | ARG  | NE-CZ   | 6.05  | 1.39        | 1.33     |
| 3   | D5    | 343 | GLU  | CD-OE1  | 5.93  | 1.36        | 1.25     |
| 3   | A9    | 208 | TYR  | C-O     | -5.93 | 1.17        | 1.24     |
| 2   | D0    | 221 | ARG  | CZ-NH1  | 5.89  | 1.41        | 1.32     |
| 2   | B2    | 393 | HIS  | CE1-NE2 | 5.79  | 1.38        | 1.32     |
| 4   | h     | 202 | ARG  | CD-NE   | 5.78  | 1.54        | 1.46     |
| 3   | C5    | 227 | HIS  | CE1-NE2 | 5.72  | 1.38        | 1.32     |
| 3   | D1    | 227 | HIS  | CE1-NE2 | 5.72  | 1.38        | 1.32     |
| 3   | E1    | 227 | HIS  | CE1-NE2 | 5.70  | 1.38        | 1.32     |
| 3   | D1    | 343 | GLU  | CG-CD   | 5.69  | 1.66        | 1.52     |
| 5   | l     | 78  | LYS  | CG-CD   | 5.69  | 1.69        | 1.52     |
| 2   | B0    | 214 | ARG  | NE-CZ   | 5.68  | 1.39        | 1.33     |
| 3   | D1    | 397 | TRP  | CD2-CE3 | 5.66  | 1.49        | 1.40     |
| 3   | C5    | 320 | ARG  | CD-NE   | 5.63  | 1.54        | 1.46     |
| 2   | D6    | 221 | ARG  | CD-NE   | 5.62  | 1.54        | 1.46     |
| 3   | E3    | 391 | ARG  | CD-NE   | 5.57  | 1.54        | 1.46     |
| 3   | D7    | 190 | HIS  | CE1-NE2 | 5.57  | 1.38        | 1.32     |
| 3   | D7    | 227 | HIS  | CG-ND1  | 5.55  | 1.44        | 1.38     |
| 3   | A1    | 122 | LYS  | CD-CE   | 5.54  | 1.69        | 1.52     |
| 3   | A1    | 379 | LYS  | CG-CD   | 5.50  | 1.69        | 1.52     |
| 3   | D1    | 3   | GLU  | CD-OE1  | 5.43  | 1.35        | 1.25     |
| 4   | g     | 13  | GLU  | CD-OE2  | -5.37 | 1.15        | 1.25     |
| 3   | D5    | 190 | HIS  | CE1-NE2 | 5.36  | 1.38        | 1.32     |
| 3   | C7    | 396 | HIS  | CE1-NE2 | 5.33  | 1.37        | 1.32     |
| 3   | D9    | 227 | HIS  | CG-ND1  | 5.31  | 1.44        | 1.38     |
| 3   | D3    | 264 | HIS  | CE1-NE2 | 5.31  | 1.37        | 1.32     |
| 3   | A1    | 122 | LYS  | CE-NZ   | 5.30  | 1.65        | 1.49     |
| 3   | C7    | 397 | TRP  | CA-C    | 5.28  | 1.59        | 1.52     |
| 3   | B9    | 227 | HIS  | CE1-NE2 | 5.25  | 1.37        | 1.32     |
| 2   | B2    | 372 | MET  | CG-SD   | 5.24  | 1.93        | 1.80     |
| 3   | D9    | 129 | CYS  | C-O     | 5.20  | 1.30        | 1.23     |
| 3   | B9    | 122 | LYS  | CG-CD   | 5.20  | 1.68        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | E7    | 105 | HIS  | CE1-NE2 | 5.19 | 1.37        | 1.32     |
| 3   | B5    | 336 | LYS  | CE-NZ   | 5.17 | 1.64        | 1.49     |
| 2   | A4    | 107 | HIS  | CE1-NE2 | 5.14 | 1.37        | 1.32     |
| 2   | E2    | 116 | ASP  | CG-OD2  | 5.12 | 1.35        | 1.25     |
| 4   | h     | 147 | HIS  | CE1-NE2 | 5.11 | 1.37        | 1.32     |
| 2   | C4    | 326 | LYS  | CG-CD   | 5.10 | 1.67        | 1.52     |
| 2   | D6    | 221 | ARG  | NE-CZ   | 5.10 | 1.38        | 1.33     |
| 2   | B6    | 8   | HIS  | CE1-NE2 | 5.09 | 1.37        | 1.32     |
| 3   | D1    | 363 | MET  | CG-SD   | 5.07 | 1.93        | 1.80     |
| 2   | C8    | 393 | HIS  | CE1-NE2 | 5.03 | 1.37        | 1.32     |
| 2   | A2    | 372 | MET  | CG-SD   | 5.02 | 1.93        | 1.80     |

All (887) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 4   | c     | 178 | ARG  | NE-CZ-NH1 | 20.78  | 142.28      | 121.50   |
| 2   | C4    | 2   | ARG  | CG-CD-NE  | 17.47  | 150.43      | 112.00   |
| 3   | D1    | 213 | ARG  | CG-CD-NE  | -15.03 | 78.93       | 112.00   |
| 4   | t     | 97  | ARG  | CD-NE-CZ  | 14.87  | 145.22      | 124.40   |
| 3   | C9    | 291 | GLN  | CB-CG-CD  | 14.39  | 137.06      | 112.60   |
| 4   | o     | 202 | ARG  | CB-CG-CD  | 14.25  | 144.08      | 111.30   |
| 4   | c     | 178 | ARG  | CD-NE-CZ  | 14.07  | 144.10      | 124.40   |
| 4   | c     | 178 | ARG  | NE-CZ-NH2 | -14.02 | 106.59      | 119.20   |
| 3   | D3    | 424 | GLN  | CB-CG-CD  | 13.39  | 135.36      | 112.60   |
| 3   | D5    | 343 | GLU  | N-CA-CB   | 13.27  | 130.58      | 110.80   |
| 2   | D4    | 123 | ARG  | CD-NE-CZ  | 12.85  | 142.39      | 124.40   |
| 3   | F1    | 177 | ASP  | CA-CB-CG  | 12.70  | 125.30      | 112.60   |
| 3   | A5    | 125 | GLU  | CB-CG-CD  | 12.53  | 133.91      | 112.60   |
| 4   | v     | 202 | ARG  | CG-CD-NE  | 12.50  | 139.51      | 112.00   |
| 4   | h     | 155 | GLU  | CB-CG-CD  | 12.31  | 133.53      | 112.60   |
| 3   | D5    | 391 | ARG  | CB-CG-CD  | 12.09  | 139.10      | 111.30   |
| 3   | E7    | 394 | PHE  | CA-CB-CG  | -11.89 | 101.91      | 113.80   |
| 2   | C8    | 420 | GLU  | CB-CG-CD  | 11.88  | 132.80      | 112.60   |
| 4   | h     | 198 | ARG  | CG-CD-NE  | 11.80  | 137.95      | 112.00   |
| 3   | A3    | 391 | ARG  | CB-CG-CD  | 11.78  | 138.39      | 111.30   |
| 2   | E2    | 156 | ARG  | CB-CG-CD  | 11.70  | 138.21      | 111.30   |
| 3   | C1    | 174 | LYS  | CB-CG-CD  | 11.64  | 138.07      | 111.30   |
| 3   | D1    | 121 | ARG  | CG-CD-NE  | 11.61  | 137.53      | 112.00   |
| 2   | B8    | 113 | GLU  | CB-CG-CD  | 11.45  | 132.07      | 112.60   |
| 2   | A6    | 279 | GLU  | CB-CG-CD  | 11.36  | 131.91      | 112.60   |
| 3   | B9    | 11  | GLN  | CB-CG-CD  | 11.10  | 131.47      | 112.60   |
| 3   | D7    | 391 | ARG  | CB-CG-CD  | 11.07  | 136.75      | 111.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3   | B3    | 280 | GLN  | CB-CG-CD  | 10.75  | 130.87      | 112.60   |
| 2   | A6    | 326 | LYS  | CG-CD-CE  | 10.47  | 135.39      | 111.30   |
| 4   | n     | 202 | ARG  | CB-CG-CD  | 10.42  | 135.27      | 111.30   |
| 3   | C1    | 204 | ASN  | CA-CB-CG  | 10.25  | 122.85      | 112.60   |
| 4   | n     | 91  | PHE  | CA-CB-CG  | -10.19 | 103.61      | 113.80   |
| 4   | d     | 117 | ARG  | CB-CG-CD  | 10.04  | 134.39      | 111.30   |
| 3   | D1    | 291 | GLN  | CB-CG-CD  | 10.03  | 129.64      | 112.60   |
| 3   | A1    | 122 | LYS  | CB-CG-CD  | 10.02  | 134.34      | 111.30   |
| 2   | D6    | 297 | GLU  | CB-CG-CD  | 9.99   | 129.58      | 112.60   |
| 3   | A5    | 227 | HIS  | CA-CB-CG  | 9.88   | 123.67      | 113.80   |
| 3   | D7    | 121 | ARG  | CG-CD-NE  | 9.82   | 133.61      | 112.00   |
| 3   | E5    | 320 | ARG  | CB-CG-CD  | 9.73   | 133.69      | 111.30   |
| 3   | D3    | 391 | ARG  | CB-CG-CD  | 9.64   | 133.47      | 111.30   |
| 4   | c     | 69  | LYS  | CG-CD-CE  | 9.63   | 133.45      | 111.30   |
| 3   | A3    | 177 | ASP  | CA-CB-CG  | 9.62   | 122.22      | 112.60   |
| 2   | A6    | 214 | ARG  | CB-CG-CD  | -9.58  | 89.27       | 111.30   |
| 1   | 12    | 242 | ASN  | CA-CB-CG  | 9.55   | 122.15      | 112.60   |
| 3   | D9    | 405 | GLU  | CB-CG-CD  | 9.50   | 128.75      | 112.60   |
| 2   | A0    | 254 | GLU  | CB-CG-CD  | 9.49   | 128.73      | 112.60   |
| 3   | D5    | 128 | ASP  | O-C-N     | 9.49   | 131.84      | 122.07   |
| 2   | A6    | 214 | ARG  | CG-CD-NE  | 9.42   | 132.73      | 112.00   |
| 3   | B1    | 280 | GLN  | CB-CG-CD  | 9.41   | 128.59      | 112.60   |
| 2   | B0    | 285 | GLN  | CB-CG-CD  | 9.39   | 128.56      | 112.60   |
| 4   | n     | 202 | ARG  | NE-CZ-NH2 | 9.35   | 127.61      | 119.20   |
| 3   | F1    | 332 | ASN  | CA-CB-CG  | 9.33   | 121.93      | 112.60   |
| 3   | C3    | 391 | ARG  | CB-CG-CD  | -9.30  | 89.90       | 111.30   |
| 2   | D2    | 339 | ARG  | N-CA-CB   | 9.30   | 124.66      | 110.61   |
| 2   | E0    | 156 | ARG  | CB-CG-CD  | 9.26   | 132.59      | 111.30   |
| 2   | D8    | 401 | LYS  | CG-CD-CE  | 9.25   | 132.57      | 111.30   |
| 2   | A8    | 85  | HIS  | CA-CB-CG  | 9.19   | 122.99      | 113.80   |
| 4   | h     | 202 | ARG  | NE-CZ-NH2 | 9.18   | 127.46      | 119.20   |
| 3   | B7    | 11  | GLN  | CB-CG-CD  | 9.10   | 128.06      | 112.60   |
| 4   | i     | 202 | ARG  | CG-CD-NE  | 9.03   | 131.87      | 112.00   |
| 3   | D5    | 121 | ARG  | NE-CZ-NH2 | 9.03   | 127.33      | 119.20   |
| 3   | E7    | 77  | ARG  | NE-CZ-NH1 | -9.02  | 112.48      | 121.50   |
| 3   | E1    | 390 | ARG  | CB-CG-CD  | 8.95   | 131.87      | 111.30   |
| 3   | B3    | 391 | ARG  | CG-CD-NE  | -8.93  | 92.35       | 112.00   |
| 2   | B0    | 401 | LYS  | N-CA-CB   | 8.91   | 129.63      | 111.36   |
| 4   | c     | 123 | GLU  | CB-CG-CD  | 8.85   | 127.64      | 112.60   |
| 3   | D1    | 194 | GLU  | CB-CG-CD  | 8.75   | 127.47      | 112.60   |
| 3   | F1    | 336 | LYS  | CA-CB-CG  | 8.74   | 131.59      | 114.10   |
| 2   | D2    | 297 | GLU  | CB-CG-CD  | 8.71   | 127.40      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | 12    | 248 | ARG  | CB-CA-C   | -8.68 | 94.00       | 110.67   |
| 3   | B3    | 213 | ARG  | CG-CD-NE  | 8.68  | 131.09      | 112.00   |
| 3   | B9    | 177 | ASP  | CA-CB-CG  | 8.67  | 121.27      | 112.60   |
| 1   | 15    | 248 | ARG  | CG-CD-NE  | 8.65  | 131.04      | 112.00   |
| 3   | D3    | 46  | ARG  | CB-CG-CD  | 8.65  | 131.20      | 111.30   |
| 3   | D1    | 392 | LYS  | CG-CD-CE  | 8.64  | 131.17      | 111.30   |
| 3   | E7    | 394 | PHE  | CB-CA-C   | 8.63  | 127.37      | 111.06   |
| 3   | E3    | 391 | ARG  | CG-CD-NE  | 8.63  | 130.98      | 112.00   |
| 3   | C9    | 390 | ARG  | CG-CD-NE  | 8.63  | 130.98      | 112.00   |
| 2   | D4    | 163 | LYS  | CG-CD-CE  | 8.62  | 131.13      | 111.30   |
| 2   | A8    | 262 | TYR  | O-C-N     | 8.62  | 127.23      | 121.71   |
| 2   | A8    | 285 | GLN  | N-CA-CB   | 8.58  | 124.39      | 110.41   |
| 3   | F1    | 118 | ASP  | CA-CB-CG  | 8.57  | 121.17      | 112.60   |
| 3   | C5    | 11  | GLN  | N-CA-CB   | -8.57 | 97.58       | 110.01   |
| 2   | C8    | 423 | GLU  | CB-CG-CD  | -8.55 | 98.06       | 112.60   |
| 2   | D4    | 162 | GLY  | CA-C-O    | -8.55 | 111.59      | 120.66   |
| 2   | D4    | 123 | ARG  | CG-CD-NE  | -8.54 | 93.21       | 112.00   |
| 3   | D5    | 410 | GLU  | CB-CG-CD  | 8.51  | 127.06      | 112.60   |
| 5   | k     | 26  | PRO  | CB-CA-C   | -8.47 | 99.82       | 111.85   |
| 4   | e     | 120 | GLU  | CB-CG-CD  | 8.47  | 126.99      | 112.60   |
| 3   | D5    | 121 | ARG  | NE-CZ-NH1 | -8.46 | 113.04      | 121.50   |
| 2   | B2    | 156 | ARG  | CB-CG-CD  | 8.45  | 130.74      | 111.30   |
| 4   | v     | 202 | ARG  | NE-CZ-NH1 | -8.45 | 113.05      | 121.50   |
| 2   | A0    | 2   | ARG  | CG-CD-NE  | 8.41  | 130.51      | 112.00   |
| 3   | D3    | 220 | PRO  | CB-CA-C   | -8.41 | 102.39      | 111.56   |
| 2   | F0    | 336 | LYS  | CB-CG-CD  | 8.38  | 130.58      | 111.30   |
| 3   | C9    | 391 | ARG  | CG-CD-NE  | -8.38 | 93.57       | 112.00   |
| 3   | E3    | 125 | GLU  | CA-C-N    | 8.37  | 129.40      | 120.03   |
| 3   | E3    | 125 | GLU  | C-N-CA    | 8.37  | 129.40      | 120.03   |
| 3   | D5    | 394 | PHE  | CA-CB-CG  | -8.36 | 105.44      | 113.80   |
| 1   | 22    | 248 | ARG  | CB-CG-CD  | 8.32  | 130.44      | 111.30   |
| 5   | x     | 54  | ARG  | CG-CD-NE  | 8.30  | 130.27      | 112.00   |
| 3   | C3    | 46  | ARG  | CB-CG-CD  | 8.28  | 130.34      | 111.30   |
| 3   | D1    | 355 | ASP  | CA-CB-CG  | 8.27  | 120.87      | 112.60   |
| 3   | D1    | 213 | ARG  | NE-CZ-NH2 | 8.27  | 126.64      | 119.20   |
| 3   | A1    | 379 | LYS  | CB-CG-CD  | -8.25 | 92.33       | 111.30   |
| 3   | E3    | 128 | ASP  | CB-CA-C   | 8.25  | 124.03      | 110.92   |
| 2   | D2    | 123 | ARG  | CB-CG-CD  | -8.24 | 92.36       | 111.30   |
| 2   | D8    | 264 | ARG  | CB-CG-CD  | 8.21  | 130.19      | 111.30   |
| 4   | t     | 178 | ARG  | CG-CD-NE  | 8.20  | 130.05      | 112.00   |
| 3   | D1    | 391 | ARG  | CG-CD-NE  | -8.20 | 93.96       | 112.00   |
| 3   | D5    | 46  | ARG  | CG-CD-NE  | 8.20  | 130.04      | 112.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | E7    | 391 | ARG  | CG-CD-NE   | -8.19 | 93.98       | 112.00   |
| 3   | D5    | 212 | PHE  | CA-CB-CG   | 8.18  | 121.97      | 113.80   |
| 2   | B6    | 339 | ARG  | CG-CD-NE   | 8.17  | 129.98      | 112.00   |
| 2   | F0    | 215 | ARG  | CG-CD-NE   | 8.16  | 129.96      | 112.00   |
| 2   | A2    | 221 | ARG  | CG-CD-NE   | 8.16  | 129.94      | 112.00   |
| 3   | C7    | 291 | GLN  | OE1-CD-NE2 | 8.13  | 130.73      | 122.60   |
| 4   | m     | 27  | GLN  | CB-CG-CD   | 8.11  | 126.39      | 112.60   |
| 4   | b     | 146 | ARG  | CG-CD-NE   | 8.09  | 129.79      | 112.00   |
| 2   | A6    | 345 | ASP  | CA-CB-CG   | 8.08  | 120.68      | 112.60   |
| 2   | D0    | 279 | GLU  | CB-CG-CD   | -8.03 | 98.95       | 112.60   |
| 4   | o     | 155 | GLU  | CB-CG-CD   | 8.03  | 126.24      | 112.60   |
| 3   | A5    | 320 | ARG  | CB-CG-CD   | 8.02  | 129.75      | 111.30   |
| 3   | E5    | 320 | ARG  | CG-CD-NE   | -8.02 | 94.35       | 112.00   |
| 4   | d     | 194 | ARG  | CG-CD-NE   | 8.01  | 129.62      | 112.00   |
| 4   | c     | 202 | ARG  | CG-CD-NE   | 7.98  | 129.56      | 112.00   |
| 2   | A8    | 214 | ARG  | CG-CD-NE   | 7.98  | 129.56      | 112.00   |
| 3   | C5    | 174 | LYS  | CB-CG-CD   | 7.95  | 129.57      | 111.30   |
| 3   | D1    | 391 | ARG  | CB-CG-CD   | 7.94  | 129.55      | 111.30   |
| 4   | b     | 194 | ARG  | CG-CD-NE   | 7.93  | 129.44      | 112.00   |
| 2   | C4    | 401 | LYS  | CB-CA-C    | 7.89  | 127.67      | 111.97   |
| 3   | E9    | 11  | GLN  | CB-CG-CD   | -7.89 | 99.19       | 112.60   |
| 3   | D1    | 343 | GLU  | N-CA-CB    | 7.88  | 122.54      | 110.80   |
| 4   | h     | 146 | ARG  | CG-CD-NE   | 7.87  | 129.31      | 112.00   |
| 2   | C4    | 326 | LYS  | CG-CD-CE   | 7.82  | 129.30      | 111.30   |
| 4   | r     | 155 | GLU  | N-CA-C     | -7.82 | 105.70      | 114.62   |
| 4   | q     | 117 | ARG  | CG-CD-NE   | 7.82  | 129.21      | 112.00   |
| 3   | D5    | 268 | ILE  | CA-C-N     | 7.81  | 127.62      | 121.61   |
| 3   | D5    | 268 | ILE  | C-N-CA     | 7.81  | 127.62      | 121.61   |
| 4   | d     | 155 | GLU  | CB-CG-CD   | 7.79  | 125.84      | 112.60   |
| 4   | d     | 202 | ARG  | CD-NE-CZ   | 7.76  | 135.26      | 124.40   |
| 3   | B7    | 426 | GLN  | CB-CA-C    | 7.71  | 124.76      | 110.10   |
| 2   | A6    | 60  | LYS  | CG-CD-CE   | 7.70  | 129.00      | 111.30   |
| 3   | B1    | 129 | CYS  | CB-CA-C    | 7.68  | 121.84      | 110.62   |
| 2   | A0    | 217 | LEU  | CA-C-N     | 7.68  | 133.29      | 122.46   |
| 2   | A0    | 217 | LEU  | C-N-CA     | 7.68  | 133.29      | 122.46   |
| 4   | s     | 16  | ARG  | CB-CG-CD   | 7.68  | 128.95      | 111.30   |
| 2   | D4    | 401 | LYS  | CB-CA-C    | 7.67  | 124.64      | 111.45   |
| 4   | i     | 202 | ARG  | CB-CG-CD   | -7.67 | 93.67       | 111.30   |
| 3   | E3    | 276 | ARG  | CB-CG-CD   | 7.66  | 128.92      | 111.30   |
| 2   | D8    | 214 | ARG  | CD-NE-CZ   | 7.64  | 135.10      | 124.40   |
| 4   | p     | 97  | ARG  | CD-NE-CZ   | 7.63  | 135.09      | 124.40   |
| 2   | D8    | 214 | ARG  | CB-CG-CD   | -7.61 | 93.80       | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | D3    | 46  | ARG  | CG-CD-NE   | -7.60 | 95.28       | 112.00   |
| 4   | s     | 97  | ARG  | CG-CD-NE   | -7.59 | 95.29       | 112.00   |
| 2   | A8    | 285 | GLN  | OE1-CD-NE2 | -7.59 | 115.01      | 122.60   |
| 2   | A2    | 214 | ARG  | CG-CD-NE   | -7.58 | 95.33       | 112.00   |
| 3   | C9    | 343 | GLU  | N-CA-CB    | 7.56  | 120.64      | 110.59   |
| 4   | t     | 97  | ARG  | NE-CZ-NH1  | 7.54  | 129.04      | 121.50   |
| 2   | E2    | 220 | GLU  | CB-CG-CD   | 7.53  | 125.40      | 112.60   |
| 3   | A9    | 252 | LYS  | CG-CD-CE   | 7.53  | 128.62      | 111.30   |
| 3   | B1    | 227 | HIS  | CA-CB-CG   | 7.52  | 121.32      | 113.80   |
| 4   | q     | 123 | GLU  | CB-CG-CD   | 7.51  | 125.38      | 112.60   |
| 3   | A1    | 383 | ASP  | CA-CB-CG   | 7.50  | 120.11      | 112.60   |
| 3   | D3    | 45  | GLU  | CB-CG-CD   | 7.50  | 125.36      | 112.60   |
| 3   | F1    | 123 | GLU  | CB-CG-CD   | 7.49  | 125.33      | 112.60   |
| 4   | m     | 19  | GLU  | CB-CG-CD   | 7.49  | 125.33      | 112.60   |
| 2   | D4    | 423 | GLU  | CB-CG-CD   | -7.48 | 99.89       | 112.60   |
| 2   | E2    | 156 | ARG  | CG-CD-NE   | -7.47 | 95.57       | 112.00   |
| 2   | D4    | 163 | LYS  | CB-CG-CD   | 7.46  | 128.46      | 111.30   |
| 3   | B7    | 320 | ARG  | CG-CD-NE   | -7.45 | 95.61       | 112.00   |
| 1   | 4     | 240 | PRO  | CB-CA-C    | 7.44  | 120.87      | 110.60   |
| 4   | c     | 52  | GLU  | CB-CG-CD   | 7.43  | 125.23      | 112.60   |
| 1   | 16    | 248 | ARG  | CG-CD-NE   | -7.41 | 95.70       | 112.00   |
| 4   | g     | 13  | GLU  | CB-CG-CD   | 7.40  | 125.19      | 112.60   |
| 3   | A3    | 125 | GLU  | CB-CG-CD   | 7.38  | 125.15      | 112.60   |
| 3   | D3    | 424 | GLN  | CG-CD-NE2  | -7.38 | 105.32      | 116.40   |
| 3   | E3    | 320 | ARG  | CB-CA-C    | 7.38  | 121.89      | 110.67   |
| 4   | u     | 65  | GLN  | CB-CG-CD   | 7.38  | 125.14      | 112.60   |
| 3   | A3    | 128 | ASP  | CB-CA-C    | 7.38  | 122.38      | 110.95   |
| 2   | A0    | 124 | LYS  | CB-CG-CD   | 7.37  | 128.24      | 111.30   |
| 2   | D2    | 85  | HIS  | CA-CB-CG   | 7.32  | 121.12      | 113.80   |
| 3   | D7    | 122 | LYS  | CG-CD-CE   | 7.28  | 128.05      | 111.30   |
| 4   | e     | 41  | ASN  | CA-CB-CG   | 7.28  | 119.88      | 112.60   |
| 3   | A5    | 122 | LYS  | CG-CD-CE   | 7.27  | 128.03      | 111.30   |
| 3   | D3    | 48  | ASN  | CA-CB-CG   | 7.25  | 119.84      | 112.60   |
| 2   | D0    | 156 | ARG  | NE-CZ-NH2  | 7.22  | 125.70      | 119.20   |
| 5   | x     | 66  | LYS  | CA-C-N     | 7.22  | 131.08      | 120.90   |
| 5   | x     | 66  | LYS  | C-N-CA     | 7.22  | 131.08      | 120.90   |
| 3   | B9    | 15  | GLN  | CB-CG-CD   | 7.22  | 124.87      | 112.60   |
| 2   | D4    | 290 | GLU  | CB-CG-CD   | 7.22  | 124.87      | 112.60   |
| 2   | C8    | 358 | GLN  | CB-CA-C    | 7.20  | 119.03      | 108.87   |
| 3   | F1    | 125 | GLU  | CB-CG-CD   | 7.19  | 124.83      | 112.60   |
| 4   | v     | 109 | GLU  | CB-CG-CD   | 7.14  | 124.73      | 112.60   |
| 3   | C5    | 15  | GLN  | CB-CG-CD   | 7.13  | 124.73      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | a     | 198 | ARG  | CB-CG-CD  | 7.13  | 127.70      | 111.30   |
| 3   | C7    | 216 | LYS  | CG-CD-CE  | 7.12  | 127.68      | 111.30   |
| 4   | g     | 16  | ARG  | CB-CG-CD  | 7.11  | 127.65      | 111.30   |
| 4   | g     | 15  | ARG  | NE-CZ-NH2 | 7.10  | 125.59      | 119.20   |
| 5   | k     | 25  | ARG  | CB-CG-CD  | 7.08  | 127.59      | 111.30   |
| 4   | o     | 91  | PHE  | CA-CB-CG  | -7.08 | 106.72      | 113.80   |
| 2   | A8    | 285 | GLN  | CB-CG-CD  | 7.06  | 124.61      | 112.60   |
| 3   | D5    | 342 | VAL  | CA-C-N    | -7.06 | 111.28      | 122.29   |
| 3   | D5    | 342 | VAL  | C-N-CA    | -7.06 | 111.28      | 122.29   |
| 3   | B9    | 337 | ASN  | N-CA-CB   | 7.05  | 118.25      | 110.35   |
| 2   | A0    | 326 | LYS  | CA-CB-CG  | 7.05  | 128.20      | 114.10   |
| 4   | p     | 95  | TYR  | CB-CA-C   | 7.05  | 122.83      | 110.85   |
| 3   | C1    | 320 | ARG  | CG-CD-NE  | 7.03  | 127.47      | 112.00   |
| 2   | D0    | 298 | PRO  | CB-CA-C   | -7.02 | 101.43      | 111.68   |
| 2   | E2    | 162 | GLY  | CA-C-O    | -7.00 | 113.06      | 120.90   |
| 2   | D6    | 393 | HIS  | CA-CB-CG  | -6.99 | 106.81      | 113.80   |
| 2   | A2    | 430 | LYS  | CB-CG-CD  | 6.99  | 127.36      | 111.30   |
| 2   | C2    | 33  | ASP  | CA-CB-CG  | -6.98 | 105.62      | 112.60   |
| 1   | 12    | 247 | TYR  | CB-CA-C   | 6.97  | 121.92      | 110.90   |
| 2   | C6    | 123 | ARG  | CG-CD-NE  | -6.97 | 96.66       | 112.00   |
| 2   | B2    | 297 | GLU  | CB-CG-CD  | 6.96  | 124.44      | 112.60   |
| 2   | E6    | 97  | GLU  | CB-CG-CD  | 6.95  | 124.42      | 112.60   |
| 4   | p     | 94  | ASN  | CA-CB-CG  | 6.95  | 119.55      | 112.60   |
| 4   | v     | 25  | GLN  | CB-CG-CD  | 6.94  | 124.40      | 112.60   |
| 2   | C4    | 220 | GLU  | CB-CG-CD  | 6.93  | 124.39      | 112.60   |
| 3   | B3    | 391 | ARG  | CB-CG-CD  | 6.92  | 127.22      | 111.30   |
| 2   | E2    | 221 | ARG  | CG-CD-NE  | -6.91 | 96.81       | 112.00   |
| 4   | j     | 97  | ARG  | CD-NE-CZ  | 6.90  | 134.06      | 124.40   |
| 1   | 17    | 248 | ARG  | CG-CD-NE  | 6.90  | 127.17      | 112.00   |
| 4   | p     | 194 | ARG  | CD-NE-CZ  | 6.89  | 134.05      | 124.40   |
| 3   | E9    | 177 | ASP  | CA-CB-CG  | 6.88  | 119.48      | 112.60   |
| 4   | r     | 117 | ARG  | CG-CD-NE  | 6.86  | 127.09      | 112.00   |
| 4   | f     | 84  | LYS  | CB-CG-CD  | 6.86  | 127.07      | 111.30   |
| 3   | A5    | 383 | ASP  | CA-CB-CG  | 6.84  | 119.44      | 112.60   |
| 2   | F0    | 280 | LYS  | CG-CD-CE  | 6.84  | 127.03      | 111.30   |
| 3   | C7    | 276 | ARG  | CB-CG-CD  | 6.83  | 127.01      | 111.30   |
| 2   | A4    | 214 | ARG  | NE-CZ-NH1 | -6.83 | 114.67      | 121.50   |
| 2   | C0    | 254 | GLU  | CB-CG-CD  | 6.83  | 124.20      | 112.60   |
| 4   | q     | 202 | ARG  | CB-CG-CD  | 6.83  | 127.00      | 111.30   |
| 3   | C3    | 388 | MET  | CB-CG-SD  | 6.82  | 133.17      | 112.70   |
| 2   | A2    | 357 | TYR  | N-CA-CB   | 6.79  | 120.91      | 110.80   |
| 3   | C1    | 174 | LYS  | CG-CD-CE  | 6.77  | 126.87      | 111.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | D7    | 162 | ARG  | CG-CD-NE  | 6.77  | 126.89      | 112.00   |
| 2   | E0    | 162 | GLY  | CA-C-N    | 6.77  | 129.35      | 120.28   |
| 2   | E0    | 162 | GLY  | C-N-CA    | 6.77  | 129.35      | 120.28   |
| 3   | C3    | 118 | ASP  | CA-CB-CG  | 6.75  | 119.35      | 112.60   |
| 2   | A8    | 284 | GLU  | CB-CG-CD  | 6.75  | 124.07      | 112.60   |
| 4   | j     | 130 | PRO  | N-CA-C    | 6.75  | 122.33      | 114.03   |
| 3   | B7    | 46  | ARG  | CG-CD-NE  | 6.74  | 126.83      | 112.00   |
| 3   | C5    | 77  | ARG  | CG-CD-NE  | 6.73  | 126.80      | 112.00   |
| 4   | h     | 178 | ARG  | CG-CD-NE  | 6.73  | 126.80      | 112.00   |
| 3   | D1    | 406 | MET  | CB-CG-SD  | 6.72  | 132.85      | 112.70   |
| 2   | B2    | 262 | TYR  | O-C-N     | 6.71  | 126.01      | 121.71   |
| 3   | B5    | 320 | ARG  | CG-CD-NE  | 6.70  | 126.75      | 112.00   |
| 2   | B2    | 85  | HIS  | CA-CB-CG  | -6.70 | 107.10      | 113.80   |
| 3   | F1    | 362 | LYS  | N-CA-CB   | 6.70  | 120.72      | 110.81   |
| 4   | r     | 59  | ASN  | N-CA-CB   | 6.69  | 120.17      | 110.47   |
| 2   | E2    | 416 | GLY  | N-CA-C    | -6.69 | 106.42      | 113.58   |
| 1   | 21    | 237 | PRO  | N-CD-CG   | 6.68  | 113.22      | 103.20   |
| 2   | A8    | 96  | LYS  | CG-CD-CE  | 6.68  | 126.66      | 111.30   |
| 3   | D1    | 421 | GLU  | CB-CG-CD  | 6.67  | 123.94      | 112.60   |
| 4   | o     | 202 | ARG  | CB-CA-C   | -6.67 | 100.61      | 110.95   |
| 3   | A7    | 227 | HIS  | CA-CB-CG  | 6.66  | 120.46      | 113.80   |
| 3   | D9    | 399 | THR  | CA-CB-OG1 | -6.66 | 99.61       | 109.60   |
| 3   | C9    | 213 | ARG  | CG-CD-NE  | 6.65  | 126.64      | 112.00   |
| 3   | C3    | 295 | ASP  | CA-CB-CG  | 6.64  | 119.25      | 112.60   |
| 2   | A6    | 326 | LYS  | CB-CA-C   | 6.64  | 123.86      | 109.99   |
| 3   | D5    | 48  | ASN  | CA-CB-CG  | 6.64  | 119.24      | 112.60   |
| 4   | i     | 64  | PRO  | CA-C-N    | 6.64  | 129.50      | 120.54   |
| 4   | i     | 64  | PRO  | C-N-CA    | 6.64  | 129.50      | 120.54   |
| 2   | D0    | 339 | ARG  | CB-CA-C   | -6.63 | 99.35       | 110.56   |
| 4   | p     | 95  | TYR  | N-CA-CB   | -6.63 | 100.35      | 110.16   |
| 4   | j     | 117 | ARG  | CG-CD-NE  | 6.63  | 126.58      | 112.00   |
| 2   | B0    | 156 | ARG  | CG-CD-NE  | 6.62  | 126.58      | 112.00   |
| 3   | E7    | 291 | GLN  | CB-CG-CD  | 6.62  | 123.86      | 112.60   |
| 2   | A4    | 64  | ARG  | NE-CZ-NH2 | 6.62  | 125.16      | 119.20   |
| 1   | 9     | 257 | PRO  | O-C-N     | 6.60  | 124.25      | 121.15   |
| 2   | D0    | 35  | GLN  | CB-CG-CD  | 6.60  | 123.83      | 112.60   |
| 3   | D1    | 291 | GLN  | CB-CA-C   | 6.60  | 121.25      | 110.88   |
| 3   | A5    | 212 | PHE  | CA-CB-CG  | -6.60 | 107.20      | 113.80   |
| 3   | B3    | 122 | LYS  | CG-CD-CE  | 6.60  | 126.47      | 111.30   |
| 2   | A4    | 162 | GLY  | CA-C-N    | 6.59  | 131.14      | 120.60   |
| 2   | A4    | 162 | GLY  | C-N-CA    | 6.59  | 131.14      | 120.60   |
| 3   | E5    | 194 | GLU  | CB-CG-CD  | 6.59  | 123.80      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | x     | 85  | ARG  | CB-CG-CD   | 6.58  | 126.44      | 111.30   |
| 2   | B6    | 286 | LEU  | N-CA-CB    | -6.56 | 100.69      | 110.60   |
| 4   | p     | 42  | TYR  | CA-C-N     | 6.56  | 128.40      | 120.13   |
| 4   | p     | 42  | TYR  | C-N-CA     | 6.56  | 128.40      | 120.13   |
| 1   | 5     | 248 | ARG  | CG-CD-NE   | 6.56  | 126.43      | 112.00   |
| 3   | B3    | 280 | GLN  | CB-CA-C    | 6.56  | 123.76      | 110.38   |
| 2   | D2    | 123 | ARG  | CD-NE-CZ   | 6.55  | 133.57      | 124.40   |
| 1   | 0     | 250 | GLU  | CB-CG-CD   | 6.54  | 123.72      | 112.60   |
| 2   | A6    | 156 | ARG  | CB-CG-CD   | 6.54  | 126.35      | 111.30   |
| 3   | F1    | 394 | PHE  | CA-CB-CG   | 6.53  | 120.33      | 113.80   |
| 3   | D1    | 291 | GLN  | N-CA-C     | 6.53  | 118.06      | 111.07   |
| 3   | B9    | 291 | GLN  | CB-CA-C    | -6.52 | 99.76       | 110.85   |
| 2   | D8    | 371 | VAL  | CA-C-N     | 6.52  | 129.55      | 120.29   |
| 2   | D8    | 371 | VAL  | C-N-CA     | 6.52  | 129.55      | 120.29   |
| 2   | D2    | 284 | GLU  | CB-CG-CD   | 6.51  | 123.67      | 112.60   |
| 2   | B2    | 262 | TYR  | CA-C-N     | 6.51  | 126.01      | 119.24   |
| 2   | B2    | 262 | TYR  | C-N-CA     | 6.51  | 126.01      | 119.24   |
| 3   | D1    | 74  | ASP  | CA-CB-CG   | 6.50  | 119.10      | 112.60   |
| 4   | s     | 13  | GLU  | CB-CG-CD   | 6.50  | 123.65      | 112.60   |
| 2   | A6    | 173 | PRO  | CB-CA-C    | -6.50 | 103.59      | 111.46   |
| 1   | 6     | 245 | SER  | CA-C-N     | 6.50  | 129.31      | 120.54   |
| 1   | 6     | 245 | SER  | C-N-CA     | 6.50  | 129.31      | 120.54   |
| 3   | D9    | 394 | PHE  | CG-CD1-CE1 | 6.49  | 131.74      | 120.70   |
| 2   | D2    | 123 | ARG  | CG-CD-NE   | -6.49 | 97.72       | 112.00   |
| 3   | E9    | 410 | GLU  | CB-CA-C    | -6.49 | 99.82       | 110.85   |
| 3   | D5    | 309 | ARG  | NE-CZ-NH1  | -6.47 | 115.03      | 121.50   |
| 2   | A2    | 373 | ARG  | CG-CD-NE   | 6.47  | 126.24      | 112.00   |
| 4   | a     | 202 | ARG  | CG-CD-NE   | 6.47  | 126.24      | 112.00   |
| 3   | B9    | 380 | ARG  | NE-CZ-NH2  | 6.47  | 125.02      | 119.20   |
| 2   | C6    | 35  | GLN  | CA-C-N     | 6.46  | 129.88      | 120.51   |
| 2   | C6    | 35  | GLN  | C-N-CA     | 6.46  | 129.88      | 120.51   |
| 3   | C5    | 320 | ARG  | CG-CD-NE   | 6.46  | 126.21      | 112.00   |
| 3   | E3    | 407 | GLU  | CB-CA-C    | -6.45 | 98.69       | 110.63   |
| 3   | A1    | 309 | ARG  | CG-CD-NE   | -6.44 | 97.83       | 112.00   |
| 4   | n     | 202 | ARG  | NE-CZ-NH1  | -6.44 | 115.06      | 121.50   |
| 4   | t     | 97  | ARG  | NH1-CZ-NH2 | -6.43 | 110.94      | 119.30   |
| 2   | C4    | 2   | ARG  | CD-NE-CZ   | 6.43  | 133.40      | 124.40   |
| 5   | l     | 58  | LYS  | CB-CG-CD   | 6.43  | 126.09      | 111.30   |
| 4   | p     | 97  | ARG  | NE-CZ-NH2  | 6.43  | 124.98      | 119.20   |
| 3   | B9    | 122 | LYS  | CG-CD-CE   | 6.42  | 126.07      | 111.30   |
| 3   | E5    | 320 | ARG  | CD-NE-CZ   | 6.42  | 133.39      | 124.40   |
| 2   | A6    | 77  | GLU  | CB-CG-CD   | 6.41  | 123.50      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | A8    | 64  | ARG  | NE-CZ-NH1  | -6.41 | 115.09      | 121.50   |
| 2   | E0    | 206 | ASN  | CB-CA-C    | 6.41  | 121.55      | 110.79   |
| 3   | C9    | 291 | GLN  | CB-CA-C    | 6.40  | 122.42      | 110.70   |
| 2   | D8    | 290 | GLU  | CB-CG-CD   | 6.40  | 123.48      | 112.60   |
| 3   | D9    | 157 | GLU  | CB-CG-CD   | 6.40  | 123.48      | 112.60   |
| 3   | E7    | 77  | ARG  | CB-CG-CD   | 6.39  | 126.01      | 111.30   |
| 4   | n     | 120 | GLU  | CB-CG-CD   | 6.39  | 123.47      | 112.60   |
| 4   | v     | 202 | ARG  | CD-NE-CZ   | 6.39  | 133.34      | 124.40   |
| 2   | C6    | 372 | MET  | CB-CG-SD   | 6.38  | 131.85      | 112.70   |
| 2   | A8    | 224 | TYR  | N-CA-CB    | 6.38  | 121.56      | 110.39   |
| 4   | m     | 202 | ARG  | CG-CD-NE   | 6.38  | 126.04      | 112.00   |
| 4   | t     | 56  | LYS  | CB-CG-CD   | 6.38  | 125.97      | 111.30   |
| 4   | a     | 193 | ASP  | N-CA-CB    | -6.38 | 102.37      | 112.63   |
| 4   | a     | 164 | ARG  | NE-CZ-NH2  | 6.36  | 124.92      | 119.20   |
| 4   | e     | 106 | GLN  | N-CA-CB    | 6.36  | 120.11      | 109.94   |
| 2   | A2    | 214 | ARG  | NE-CZ-NH1  | -6.36 | 115.14      | 121.50   |
| 2   | A0    | 326 | LYS  | CB-CA-C    | -6.35 | 100.91      | 110.88   |
| 2   | E6    | 280 | LYS  | CB-CG-CD   | 6.35  | 125.91      | 111.30   |
| 4   | b     | 97  | ARG  | CB-CG-CD   | 6.34  | 125.88      | 111.30   |
| 3   | B5    | 332 | ASN  | CA-CB-CG   | 6.34  | 118.94      | 112.60   |
| 3   | C1    | 384 | GLN  | CB-CG-CD   | 6.33  | 123.36      | 112.60   |
| 3   | E7    | 320 | ARG  | CB-CG-CD   | 6.32  | 125.84      | 111.30   |
| 3   | D1    | 155 | VAL  | O-C-N      | 6.32  | 128.00      | 121.87   |
| 4   | v     | 69  | LYS  | CG-CD-CE   | 6.31  | 125.81      | 111.30   |
| 3   | C9    | 276 | ARG  | NE-CZ-NH2  | 6.30  | 124.87      | 119.20   |
| 3   | D3    | 53  | GLU  | CB-CG-CD   | 6.30  | 123.31      | 112.60   |
| 3   | D3    | 213 | ARG  | CD-NE-CZ   | 6.30  | 133.22      | 124.40   |
| 2   | D8    | 282 | TYR  | N-CA-CB    | 6.29  | 119.75      | 110.56   |
| 4   | c     | 178 | ARG  | NH1-CZ-NH2 | -6.29 | 111.12      | 119.30   |
| 4   | q     | 97  | ARG  | CD-NE-CZ   | 6.28  | 133.20      | 124.40   |
| 4   | b     | 178 | ARG  | CD-NE-CZ   | 6.27  | 133.18      | 124.40   |
| 4   | m     | 39  | PRO  | CA-C-N     | 6.26  | 126.62      | 119.92   |
| 4   | m     | 39  | PRO  | C-N-CA     | 6.26  | 126.62      | 119.92   |
| 3   | E7    | 424 | GLN  | CB-CG-CD   | 6.25  | 123.23      | 112.60   |
| 4   | r     | 198 | ARG  | CG-CD-NE   | 6.25  | 125.76      | 112.00   |
| 2   | A8    | 280 | LYS  | CG-CD-CE   | 6.25  | 125.67      | 111.30   |
| 2   | B0    | 336 | LYS  | CB-CG-CD   | 6.25  | 125.67      | 111.30   |
| 3   | D5    | 209 | ASP  | CA-CB-CG   | 6.24  | 118.84      | 112.60   |
| 3   | C1    | 296 | ALA  | CA-C-N     | 6.23  | 128.91      | 120.38   |
| 3   | C1    | 296 | ALA  | C-N-CA     | 6.23  | 128.91      | 120.38   |
| 4   | f     | 3   | GLN  | CB-CA-C    | -6.21 | 101.90      | 110.16   |
| 3   | C5    | 122 | LYS  | CB-CG-CD   | 6.19  | 125.54      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | D1    | 275 | SER  | CA-C-N     | 6.19  | 130.11      | 120.82   |
| 3   | D1    | 275 | SER  | C-N-CA     | 6.19  | 130.11      | 120.82   |
| 2   | A2    | 214 | ARG  | CD-NE-CZ   | -6.18 | 115.74      | 124.40   |
| 4   | i     | 36  | ILE  | CA-C-N     | 6.18  | 129.49      | 120.71   |
| 4   | i     | 36  | ILE  | C-N-CA     | 6.18  | 129.49      | 120.71   |
| 2   | D0    | 420 | GLU  | CB-CG-CD   | 6.18  | 123.11      | 112.60   |
| 3   | F1    | 209 | ASP  | CA-CB-CG   | -6.18 | 106.42      | 112.60   |
| 4   | d     | 117 | ARG  | CG-CD-NE   | 6.17  | 125.58      | 112.00   |
| 3   | A9    | 391 | ARG  | CB-CA-C    | 6.16  | 121.05      | 111.13   |
| 4   | o     | 137 | GLU  | CB-CG-CD   | 6.16  | 123.07      | 112.60   |
| 3   | E3    | 26  | ASP  | CA-CB-CG   | 6.16  | 118.76      | 112.60   |
| 3   | F1    | 336 | LYS  | CB-CA-C    | -6.16 | 101.17      | 110.90   |
| 3   | B7    | 212 | PHE  | CA-CB-CG   | 6.15  | 119.95      | 113.80   |
| 2   | A6    | 214 | ARG  | CA-CB-CG   | 6.15  | 126.39      | 114.10   |
| 2   | D2    | 221 | ARG  | CG-CD-NE   | -6.14 | 98.50       | 112.00   |
| 3   | A9    | 252 | LYS  | CB-CG-CD   | 6.14  | 125.42      | 111.30   |
| 1   | 5     | 240 | PRO  | CB-CA-C    | -6.14 | 103.54      | 111.46   |
| 4   | a     | 101 | GLU  | CB-CA-C    | -6.13 | 101.25      | 110.88   |
| 4   | p     | 16  | ARG  | CG-CD-NE   | 6.13  | 125.49      | 112.00   |
| 3   | D1    | 77  | ARG  | NE-CZ-NH1  | 6.12  | 127.62      | 121.50   |
| 2   | A8    | 336 | LYS  | CB-CA-C    | -6.12 | 101.28      | 110.88   |
| 2   | B0    | 262 | TYR  | O-C-N      | 6.12  | 126.32      | 121.55   |
| 3   | D7    | 174 | LYS  | CB-CG-CD   | 6.11  | 125.36      | 111.30   |
| 3   | D3    | 424 | GLN  | OE1-CD-NE2 | 6.11  | 128.71      | 122.60   |
| 4   | n     | 119 | ARG  | NE-CZ-NH1  | -6.11 | 115.39      | 121.50   |
| 3   | D3    | 90  | PHE  | CA-CB-CG   | 6.10  | 119.90      | 113.80   |
| 3   | B9    | 380 | ARG  | CB-CG-CD   | 6.10  | 125.32      | 111.30   |
| 2   | E0    | 156 | ARG  | CG-CD-NE   | -6.09 | 98.59       | 112.00   |
| 2   | D4    | 203 | MET  | CB-CG-SD   | -6.09 | 94.43       | 112.70   |
| 4   | u     | 79  | ASP  | CA-C-N     | 6.09  | 126.87      | 119.99   |
| 4   | u     | 79  | ASP  | C-N-CA     | 6.09  | 126.87      | 119.99   |
| 2   | D4    | 123 | ARG  | NE-CZ-NH1  | 6.09  | 127.59      | 121.50   |
| 2   | C4    | 339 | ARG  | CB-CG-CD   | 6.09  | 125.30      | 111.30   |
| 5   | k     | 58  | LYS  | CB-CG-CD   | 6.08  | 125.29      | 111.30   |
| 1   | 11    | 246 | CYS  | CA-CB-SG   | 6.08  | 128.39      | 114.40   |
| 3   | C9    | 343 | GLU  | CB-CG-CD   | 6.08  | 122.94      | 112.60   |
| 3   | A5    | 140 | GLY  | CA-C-N     | 6.08  | 130.35      | 121.96   |
| 3   | A5    | 140 | GLY  | C-N-CA     | 6.08  | 130.35      | 121.96   |
| 3   | E3    | 128 | ASP  | CA-C-O     | -6.07 | 114.39      | 121.07   |
| 3   | A1    | 80  | PRO  | CA-C-N     | 6.06  | 130.74      | 122.07   |
| 3   | A1    | 80  | PRO  | C-N-CA     | 6.06  | 130.74      | 122.07   |
| 3   | D3    | 213 | ARG  | CG-CD-NE   | 6.06  | 125.33      | 112.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D4    | 96  | LYS  | CG-CD-CE   | 6.05  | 125.21      | 111.30   |
| 2   | E2    | 123 | ARG  | NE-CZ-NH1  | -6.04 | 115.46      | 121.50   |
| 2   | B6    | 247 | ALA  | N-CA-CB    | 6.03  | 119.19      | 110.20   |
| 2   | E2    | 85  | HIS  | CA-CB-CG   | -6.03 | 107.77      | 113.80   |
| 5   | l     | 96  | GLU  | CA-C-N     | 6.03  | 128.64      | 120.38   |
| 5   | l     | 96  | GLU  | C-N-CA     | 6.03  | 128.64      | 120.38   |
| 3   | D9    | 320 | ARG  | CG-CD-NE   | 6.03  | 125.26      | 112.00   |
| 4   | n     | 156 | VAL  | CA-C-O     | 6.03  | 123.60      | 119.20   |
| 3   | B9    | 157 | GLU  | CB-CG-CD   | 6.03  | 122.85      | 112.60   |
| 3   | F1    | 285 | SER  | CA-C-N     | 6.03  | 124.04      | 120.24   |
| 3   | F1    | 285 | SER  | C-N-CA     | 6.03  | 124.04      | 120.24   |
| 2   | D6    | 221 | ARG  | NE-CZ-NH2  | 6.02  | 124.62      | 119.20   |
| 4   | b     | 97  | ARG  | CG-CD-NE   | 6.02  | 125.25      | 112.00   |
| 2   | C8    | 340 | THR  | N-CA-CB    | 6.02  | 119.58      | 110.30   |
| 3   | C7    | 143 | THR  | OG1-CB-CG2 | -6.02 | 97.26       | 109.30   |
| 2   | A8    | 155 | GLU  | CB-CG-CD   | 6.02  | 122.83      | 112.60   |
| 2   | F0    | 370 | LYS  | CB-CG-CD   | 6.01  | 125.12      | 111.30   |
| 2   | B6    | 49  | PHE  | N-CA-CB    | 6.01  | 119.33      | 110.56   |
| 4   | p     | 97  | ARG  | NE-CZ-NH1  | -6.01 | 115.49      | 121.50   |
| 3   | C1    | 252 | LYS  | CB-CG-CD   | 6.00  | 125.11      | 111.30   |
| 3   | A7    | 324 | LYS  | CG-CD-CE   | 6.00  | 125.10      | 111.30   |
| 2   | D6    | 79  | ARG  | CB-CG-CD   | -6.00 | 97.50       | 111.30   |
| 3   | E9    | 129 | CYS  | CA-C-N     | 5.99  | 130.35      | 120.94   |
| 3   | E9    | 129 | CYS  | C-N-CA     | 5.99  | 130.35      | 120.94   |
| 1   | 1     | 248 | ARG  | CG-CD-NE   | 5.99  | 125.18      | 112.00   |
| 4   | g     | 15  | ARG  | NE-CZ-NH1  | -5.99 | 115.51      | 121.50   |
| 3   | E5    | 12  | CYS  | N-CA-C     | -5.99 | 104.33      | 111.69   |
| 2   | A6    | 214 | ARG  | NE-CZ-NH1  | -5.99 | 115.52      | 121.50   |
| 2   | D8    | 264 | ARG  | CG-CD-NE   | -5.99 | 98.83       | 112.00   |
| 3   | D3    | 54  | ALA  | CA-C-N     | 5.98  | 132.97      | 121.54   |
| 3   | D3    | 54  | ALA  | C-N-CA     | 5.98  | 132.97      | 121.54   |
| 4   | i     | 37  | GLN  | CB-CG-CD   | 5.98  | 122.77      | 112.60   |
| 4   | n     | 91  | PHE  | CB-CA-C    | -5.98 | 99.19       | 110.67   |
| 3   | A5    | 276 | ARG  | CA-C-N     | 5.97  | 126.74      | 119.99   |
| 3   | A5    | 276 | ARG  | C-N-CA     | 5.97  | 126.74      | 119.99   |
| 3   | C7    | 367 | PHE  | CB-CA-C    | 5.97  | 120.07      | 110.16   |
| 3   | D3    | 410 | GLU  | CB-CG-CD   | 5.97  | 122.75      | 112.60   |
| 2   | D6    | 96  | LYS  | CG-CD-CE   | 5.97  | 125.02      | 111.30   |
| 3   | C1    | 88  | ASP  | CB-CA-C    | -5.96 | 99.60       | 110.63   |
| 2   | A0    | 285 | GLN  | CB-CA-C    | -5.96 | 100.19      | 109.61   |
| 4   | j     | 198 | ARG  | CG-CD-NE   | 5.96  | 125.11      | 112.00   |
| 3   | B5    | 177 | ASP  | CA-CB-CG   | 5.96  | 118.56      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | F1    | 177 | ASP  | CA-C-O     | -5.95 | 115.08      | 121.56   |
| 2   | A0    | 96  | LYS  | CB-CG-CD   | 5.94  | 124.97      | 111.30   |
| 3   | D1    | 342 | VAL  | CA-C-N     | -5.94 | 113.02      | 122.29   |
| 3   | D1    | 342 | VAL  | C-N-CA     | -5.94 | 113.02      | 122.29   |
| 2   | D0    | 221 | ARG  | NE-CZ-NH1  | -5.94 | 115.56      | 121.50   |
| 2   | A6    | 176 | GLN  | CB-CG-CD   | 5.93  | 122.68      | 112.60   |
| 2   | F0    | 336 | LYS  | CG-CD-CE   | -5.92 | 97.69       | 111.30   |
| 2   | A8    | 211 | ASP  | CA-CB-CG   | 5.92  | 118.52      | 112.60   |
| 3   | E7    | 320 | ARG  | CB-CA-C    | 5.92  | 119.13      | 110.26   |
| 2   | A8    | 262 | TYR  | CA-C-N     | 5.92  | 126.06      | 119.32   |
| 2   | A8    | 262 | TYR  | C-N-CA     | 5.92  | 126.06      | 119.32   |
| 2   | D2    | 285 | GLN  | CB-CG-CD   | -5.91 | 102.55      | 112.60   |
| 3   | D5    | 48  | ASN  | CB-CA-C    | -5.91 | 99.70       | 110.63   |
| 4   | d     | 101 | GLU  | CB-CG-CD   | 5.91  | 122.64      | 112.60   |
| 3   | D5    | 343 | GLU  | CB-CA-C    | -5.91 | 99.71       | 109.99   |
| 3   | F1    | 332 | ASN  | O-C-N      | 5.90  | 128.15      | 122.07   |
| 2   | C8    | 155 | GLU  | CB-CG-CD   | 5.89  | 122.62      | 112.60   |
| 2   | B4    | 415 | GLU  | CB-CG-CD   | 5.89  | 122.61      | 112.60   |
| 3   | A7    | 410 | GLU  | CB-CG-CD   | 5.88  | 122.60      | 112.60   |
| 3   | B5    | 99  | ASN  | OD1-CG-ND2 | -5.87 | 116.73      | 122.60   |
| 2   | D4    | 373 | ARG  | CG-CD-NE   | 5.87  | 124.90      | 112.00   |
| 2   | E2    | 102 | ASN  | OD1-CG-ND2 | -5.87 | 116.73      | 122.60   |
| 3   | E3    | 380 | ARG  | CB-CG-CD   | 5.87  | 124.79      | 111.30   |
| 2   | E4    | 221 | ARG  | CB-CG-CD   | -5.86 | 97.82       | 111.30   |
| 3   | D5    | 390 | ARG  | NE-CZ-NH2  | 5.86  | 124.47      | 119.20   |
| 5   | k     | 80  | GLU  | CB-CG-CD   | 5.85  | 122.55      | 112.60   |
| 3   | E3    | 77  | ARG  | NE-CZ-NH1  | -5.85 | 115.65      | 121.50   |
| 4   | e     | 44  | ASP  | CA-CB-CG   | 5.85  | 118.45      | 112.60   |
| 4   | u     | 202 | ARG  | CG-CD-NE   | 5.85  | 124.87      | 112.00   |
| 2   | A2    | 372 | MET  | CG-SD-CE   | -5.84 | 88.05       | 100.90   |
| 3   | D3    | 48  | ASN  | CB-CA-C    | -5.84 | 99.12       | 110.46   |
| 4   | n     | 202 | ARG  | CD-NE-CZ   | 5.84  | 132.58      | 124.40   |
| 4   | e     | 95  | TYR  | CB-CA-C    | 5.84  | 120.78      | 110.85   |
| 1   | 6     | 241 | PHE  | CA-CB-CG   | 5.84  | 119.64      | 113.80   |
| 2   | D6    | 163 | LYS  | CB-CG-CD   | 5.84  | 124.73      | 111.30   |
| 3   | C5    | 10  | GLY  | CA-C-N     | 5.84  | 128.03      | 120.44   |
| 3   | C5    | 10  | GLY  | C-N-CA     | 5.84  | 128.03      | 120.44   |
| 2   | D4    | 285 | GLN  | N-CA-CB    | 5.84  | 119.97      | 110.17   |
| 3   | A1    | 379 | LYS  | CG-CD-CE   | 5.83  | 124.72      | 111.30   |
| 3   | D9    | 31  | ASP  | CA-CB-CG   | 5.83  | 118.43      | 112.60   |
| 4   | e     | 42  | TYR  | CA-C-N     | 5.83  | 126.58      | 119.99   |
| 4   | e     | 42  | TYR  | C-N-CA     | 5.83  | 126.58      | 119.99   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | D5    | 70  | PRO  | CA-C-N     | 5.83  | 126.41      | 119.94   |
| 3   | D5    | 70  | PRO  | C-N-CA     | 5.83  | 126.41      | 119.94   |
| 3   | D5    | 164 | MET  | CB-CG-SD   | -5.83 | 95.22       | 112.70   |
| 2   | A8    | 224 | TYR  | CB-CA-C    | -5.82 | 98.29       | 110.17   |
| 3   | B5    | 122 | LYS  | CG-CD-CE   | 5.82  | 124.69      | 111.30   |
| 1   | 19    | 248 | ARG  | CB-CG-CD   | 5.82  | 124.69      | 111.30   |
| 3   | C9    | 324 | LYS  | CB-CG-CD   | 5.82  | 124.69      | 111.30   |
| 5   | w     | 54  | ARG  | CB-CG-CD   | 5.82  | 124.69      | 111.30   |
| 2   | B0    | 339 | ARG  | NE-CZ-NH2  | 5.82  | 124.44      | 119.20   |
| 2   | D0    | 123 | ARG  | CG-CD-NE   | 5.81  | 124.78      | 112.00   |
| 4   | i     | 69  | LYS  | CB-CA-C    | 5.81  | 119.58      | 109.65   |
| 2   | B6    | 372 | MET  | CA-C-O     | 5.81  | 125.80      | 119.24   |
| 2   | B4    | 162 | GLY  | CA-C-N     | 5.80  | 132.90      | 121.58   |
| 2   | B4    | 162 | GLY  | C-N-CA     | 5.80  | 132.90      | 121.58   |
| 2   | A8    | 264 | ARG  | CB-CA-C    | 5.80  | 120.86      | 109.72   |
| 3   | F1    | 262 | ARG  | CB-CG-CD   | 5.80  | 124.64      | 111.30   |
| 3   | B3    | 204 | ASN  | CA-CB-CG   | 5.79  | 118.39      | 112.60   |
| 3   | D7    | 121 | ARG  | NE-CZ-NH2  | 5.79  | 124.41      | 119.20   |
| 4   | p     | 126 | ARG  | NE-CZ-NH1  | -5.79 | 115.71      | 121.50   |
| 3   | C3    | 391 | ARG  | CG-CD-NE   | 5.79  | 124.73      | 112.00   |
| 2   | B2    | 156 | ARG  | NE-CZ-NH2  | 5.78  | 124.41      | 119.20   |
| 4   | m     | 79  | ASP  | CA-C-N     | 5.78  | 126.35      | 119.94   |
| 4   | m     | 79  | ASP  | C-N-CA     | 5.78  | 126.35      | 119.94   |
| 3   | D9    | 122 | LYS  | CB-CG-CD   | 5.77  | 124.58      | 111.30   |
| 3   | C9    | 276 | ARG  | CD-NE-CZ   | 5.77  | 132.47      | 124.40   |
| 5   | x     | 25  | ARG  | CB-CA-C    | 5.76  | 117.68      | 109.38   |
| 2   | B4    | 262 | TYR  | O-C-N      | 5.76  | 125.40      | 121.71   |
| 2   | D4    | 401 | LYS  | N-CA-CB    | -5.76 | 102.99      | 111.51   |
| 3   | A1    | 309 | ARG  | CB-CG-CD   | 5.76  | 124.54      | 111.30   |
| 3   | B7    | 372 | THR  | CA-CB-CG2  | 5.76  | 120.29      | 110.50   |
| 5   | k     | 126 | THR  | CA-C-N     | 5.76  | 132.53      | 121.54   |
| 5   | k     | 126 | THR  | C-N-CA     | 5.76  | 132.53      | 121.54   |
| 2   | A8    | 101 | ASN  | OD1-CG-ND2 | -5.75 | 116.85      | 122.60   |
| 2   | A0    | 339 | ARG  | CG-CD-NE   | 5.74  | 124.63      | 112.00   |
| 3   | B1    | 209 | ASP  | CA-CB-CG   | 5.74  | 118.34      | 112.60   |
| 3   | E7    | 391 | ARG  | CD-NE-CZ   | 5.74  | 132.44      | 124.40   |
| 2   | B6    | 285 | GLN  | CB-CA-C    | 5.74  | 119.70      | 110.29   |
| 3   | A5    | 114 | ASP  | CB-CA-C    | 5.73  | 121.68      | 110.67   |
| 3   | D5    | 209 | ASP  | CB-CA-C    | 5.73  | 120.31      | 110.79   |
| 2   | D2    | 336 | LYS  | CB-CA-C    | -5.73 | 101.11      | 110.85   |
| 2   | A0    | 163 | LYS  | CG-CD-CE   | 5.73  | 124.47      | 111.30   |
| 1   | 15    | 257 | PRO  | CB-CA-C    | -5.72 | 103.94      | 110.92   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | j     | 97  | ARG  | CG-CD-NE   | 5.72  | 124.59      | 112.00   |
| 2   | A0    | 156 | ARG  | CG-CD-NE   | -5.72 | 99.42       | 112.00   |
| 3   | B5    | 227 | HIS  | CA-CB-CG   | 5.72  | 119.52      | 113.80   |
| 3   | D3    | 52  | ASN  | CB-CA-C    | 5.72  | 119.67      | 109.38   |
| 4   | p     | 198 | ARG  | CG-CD-NE   | -5.71 | 99.44       | 112.00   |
| 2   | B0    | 163 | LYS  | CB-CA-C    | 5.71  | 121.14      | 109.55   |
| 4   | s     | 128 | HIS  | CA-CB-CG   | 5.71  | 119.51      | 113.80   |
| 2   | A0    | 218 | ASP  | CA-CB-CG   | 5.70  | 118.30      | 112.60   |
| 2   | A8    | 117 | LEU  | O-C-N      | 5.70  | 128.16      | 122.12   |
| 3   | E5    | 11  | GLN  | CA-CB-CG   | 5.70  | 125.50      | 114.10   |
| 4   | o     | 139 | PRO  | CB-CA-C    | -5.69 | 103.33      | 112.21   |
| 3   | D5    | 324 | LYS  | N-CA-CB    | 5.68  | 119.09      | 110.28   |
| 4   | g     | 16  | ARG  | CA-CB-CG   | -5.68 | 102.74      | 114.10   |
| 2   | B6    | 113 | GLU  | CB-CA-C    | -5.67 | 101.20      | 110.85   |
| 4   | p     | 120 | GLU  | CB-CG-CD   | 5.67  | 122.25      | 112.60   |
| 3   | C1    | 123 | GLU  | CB-CG-CD   | 5.67  | 122.24      | 112.60   |
| 2   | C6    | 156 | ARG  | CG-CD-NE   | -5.67 | 99.52       | 112.00   |
| 4   | q     | 152 | LYS  | CG-CD-CE   | 5.67  | 124.34      | 111.30   |
| 3   | D1    | 213 | ARG  | NE-CZ-NH1  | -5.67 | 115.83      | 121.50   |
| 3   | A3    | 11  | GLN  | CB-CA-C    | 5.67  | 119.78      | 110.88   |
| 2   | C6    | 112 | LYS  | CB-CG-CD   | 5.66  | 124.33      | 111.30   |
| 2   | A8    | 131 | GLY  | CA-C-O     | 5.66  | 126.10      | 119.19   |
| 3   | D5    | 340 | TYR  | CB-CA-C    | -5.66 | 100.64      | 110.09   |
| 2   | D4    | 336 | LYS  | CB-CA-C    | -5.65 | 101.41      | 110.79   |
| 2   | B0    | 423 | GLU  | CB-CG-CD   | 5.65  | 122.20      | 112.60   |
| 3   | B7    | 26  | ASP  | CA-CB-CG   | 5.65  | 118.25      | 112.60   |
| 4   | b     | 94  | ASN  | CA-CB-CG   | 5.65  | 118.25      | 112.60   |
| 4   | m     | 183 | LEU  | CA-C-O     | 5.62  | 123.78      | 119.46   |
| 4   | g     | 46  | ASP  | O-C-N      | -5.62 | 116.98      | 123.33   |
| 3   | E7    | 76  | VAL  | CA-C-N     | 5.61  | 128.07      | 120.38   |
| 3   | E7    | 76  | VAL  | C-N-CA     | 5.61  | 128.07      | 120.38   |
| 2   | A8    | 214 | ARG  | CB-CG-CD   | -5.61 | 98.40       | 111.30   |
| 3   | C3    | 203 | ASP  | CA-C-N     | 5.61  | 128.11      | 120.54   |
| 3   | C3    | 203 | ASP  | C-N-CA     | 5.61  | 128.11      | 120.54   |
| 3   | B7    | 319 | GLY  | CA-C-N     | 5.60  | 132.24      | 121.54   |
| 3   | B7    | 319 | GLY  | C-N-CA     | 5.60  | 132.24      | 121.54   |
| 2   | D2    | 33  | ASP  | CA-CB-CG   | 5.60  | 118.20      | 112.60   |
| 4   | b     | 141 | THR  | OG1-CB-CG2 | 5.60  | 120.50      | 109.30   |
| 2   | A8    | 264 | ARG  | CD-NE-CZ   | 5.60  | 132.24      | 124.40   |
| 2   | A2    | 261 | PRO  | CB-CA-C    | -5.59 | 104.16      | 113.06   |
| 3   | E3    | 180 | VAL  | CB-CA-C    | 5.59  | 120.46      | 111.29   |
| 1   | 4     | 241 | PHE  | CA-CB-CG   | 5.59  | 119.39      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D4    | 417 | GLU  | CB-CG-CD   | 5.59  | 122.10      | 112.60   |
| 2   | A4    | 173 | PRO  | CB-CA-C    | -5.58 | 104.61      | 111.64   |
| 3   | B1    | 83  | GLN  | CB-CG-CD   | -5.58 | 103.11      | 112.60   |
| 4   | m     | 179 | GLU  | CB-CA-C    | 5.58  | 118.64      | 110.26   |
| 2   | A4    | 123 | ARG  | CG-CD-NE   | -5.58 | 99.72       | 112.00   |
| 3   | A5    | 19  | LYS  | CB-CG-CD   | 5.58  | 124.14      | 111.30   |
| 3   | B9    | 212 | PHE  | CA-CB-CG   | 5.58  | 119.38      | 113.80   |
| 4   | o     | 202 | ARG  | CA-CB-CG   | 5.58  | 125.26      | 114.10   |
| 3   | C1    | 83  | GLN  | CB-CG-CD   | 5.58  | 122.09      | 112.60   |
| 3   | B3    | 216 | LYS  | CB-CG-CD   | 5.57  | 124.11      | 111.30   |
| 1   | 14    | 237 | PRO  | CB-CA-C    | 5.57  | 120.67      | 110.10   |
| 2   | D0    | 401 | LYS  | N-CA-CB    | 5.56  | 122.76      | 111.36   |
| 3   | D3    | 320 | ARG  | CB-CG-CD   | -5.56 | 98.51       | 111.30   |
| 4   | j     | 97  | ARG  | NH1-CZ-NH2 | -5.56 | 112.07      | 119.30   |
| 2   | D4    | 49  | PHE  | N-CA-CB    | 5.56  | 118.72      | 110.49   |
| 3   | B5    | 10  | GLY  | CA-C-N     | 5.55  | 127.99      | 120.38   |
| 3   | B5    | 10  | GLY  | C-N-CA     | 5.55  | 127.99      | 120.38   |
| 4   | c     | 158 | THR  | CA-CB-OG1  | -5.55 | 101.27      | 109.60   |
| 1   | 6     | 237 | PRO  | N-CD-CG    | 5.54  | 111.51      | 103.20   |
| 2   | A8    | 120 | ASP  | CA-CB-CG   | -5.53 | 107.07      | 112.60   |
| 2   | E6    | 401 | LYS  | CG-CD-CE   | 5.53  | 124.01      | 111.30   |
| 4   | o     | 194 | ARG  | CD-NE-CZ   | 5.53  | 132.14      | 124.40   |
| 5   | k     | 13  | VAL  | N-CA-CB    | 5.52  | 119.03      | 111.41   |
| 4   | o     | 103 | GLY  | CA-C-N     | 5.52  | 127.68      | 120.28   |
| 4   | o     | 103 | GLY  | C-N-CA     | 5.52  | 127.68      | 120.28   |
| 2   | B4    | 339 | ARG  | CB-CG-CD   | 5.52  | 124.00      | 111.30   |
| 4   | j     | 15  | ARG  | NE-CZ-NH2  | 5.52  | 124.17      | 119.20   |
| 4   | a     | 164 | ARG  | CD-NE-CZ   | 5.52  | 132.12      | 124.40   |
| 3   | A5    | 12  | CYS  | N-CA-C     | -5.51 | 104.91      | 111.69   |
| 3   | D3    | 171 | PRO  | N-CA-CB    | 5.50  | 108.14      | 103.19   |
| 2   | B0    | 64  | ARG  | NE-CZ-NH1  | -5.50 | 116.00      | 121.50   |
| 3   | C1    | 203 | ASP  | CA-C-N     | 5.50  | 127.96      | 120.54   |
| 3   | C1    | 203 | ASP  | C-N-CA     | 5.50  | 127.96      | 120.54   |
| 3   | D9    | 127 | CYS  | CA-C-N     | 5.49  | 127.90      | 120.65   |
| 3   | D9    | 127 | CYS  | C-N-CA     | 5.49  | 127.90      | 120.65   |
| 2   | C8    | 420 | GLU  | CA-CB-CG   | -5.49 | 103.12      | 114.10   |
| 3   | A3    | 320 | ARG  | CB-CG-CD   | 5.49  | 123.92      | 111.30   |
| 2   | E0    | 221 | ARG  | CG-CD-NE   | -5.49 | 99.93       | 112.00   |
| 4   | s     | 152 | LYS  | CG-CD-CE   | 5.49  | 123.91      | 111.30   |
| 3   | D3    | 343 | GLU  | CB-CG-CD   | 5.48  | 121.92      | 112.60   |
| 4   | h     | 202 | ARG  | NH1-CZ-NH2 | -5.48 | 112.17      | 119.30   |
| 3   | D3    | 366 | THR  | CA-CB-CG2  | 5.48  | 119.82      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | A5    | 320 | ARG  | NE-CZ-NH2  | 5.48  | 124.13      | 119.20   |
| 2   | D0    | 116 | ASP  | CB-CA-C    | 5.48  | 121.18      | 110.67   |
| 2   | E2    | 284 | GLU  | CB-CG-CD   | 5.48  | 121.91      | 112.60   |
| 2   | B6    | 279 | GLU  | CB-CG-CD   | 5.47  | 121.91      | 112.60   |
| 3   | D5    | 319 | GLY  | CA-C-N     | 5.47  | 130.15      | 121.99   |
| 3   | D5    | 319 | GLY  | C-N-CA     | 5.47  | 130.15      | 121.99   |
| 4   | a     | 179 | GLU  | CB-CA-C    | 5.47  | 118.44      | 109.90   |
| 4   | b     | 138 | ASN  | CA-CB-CG   | 5.47  | 118.07      | 112.60   |
| 2   | D6    | 71  | GLU  | CB-CA-C    | 5.47  | 116.25      | 108.76   |
| 2   | D4    | 221 | ARG  | CB-CA-C    | 5.46  | 118.37      | 111.21   |
| 3   | A5    | 11  | GLN  | CA-CB-CG   | 5.46  | 125.01      | 114.10   |
| 3   | B5    | 212 | PHE  | CA-CB-CG   | 5.45  | 119.25      | 113.80   |
| 3   | C9    | 276 | ARG  | CG-CD-NE   | 5.45  | 123.99      | 112.00   |
| 4   | s     | 191 | GLU  | CB-CG-CD   | 5.45  | 121.86      | 112.60   |
| 3   | E3    | 276 | ARG  | NE-CZ-NH1  | -5.45 | 116.05      | 121.50   |
| 3   | E3    | 174 | LYS  | CG-CD-CE   | 5.45  | 123.82      | 111.30   |
| 3   | D1    | 227 | HIS  | CA-CB-CG   | 5.44  | 119.24      | 113.80   |
| 3   | D1    | 276 | ARG  | NE-CZ-NH2  | 5.44  | 124.10      | 119.20   |
| 2   | D6    | 85  | HIS  | CA-CB-CG   | 5.44  | 119.24      | 113.80   |
| 1   | 12    | 242 | ASN  | N-CA-CB    | -5.44 | 103.31      | 111.25   |
| 5   | k     | 128 | ILE  | CB-CA-C    | 5.44  | 116.33      | 111.00   |
| 2   | E4    | 15  | GLN  | CB-CG-CD   | 5.44  | 121.84      | 112.60   |
| 4   | c     | 61  | THR  | OG1-CB-CG2 | 5.43  | 120.16      | 109.30   |
| 3   | D9    | 90  | PHE  | CA-CB-CG   | 5.43  | 119.23      | 113.80   |
| 2   | A2    | 142 | GLY  | CA-C-N     | 5.42  | 126.35      | 120.44   |
| 2   | A2    | 142 | GLY  | C-N-CA     | 5.42  | 126.35      | 120.44   |
| 2   | E4    | 79  | ARG  | NE-CZ-NH2  | 5.42  | 124.08      | 119.20   |
| 4   | t     | 4   | PRO  | N-CD-CG    | -5.42 | 97.29       | 103.80   |
| 2   | B4    | 285 | GLN  | CB-CG-CD   | 5.42  | 121.81      | 112.60   |
| 4   | s     | 119 | ARG  | CB-CG-CD   | 5.42  | 123.76      | 111.30   |
| 3   | A1    | 122 | LYS  | CA-CB-CG   | -5.42 | 103.27      | 114.10   |
| 3   | A5    | 125 | GLU  | CB-CA-C    | 5.42  | 120.73      | 109.95   |
| 2   | A6    | 71  | GLU  | CB-CA-C    | 5.42  | 115.86      | 109.47   |
| 3   | A9    | 37  | CYS  | CB-CA-C    | 5.41  | 118.14      | 110.24   |
| 4   | i     | 69  | LYS  | CB-CG-CD   | 5.41  | 123.73      | 111.30   |
| 4   | r     | 15  | ARG  | NE-CZ-NH2  | 5.41  | 124.07      | 119.20   |
| 3   | C3    | 251 | ARG  | CG-CD-NE   | -5.40 | 100.12      | 112.00   |
| 3   | D3    | 320 | ARG  | NE-CZ-NH2  | 5.40  | 124.06      | 119.20   |
| 3   | C9    | 227 | HIS  | CA-CB-CG   | 5.40  | 119.20      | 113.80   |
| 3   | D3    | 22  | GLU  | CB-CG-CD   | 5.40  | 121.78      | 112.60   |
| 2   | D8    | 220 | GLU  | CB-CG-CD   | 5.40  | 121.78      | 112.60   |
| 3   | A5    | 15  | GLN  | OE1-CD-NE2 | -5.40 | 117.20      | 122.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | A0    | 123 | ARG  | NE-CZ-NH1 | -5.39 | 116.11      | 121.50   |
| 2   | A0    | 326 | LYS  | N-CA-CB   | 5.38  | 117.82      | 110.01   |
| 1   | 1     | 250 | GLU  | CB-CG-CD  | 5.38  | 121.74      | 112.60   |
| 1   | 21    | 248 | ARG  | CB-CG-CD  | 5.38  | 123.67      | 111.30   |
| 2   | A0    | 251 | ASP  | CA-C-N    | 5.38  | 127.33      | 120.56   |
| 2   | A0    | 251 | ASP  | C-N-CA    | 5.38  | 127.33      | 120.56   |
| 2   | B0    | 141 | VAL  | CA-C-N    | 5.38  | 126.05      | 120.03   |
| 2   | B0    | 141 | VAL  | C-N-CA    | 5.38  | 126.05      | 120.03   |
| 3   | A7    | 380 | ARG  | NE-CZ-NH2 | 5.37  | 124.03      | 119.20   |
| 3   | A5    | 56  | GLY  | CA-C-N    | 5.37  | 131.06      | 122.25   |
| 3   | A5    | 56  | GLY  | C-N-CA    | 5.37  | 131.06      | 122.25   |
| 3   | A9    | 379 | LYS  | CG-CD-CE  | 5.37  | 123.64      | 111.30   |
| 2   | B0    | 173 | PRO  | CB-CA-C   | -5.37 | 104.88      | 111.64   |
| 1   | 13    | 258 | PRO  | N-CA-CB   | 5.36  | 108.90      | 103.00   |
| 2   | B2    | 156 | ARG  | NE-CZ-NH1 | -5.36 | 116.14      | 121.50   |
| 3   | C7    | 291 | GLN  | CG-CD-NE2 | -5.36 | 108.36      | 116.40   |
| 3   | D3    | 69  | GLU  | CB-CG-CD  | 5.36  | 121.71      | 112.60   |
| 2   | E2    | 160 | ASP  | CB-CA-C   | 5.36  | 118.49      | 110.08   |
| 3   | B3    | 118 | ASP  | CA-CB-CG  | -5.36 | 107.25      | 112.60   |
| 3   | C7    | 396 | HIS  | CA-C-N    | 5.35  | 127.99      | 120.28   |
| 3   | C7    | 396 | HIS  | C-N-CA    | 5.35  | 127.99      | 120.28   |
| 3   | C3    | 114 | ASP  | CB-CA-C   | -5.35 | 101.76      | 110.85   |
| 3   | A7    | 54  | ALA  | CA-C-N    | 5.34  | 131.75      | 121.54   |
| 3   | A7    | 54  | ALA  | C-N-CA    | 5.34  | 131.75      | 121.54   |
| 2   | B8    | 229 | ARG  | CB-CA-C   | -5.34 | 102.49      | 110.88   |
| 2   | A4    | 145 | THR  | CA-C-N    | 5.34  | 125.91      | 119.98   |
| 2   | A4    | 145 | THR  | C-N-CA    | 5.34  | 125.91      | 119.98   |
| 2   | C4    | 84  | ARG  | CD-NE-CZ  | 5.34  | 131.88      | 124.40   |
| 2   | A8    | 64  | ARG  | NE-CZ-NH2 | 5.34  | 124.00      | 119.20   |
| 3   | A9    | 251 | ARG  | N-CA-CB   | 5.34  | 118.52      | 110.30   |
| 3   | B1    | 204 | ASN  | CB-CG-ND2 | 5.33  | 124.40      | 116.40   |
| 2   | B8    | 22  | GLU  | CB-CG-CD  | 5.33  | 121.67      | 112.60   |
| 2   | A8    | 264 | ARG  | CB-CG-CD  | 5.33  | 123.56      | 111.30   |
| 3   | C9    | 86  | ARG  | CG-CD-NE  | -5.33 | 100.28      | 112.00   |
| 2   | A8    | 72  | PRO  | CB-CA-C   | -5.32 | 103.91      | 111.68   |
| 2   | D2    | 211 | ASP  | CA-CB-CG  | 5.32  | 117.92      | 112.60   |
| 3   | C7    | 213 | ARG  | CG-CD-NE  | -5.32 | 100.31      | 112.00   |
| 2   | D4    | 48  | ALA  | CA-C-N    | -5.32 | 113.77      | 122.54   |
| 2   | D4    | 48  | ALA  | C-N-CA    | -5.32 | 113.77      | 122.54   |
| 3   | A5    | 181 | GLU  | CB-CG-CD  | 5.31  | 121.64      | 112.60   |
| 2   | D8    | 262 | TYR  | CA-C-N    | 5.31  | 124.76      | 119.24   |
| 2   | D8    | 262 | TYR  | C-N-CA    | 5.31  | 124.76      | 119.24   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | A2    | 402 | ARG  | NE-CZ-NH2  | 5.31  | 123.98      | 119.20   |
| 3   | D1    | 362 | LYS  | CG-CD-CE   | 5.31  | 123.51      | 111.30   |
| 2   | C6    | 393 | HIS  | CA-CB-CG   | -5.31 | 108.49      | 113.80   |
| 5   | l     | 78  | LYS  | CG-CD-CE   | 5.30  | 123.50      | 111.30   |
| 2   | D8    | 95  | GLY  | O-C-N      | 5.30  | 128.44      | 122.82   |
| 2   | D2    | 326 | LYS  | CB-CG-CD   | 5.30  | 123.49      | 111.30   |
| 3   | C5    | 251 | ARG  | CG-CD-NE   | 5.30  | 123.66      | 112.00   |
| 3   | A9    | 174 | LYS  | CG-CD-CE   | 5.29  | 123.47      | 111.30   |
| 2   | C2    | 370 | LYS  | CB-CA-C    | 5.29  | 120.29      | 111.83   |
| 2   | A4    | 142 | GLY  | CA-C-N     | 5.29  | 131.77      | 121.41   |
| 2   | A4    | 142 | GLY  | C-N-CA     | 5.29  | 131.77      | 121.41   |
| 3   | D7    | 414 | ASN  | CA-CB-CG   | 5.29  | 117.89      | 112.60   |
| 1   | 8     | 248 | ARG  | CB-CA-C    | -5.29 | 99.26       | 110.31   |
| 2   | E4    | 221 | ARG  | CG-CD-NE   | 5.29  | 123.63      | 112.00   |
| 1   | 12    | 245 | SER  | CA-C-N     | 5.28  | 127.62      | 120.38   |
| 1   | 12    | 245 | SER  | C-N-CA     | 5.28  | 127.62      | 120.38   |
| 2   | A0    | 156 | ARG  | CB-CG-CD   | 5.28  | 123.44      | 111.30   |
| 5   | x     | 158 | ASP  | CA-CB-CG   | 5.28  | 117.88      | 112.60   |
| 2   | A4    | 342 | GLN  | CB-CG-CD   | -5.28 | 103.63      | 112.60   |
| 4   | p     | 97  | ARG  | CB-CG-CD   | 5.27  | 123.42      | 111.30   |
| 3   | F1    | 332 | ASN  | OD1-CG-ND2 | 5.27  | 127.87      | 122.60   |
| 2   | B8    | 391 | MET  | CB-CG-SD   | -5.26 | 96.91       | 112.70   |
| 1   | 19    | 245 | SER  | CA-C-N     | 5.26  | 127.33      | 120.28   |
| 1   | 19    | 245 | SER  | C-N-CA     | 5.26  | 127.33      | 120.28   |
| 2   | A0    | 279 | GLU  | CB-CG-CD   | 5.26  | 121.54      | 112.60   |
| 3   | B7    | 401 | GLU  | CB-CA-C    | 5.26  | 117.91      | 109.07   |
| 3   | D3    | 276 | ARG  | CB-CG-CD   | 5.26  | 123.40      | 111.30   |
| 2   | D4    | 436 | GLY  | N-CA-C     | 5.26  | 120.24      | 114.40   |
| 5   | k     | 26  | PRO  | CA-C-N     | 5.26  | 129.50      | 120.72   |
| 5   | k     | 26  | PRO  | C-N-CA     | 5.26  | 129.50      | 120.72   |
| 3   | D3    | 41  | ASP  | CA-C-N     | 5.26  | 131.58      | 121.54   |
| 3   | D3    | 41  | ASP  | C-N-CA     | 5.26  | 131.58      | 121.54   |
| 3   | D7    | 268 | ILE  | CA-C-N     | 5.26  | 126.45      | 121.46   |
| 3   | D7    | 268 | ILE  | C-N-CA     | 5.26  | 126.45      | 121.46   |
| 3   | E5    | 10  | GLY  | CA-C-N     | 5.25  | 127.27      | 120.44   |
| 3   | E5    | 10  | GLY  | C-N-CA     | 5.25  | 127.27      | 120.44   |
| 2   | C0    | 308 | ARG  | NE-CZ-NH1  | -5.25 | 116.25      | 121.50   |
| 4   | f     | 120 | GLU  | CB-CG-CD   | 5.25  | 121.53      | 112.60   |
| 3   | C1    | 271 | ALA  | O-C-N      | -5.25 | 118.15      | 121.88   |
| 3   | D1    | 129 | CYS  | CB-CA-C    | 5.25  | 119.77      | 110.16   |
| 3   | D5    | 262 | ARG  | NE-CZ-NH1  | -5.25 | 116.25      | 121.50   |
| 1   | 11    | 246 | CYS  | N-CA-CB    | 5.25  | 118.64      | 109.72   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | m     | 202 | ARG  | CA-CB-CG   | 5.24  | 124.58      | 114.10   |
| 4   | g     | 47  | LEU  | CD1-CG-CD2 | -5.24 | 99.28       | 110.80   |
| 2   | D8    | 11  | GLN  | O-C-N      | 5.24  | 127.46      | 122.07   |
| 4   | o     | 151 | MET  | CA-C-N     | 5.23  | 127.72      | 120.29   |
| 4   | o     | 151 | MET  | C-N-CA     | 5.23  | 127.72      | 120.29   |
| 3   | D5    | 251 | ARG  | CG-CD-NE   | 5.23  | 123.50      | 112.00   |
| 2   | C4    | 206 | ASN  | CB-CG-ND2  | 5.22  | 124.23      | 116.40   |
| 3   | A9    | 410 | GLU  | CB-CG-CD   | 5.22  | 121.47      | 112.60   |
| 4   | i     | 146 | ARG  | CD-NE-CZ   | -5.22 | 117.09      | 124.40   |
| 3   | E1    | 125 | GLU  | CA-C-N     | 5.22  | 126.70      | 120.13   |
| 3   | E1    | 125 | GLU  | C-N-CA     | 5.22  | 126.70      | 120.13   |
| 4   | e     | 99  | MET  | CB-CG-SD   | -5.21 | 97.06       | 112.70   |
| 3   | A7    | 252 | LYS  | CB-CG-CD   | 5.21  | 123.28      | 111.30   |
| 2   | C8    | 214 | ARG  | CG-CD-NE   | 5.21  | 123.46      | 112.00   |
| 2   | A4    | 214 | ARG  | CB-CG-CD   | -5.21 | 99.32       | 111.30   |
| 3   | C7    | 379 | LYS  | CB-CG-CD   | 5.21  | 123.27      | 111.30   |
| 3   | F1    | 401 | GLU  | CB-CG-CD   | 5.20  | 121.44      | 112.60   |
| 3   | E9    | 74  | ASP  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 3   | E3    | 347 | ASN  | CB-CA-C    | 5.20  | 120.09      | 112.09   |
| 2   | A0    | 97  | GLU  | CB-CG-CD   | 5.19  | 121.43      | 112.60   |
| 4   | r     | 146 | ARG  | CB-CG-CD   | 5.19  | 123.24      | 111.30   |
| 2   | A8    | 156 | ARG  | CB-CG-CD   | 5.19  | 123.23      | 111.30   |
| 2   | C2    | 336 | LYS  | CB-CG-CD   | 5.19  | 123.23      | 111.30   |
| 2   | F0    | 285 | GLN  | CB-CA-C    | 5.19  | 119.82      | 111.05   |
| 4   | e     | 15  | ARG  | NE-CZ-NH2  | 5.19  | 123.87      | 119.20   |
| 3   | D5    | 47  | ILE  | CA-C-O     | -5.18 | 114.30      | 120.78   |
| 4   | c     | 80  | GLY  | CA-C-N     | 5.18  | 129.38      | 120.72   |
| 4   | c     | 80  | GLY  | C-N-CA     | 5.18  | 129.38      | 120.72   |
| 4   | o     | 84  | LYS  | CB-CG-CD   | 5.18  | 123.22      | 111.30   |
| 2   | A6    | 124 | LYS  | CB-CG-CD   | 5.18  | 123.21      | 111.30   |
| 2   | A8    | 179 | THR  | CA-CB-CG2  | 5.18  | 119.30      | 110.50   |
| 2   | C6    | 156 | ARG  | CB-CG-CD   | 5.17  | 123.20      | 111.30   |
| 4   | d     | 28  | LYS  | CG-CD-CE   | 5.17  | 123.20      | 111.30   |
| 2   | A2    | 221 | ARG  | CD-NE-CZ   | 5.17  | 131.63      | 124.40   |
| 3   | A7    | 162 | ARG  | CB-CG-CD   | 5.17  | 123.18      | 111.30   |
| 3   | E7    | 262 | ARG  | CG-CD-NE   | 5.17  | 123.37      | 112.00   |
| 2   | D2    | 339 | ARG  | CB-CG-CD   | 5.17  | 123.18      | 111.30   |
| 2   | A4    | 222 | PRO  | N-CA-CB    | -5.16 | 98.14       | 103.15   |
| 4   | g     | 16  | ARG  | NE-CZ-NH2  | 5.16  | 123.84      | 119.20   |
| 4   | i     | 7   | ALA  | N-CA-CB    | 5.16  | 119.10      | 110.53   |
| 3   | A1    | 11  | GLN  | CB-CG-CD   | -5.16 | 103.83      | 112.60   |
| 3   | D7    | 122 | LYS  | CB-CG-CD   | 5.15  | 123.15      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | C5    | 174 | LYS  | N-CA-CB    | 5.15  | 117.42      | 110.10   |
| 3   | D5    | 112 | LEU  | N-CA-CB    | -5.15 | 103.63      | 111.15   |
| 2   | D8    | 408 | TYR  | CA-C-O     | -5.15 | 114.52      | 120.24   |
| 4   | i     | 21  | ARG  | CG-CD-NE   | 5.15  | 123.33      | 112.00   |
| 2   | B8    | 142 | GLY  | CA-C-N     | 5.15  | 129.00      | 122.77   |
| 2   | B8    | 142 | GLY  | C-N-CA     | 5.15  | 129.00      | 122.77   |
| 2   | A4    | 116 | ASP  | CB-CA-C    | 5.14  | 120.55      | 110.67   |
| 4   | n     | 24  | MET  | CB-CG-SD   | 5.14  | 128.13      | 112.70   |
| 2   | C0    | 84  | ARG  | CB-CA-C    | -5.14 | 99.89       | 110.38   |
| 2   | D2    | 349 | THR  | N-CA-CB    | 5.14  | 117.51      | 110.57   |
| 4   | a     | 141 | THR  | OG1-CB-CG2 | 5.14  | 119.58      | 109.30   |
| 4   | u     | 52  | GLU  | CB-CG-CD   | 5.14  | 121.34      | 112.60   |
| 2   | A8    | 211 | ASP  | CB-CA-C    | 5.14  | 118.59      | 109.65   |
| 3   | A7    | 282 | ARG  | CD-NE-CZ   | 5.14  | 131.59      | 124.40   |
| 2   | D4    | 79  | ARG  | NE-CZ-NH2  | -5.14 | 114.57      | 119.20   |
| 3   | D1    | 3   | GLU  | N-CA-CB    | 5.14  | 119.77      | 110.83   |
| 4   | q     | 24  | MET  | CB-CG-SD   | -5.14 | 97.29       | 112.70   |
| 2   | B0    | 343 | PHE  | CA-CB-CG   | -5.13 | 108.67      | 113.80   |
| 3   | E1    | 328 | GLU  | CB-CG-CD   | 5.13  | 121.32      | 112.60   |
| 3   | D9    | 276 | ARG  | CD-NE-CZ   | 5.13  | 131.58      | 124.40   |
| 5   | l     | 96  | GLU  | CB-CG-CD   | 5.13  | 121.32      | 112.60   |
| 4   | c     | 154 | TYR  | CB-CA-C    | 5.13  | 120.25      | 112.00   |
| 2   | D8    | 123 | ARG  | NE-CZ-NH1  | 5.12  | 126.62      | 121.50   |
| 2   | C6    | 36  | MET  | CB-CG-SD   | 5.12  | 128.06      | 112.70   |
| 3   | B3    | 47  | ILE  | N-CA-C     | -5.12 | 108.51      | 113.53   |
| 2   | D8    | 264 | ARG  | CB-CA-C    | 5.12  | 120.50      | 110.67   |
| 4   | n     | 19  | GLU  | CB-CG-CD   | 5.12  | 121.30      | 112.60   |
| 3   | B7    | 309 | ARG  | CG-CD-NE   | 5.11  | 123.25      | 112.00   |
| 2   | A4    | 36  | MET  | CG-SD-CE   | -5.11 | 89.66       | 100.90   |
| 2   | C8    | 338 | LYS  | CG-CD-CE   | 5.11  | 123.05      | 111.30   |
| 2   | A4    | 123 | ARG  | NE-CZ-NH1  | -5.11 | 116.39      | 121.50   |
| 2   | C6    | 306 | ASP  | CA-CB-CG   | 5.11  | 117.71      | 112.60   |
| 4   | f     | 2   | SER  | CB-CA-C    | 5.11  | 119.80      | 110.10   |
| 1   | 17    | 244 | GLN  | CA-C-N     | 5.10  | 128.46      | 120.75   |
| 1   | 17    | 244 | GLN  | C-N-CA     | 5.10  | 128.46      | 120.75   |
| 3   | D9    | 160 | PRO  | CB-CA-C    | 5.10  | 120.20      | 112.55   |
| 4   | f     | 99  | MET  | CB-CG-SD   | -5.10 | 97.40       | 112.70   |
| 2   | B0    | 81  | GLY  | CA-C-N     | 5.10  | 127.11      | 120.28   |
| 2   | B0    | 81  | GLY  | C-N-CA     | 5.10  | 127.11      | 120.28   |
| 3   | C9    | 95  | THR  | CA-CB-OG1  | -5.10 | 101.95      | 109.60   |
| 3   | E9    | 279 | GLN  | CB-CG-CD   | 5.10  | 121.27      | 112.60   |
| 3   | D5    | 130 | LEU  | CD1-CG-CD2 | -5.10 | 99.58       | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D8    | 33  | ASP  | CA-CB-CG   | 5.10  | 117.70      | 112.60   |
| 2   | D0    | 47  | ASP  | CB-CA-C    | 5.10  | 119.78      | 110.10   |
| 2   | A4    | 358 | GLN  | CG-CD-NE2  | -5.09 | 108.77      | 116.40   |
| 2   | E2    | 372 | MET  | CB-CG-SD   | 5.09  | 127.96      | 112.70   |
| 5   | x     | 66  | LYS  | N-CA-CB    | 5.09  | 118.69      | 110.85   |
| 3   | D3    | 258 | ILE  | CA-C-O     | 5.08  | 122.15      | 119.15   |
| 4   | q     | 194 | ARG  | CG-CD-NE   | -5.08 | 100.81      | 112.00   |
| 3   | A1    | 391 | ARG  | CG-CD-NE   | -5.08 | 100.82      | 112.00   |
| 2   | C6    | 408 | TYR  | CA-C-N     | 5.08  | 126.96      | 120.56   |
| 2   | C6    | 408 | TYR  | C-N-CA     | 5.08  | 126.96      | 120.56   |
| 2   | D0    | 142 | GLY  | CA-C-N     | 5.08  | 124.80      | 119.92   |
| 2   | D0    | 142 | GLY  | C-N-CA     | 5.08  | 124.80      | 119.92   |
| 4   | c     | 150 | VAL  | CA-CB-CG1  | 5.08  | 119.03      | 110.40   |
| 4   | n     | 128 | HIS  | CA-CB-CG   | 5.08  | 118.88      | 113.80   |
| 2   | C6    | 336 | LYS  | CG-CD-CE   | 5.08  | 122.97      | 111.30   |
| 3   | C9    | 140 | GLY  | CA-C-N     | 5.08  | 127.30      | 122.27   |
| 3   | C9    | 140 | GLY  | C-N-CA     | 5.08  | 127.30      | 122.27   |
| 3   | D3    | 257 | LEU  | CA-C-N     | -5.07 | 118.94      | 122.59   |
| 3   | D3    | 257 | LEU  | C-N-CA     | -5.07 | 118.94      | 122.59   |
| 3   | A5    | 227 | HIS  | ND1-CG-CD2 | 5.07  | 111.17      | 106.10   |
| 2   | A8    | 349 | THR  | N-CA-CB    | 5.07  | 118.51      | 110.55   |
| 3   | D7    | 319 | GLY  | CA-C-N     | 5.07  | 131.22      | 121.54   |
| 3   | D7    | 319 | GLY  | C-N-CA     | 5.07  | 131.22      | 121.54   |
| 4   | s     | 42  | TYR  | CA-C-N     | 5.07  | 125.61      | 119.98   |
| 4   | s     | 42  | TYR  | C-N-CA     | 5.07  | 125.61      | 119.98   |
| 2   | D6    | 50  | ASN  | OD1-CG-ND2 | 5.07  | 127.67      | 122.60   |
| 3   | A3    | 213 | ARG  | CB-CG-CD   | 5.07  | 122.95      | 111.30   |
| 4   | r     | 202 | ARG  | N-CA-CB    | 5.07  | 117.93      | 110.33   |
| 2   | B8    | 36  | MET  | CB-CA-C    | 5.06  | 116.01      | 108.87   |
| 1   | 15    | 241 | PHE  | CB-CA-C    | 5.06  | 118.97      | 109.71   |
| 3   | E5    | 256 | ASN  | CA-CB-CG   | 5.06  | 117.66      | 112.60   |
| 3   | A1    | 390 | ARG  | CG-CD-NE   | 5.05  | 123.12      | 112.00   |
| 3   | E9    | 121 | ARG  | CB-CG-CD   | -5.05 | 99.68       | 111.30   |
| 3   | F1    | 336 | LYS  | CG-CD-CE   | 5.05  | 122.92      | 111.30   |
| 4   | d     | 117 | ARG  | CD-NE-CZ   | 5.05  | 131.47      | 124.40   |
| 2   | A6    | 179 | THR  | CA-CB-CG2  | 5.05  | 119.08      | 110.50   |
| 3   | C7    | 401 | GLU  | CB-CA-C    | 5.05  | 117.16      | 109.34   |
| 2   | D8    | 281 | ALA  | CA-C-N     | -5.05 | 114.58      | 122.65   |
| 2   | D8    | 281 | ALA  | C-N-CA     | -5.05 | 114.58      | 122.65   |
| 4   | d     | 15  | ARG  | NE-CZ-NH2  | 5.05  | 123.74      | 119.20   |
| 4   | r     | 156 | VAL  | N-CA-CB    | 5.04  | 114.77      | 110.08   |
| 4   | n     | 93  | LEU  | CA-C-N     | 5.04  | 127.03      | 120.28   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | n     | 93  | LEU  | C-N-CA   | 5.04  | 127.03      | 120.28   |
| 2   | B2    | 418 | PHE  | CA-CB-CG | 5.04  | 118.84      | 113.80   |
| 3   | E3    | 174 | LYS  | CB-CG-CD | 5.04  | 122.89      | 111.30   |
| 3   | F1    | 249 | ASP  | CA-CB-CG | 5.04  | 117.64      | 112.60   |
| 3   | D5    | 128 | ASP  | CA-C-O   | -5.03 | 115.54      | 120.82   |
| 2   | D6    | 50  | ASN  | CB-CA-C  | -5.03 | 101.02      | 110.67   |
| 5   | x     | 102 | ARG  | CB-CA-C  | 5.03  | 118.85      | 110.90   |
| 3   | A5    | 90  | PHE  | CA-CB-CG | 5.03  | 118.83      | 113.80   |
| 4   | i     | 50  | PHE  | CB-CA-C  | 5.03  | 115.75      | 110.17   |
| 3   | C5    | 291 | GLN  | CB-CG-CD | 5.03  | 121.14      | 112.60   |
| 5   | x     | 65  | GLU  | CB-CG-CD | 5.02  | 121.14      | 112.60   |
| 2   | C4    | 255 | PHE  | CB-CA-C  | 5.02  | 118.03      | 109.24   |
| 3   | B1    | 401 | GLU  | CB-CG-CD | 5.01  | 121.12      | 112.60   |
| 2   | A6    | 264 | ARG  | CG-CD-NE | 5.01  | 123.02      | 112.00   |
| 4   | i     | 130 | PRO  | N-CA-C   | 5.01  | 120.12      | 113.86   |
| 4   | n     | 94  | ASN  | CA-CB-CG | 5.00  | 117.61      | 112.60   |
| 4   | r     | 91  | PHE  | CB-CA-C  | -5.00 | 102.34      | 110.85   |
| 3   | B9    | 86  | ARG  | CG-CD-NE | 5.00  | 123.01      | 112.00   |
| 4   | r     | 117 | ARG  | CD-NE-CZ | 5.00  | 131.41      | 124.40   |
| 2   | C4    | 275 | ILE  | N-CA-CB  | -5.00 | 107.65      | 112.65   |

There are no chirality outliers.

All (35) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 13    | 255 | PRO  | Peptide |
| 1   | 15    | 237 | PRO  | Peptide |
| 1   | 15    | 240 | PRO  | Peptide |
| 1   | 18    | 242 | ASN  | Peptide |
| 1   | 23    | 239 | LEU  | Peptide |
| 1   | 23    | 255 | PRO  | Peptide |
| 1   | 4     | 240 | PRO  | Peptide |
| 1   | 7     | 237 | PRO  | Peptide |
| 2   | A0    | 401 | LYS  | Peptide |
| 2   | A2    | 284 | GLU  | Peptide |
| 2   | A2    | 401 | LYS  | Peptide |
| 2   | A4    | 254 | GLU  | Peptide |
| 2   | A4    | 401 | LYS  | Peptide |
| 2   | A8    | 107 | HIS  | Peptide |
| 2   | A8    | 284 | GLU  | Peptide |
| 2   | A8    | 401 | LYS  | Peptide |
| 2   | B0    | 401 | LYS  | Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | B3    | 43  | GLN  | Peptide   |
| 2   | B4    | 284 | GLU  | Peptide   |
| 2   | B6    | 338 | LYS  | Peptide   |
| 3   | B9    | 200 | GLN  | Peptide   |
| 2   | C4    | 401 | LYS  | Peptide   |
| 2   | C8    | 284 | GLU  | Peptide   |
| 2   | D0    | 36  | MET  | Peptide   |
| 2   | D0    | 401 | LYS  | Peptide   |
| 2   | D2    | 284 | GLU  | Peptide   |
| 2   | E2    | 162 | GLY  | Peptide   |
| 3   | E5    | 321 | MET  | Peptide   |
| 3   | E5    | 322 | SER  | Peptide   |
| 4   | c     | 161 | TYR  | Peptide   |
| 4   | e     | 35  | ASN  | Peptide   |
| 5   | k     | 13  | VAL  | Peptide   |
| 5   | l     | 13  | VAL  | Peptide   |
| 4   | o     | 91  | PHE  | Sidechain |
| 4   | t     | 35  | ASN  | Peptide   |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 174   | 0        | 171      | 25      | 0            |
| 1   | 1     | 174   | 0        | 171      | 6       | 0            |
| 1   | 10    | 174   | 0        | 171      | 29      | 0            |
| 1   | 11    | 174   | 0        | 171      | 28      | 0            |
| 1   | 12    | 174   | 0        | 171      | 9       | 0            |
| 1   | 13    | 174   | 0        | 171      | 16      | 0            |
| 1   | 14    | 174   | 0        | 171      | 8       | 0            |
| 1   | 15    | 174   | 0        | 171      | 20      | 0            |
| 1   | 16    | 174   | 0        | 171      | 18      | 0            |
| 1   | 17    | 174   | 0        | 171      | 12      | 0            |
| 1   | 18    | 174   | 0        | 171      | 8       | 0            |
| 1   | 19    | 174   | 0        | 171      | 24      | 0            |
| 1   | 2     | 174   | 0        | 171      | 29      | 0            |
| 1   | 20    | 174   | 0        | 171      | 13      | 0            |
| 1   | 21    | 174   | 0        | 171      | 20      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 22    | 160   | 0        | 156      | 8       | 0            |
| 1   | 23    | 160   | 0        | 156      | 11      | 0            |
| 1   | 3     | 174   | 0        | 171      | 8       | 0            |
| 1   | 4     | 174   | 0        | 171      | 28      | 0            |
| 1   | 5     | 174   | 0        | 171      | 23      | 0            |
| 1   | 6     | 174   | 0        | 171      | 22      | 0            |
| 1   | 7     | 174   | 0        | 171      | 23      | 0            |
| 1   | 8     | 174   | 0        | 171      | 32      | 0            |
| 1   | 9     | 174   | 0        | 171      | 33      | 0            |
| 2   | A0    | 3325  | 0        | 3252     | 99      | 0            |
| 2   | A2    | 3325  | 0        | 3252     | 80      | 0            |
| 2   | A4    | 3325  | 0        | 3252     | 86      | 0            |
| 2   | A6    | 3325  | 0        | 3252     | 100     | 0            |
| 2   | A8    | 3325  | 0        | 3252     | 92      | 0            |
| 2   | B0    | 3325  | 0        | 3252     | 85      | 0            |
| 2   | B2    | 3325  | 0        | 3252     | 77      | 0            |
| 2   | B4    | 3325  | 0        | 3252     | 89      | 0            |
| 2   | B6    | 3325  | 0        | 3252     | 76      | 0            |
| 2   | B8    | 3325  | 0        | 3252     | 98      | 0            |
| 2   | C0    | 3325  | 0        | 3252     | 87      | 0            |
| 2   | C2    | 3325  | 0        | 3252     | 108     | 0            |
| 2   | C4    | 3325  | 0        | 3252     | 107     | 0            |
| 2   | C6    | 3325  | 0        | 3252     | 125     | 0            |
| 2   | C8    | 3325  | 0        | 3252     | 91      | 0            |
| 2   | D0    | 3325  | 0        | 3252     | 114     | 0            |
| 2   | D2    | 3325  | 0        | 3252     | 88      | 0            |
| 2   | D4    | 3325  | 0        | 3252     | 126     | 0            |
| 2   | D6    | 3325  | 0        | 3252     | 66      | 0            |
| 2   | D8    | 3325  | 0        | 3252     | 107     | 0            |
| 2   | E0    | 3325  | 0        | 3252     | 81      | 0            |
| 2   | E2    | 3325  | 0        | 3252     | 64      | 0            |
| 2   | E4    | 3325  | 0        | 3252     | 72      | 0            |
| 2   | E6    | 3325  | 0        | 3252     | 95      | 0            |
| 2   | E8    | 3325  | 0        | 3252     | 78      | 0            |
| 2   | F0    | 3325  | 0        | 3252     | 101     | 0            |
| 3   | A1    | 3331  | 0        | 3207     | 99      | 0            |
| 3   | A3    | 3331  | 0        | 3209     | 58      | 0            |
| 3   | A5    | 3331  | 0        | 3207     | 103     | 0            |
| 3   | A7    | 3331  | 0        | 3207     | 71      | 0            |
| 3   | A9    | 3331  | 0        | 3207     | 88      | 0            |
| 3   | B1    | 3331  | 0        | 3209     | 75      | 0            |
| 3   | B3    | 3331  | 0        | 3207     | 89      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B5    | 3331  | 0        | 3207     | 73      | 0            |
| 3   | B7    | 3331  | 0        | 3209     | 66      | 0            |
| 3   | B9    | 3331  | 0        | 3209     | 66      | 0            |
| 3   | C1    | 3331  | 0        | 3209     | 115     | 0            |
| 3   | C3    | 3331  | 0        | 3209     | 99      | 0            |
| 3   | C5    | 3331  | 0        | 3209     | 86      | 0            |
| 3   | C7    | 3331  | 0        | 3209     | 96      | 0            |
| 3   | C9    | 3331  | 0        | 3209     | 110     | 0            |
| 3   | D1    | 3331  | 0        | 3209     | 89      | 0            |
| 3   | D3    | 3331  | 0        | 3207     | 111     | 0            |
| 3   | D5    | 3331  | 0        | 3207     | 121     | 0            |
| 3   | D7    | 3331  | 0        | 3207     | 91      | 0            |
| 3   | D9    | 3331  | 0        | 3207     | 84      | 0            |
| 3   | E1    | 3331  | 0        | 3207     | 80      | 0            |
| 3   | E3    | 3331  | 0        | 3209     | 65      | 0            |
| 3   | E5    | 3331  | 0        | 3207     | 80      | 0            |
| 3   | E7    | 3331  | 0        | 3207     | 97      | 0            |
| 3   | E9    | 3331  | 0        | 3207     | 84      | 0            |
| 3   | F1    | 3331  | 0        | 3207     | 96      | 0            |
| 4   | a     | 1198  | 0        | 1194     | 46      | 0            |
| 4   | b     | 1198  | 0        | 1194     | 48      | 0            |
| 4   | c     | 1608  | 0        | 1590     | 59      | 0            |
| 4   | d     | 1608  | 0        | 1590     | 66      | 0            |
| 4   | e     | 1608  | 0        | 1590     | 75      | 0            |
| 4   | f     | 1608  | 0        | 1590     | 77      | 0            |
| 4   | g     | 1608  | 0        | 1590     | 65      | 0            |
| 4   | h     | 1608  | 0        | 1590     | 54      | 0            |
| 4   | i     | 1608  | 0        | 1590     | 32      | 0            |
| 4   | j     | 1608  | 0        | 1590     | 41      | 0            |
| 4   | m     | 1608  | 0        | 1590     | 59      | 0            |
| 4   | n     | 1608  | 0        | 1590     | 62      | 0            |
| 4   | o     | 1608  | 0        | 1590     | 41      | 0            |
| 4   | p     | 1608  | 0        | 1590     | 44      | 0            |
| 4   | q     | 1608  | 0        | 1590     | 33      | 0            |
| 4   | r     | 1608  | 0        | 1590     | 50      | 0            |
| 4   | s     | 1608  | 0        | 1590     | 36      | 0            |
| 4   | t     | 1608  | 0        | 1590     | 68      | 0            |
| 4   | u     | 1608  | 0        | 1590     | 30      | 0            |
| 4   | v     | 1608  | 0        | 1588     | 58      | 0            |
| 5   | k     | 1140  | 0        | 1143     | 50      | 0            |
| 5   | l     | 1140  | 0        | 1143     | 39      | 0            |
| 5   | w     | 1172  | 0        | 1171     | 35      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 5   | x     | 1172   | 0        | 1171     | 33      | 0            |
| All | All   | 213168 | 0        | 207664   | 4846    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (4846) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:19:241:PHE:CZ  | 3:E7:356:ILE:HG23 | 1.28                     | 1.68              |
| 4:v:202:ARG:CD   | 4:v:202:ARG:NE    | 1.67                     | 1.56              |
| 2:C4:2:ARG:CG    | 2:C4:2:ARG:CD     | 1.76                     | 1.56              |
| 3:A9:252:LYS:CG  | 3:A9:252:LYS:CD   | 1.84                     | 1.55              |
| 1:19:241:PHE:HZ  | 3:E7:356:ILE:CG2  | 1.03                     | 1.54              |
| 2:C4:2:ARG:CD    | 2:C4:2:ARG:NE     | 1.70                     | 1.54              |
| 2:A4:254:GLU:CG  | 2:A4:254:GLU:CD   | 1.76                     | 1.54              |
| 3:A5:252:LYS:NZ  | 3:A5:252:LYS:CE   | 1.71                     | 1.54              |
| 3:A5:252:LYS:CE  | 3:A5:252:LYS:CD   | 1.78                     | 1.52              |
| 1:19:241:PHE:CZ  | 3:E7:356:ILE:CG2  | 1.81                     | 1.48              |
| 1:6:256:LEU:HD11 | 2:B6:31:GLN:CG    | 1.44                     | 1.44              |
| 3:A1:219:THR:HA  | 2:A2:326:LYS:NZ   | 1.24                     | 1.43              |
| 2:C0:84:ARG:NH2  | 4:i:197:LEU:HD11  | 1.33                     | 1.42              |
| 4:b:97:ARG:NH1   | 4:d:6:PHE:HB3     | 1.07                     | 1.36              |
| 4:f:105:ASN:ND2  | 4:h:37:GLN:HE22   | 1.22                     | 1.32              |
| 1:8:243:ALA:HB2  | 3:C1:357:PRO:CD   | 1.60                     | 1.31              |
| 2:B4:283:HIS:O   | 2:B8:56:THR:CB    | 1.78                     | 1.31              |
| 2:C6:407:TRP:CZ3 | 3:C7:255:VAL:HA   | 1.63                     | 1.30              |
| 1:8:243:ALA:CB   | 3:C1:357:PRO:HD2  | 1.59                     | 1.29              |
| 2:C6:218:ASP:O   | 4:n:194:ARG:NH2   | 1.66                     | 1.28              |
| 4:u:59:ASN:ND2   | 5:w:100:CYS:HB2   | 1.47                     | 1.28              |
| 3:C5:39:ASP:OD1  | 5:k:51:PRO:HG3    | 1.35                     | 1.27              |
| 3:F1:39:ASP:OD1  | 5:x:51:PRO:HG3    | 1.19                     | 1.24              |
| 1:0:244:GLN:NE2  | 4:c:162:GLY:HA3   | 1.51                     | 1.24              |
| 2:C0:84:ARG:HH22 | 4:i:197:LEU:CD1   | 1.49                     | 1.24              |
| 4:b:97:ARG:NH1   | 4:d:6:PHE:CB      | 2.01                     | 1.23              |
| 1:19:243:ALA:CB  | 3:E7:357:PRO:HD2  | 1.71                     | 1.21              |
| 1:6:256:LEU:CD1  | 2:B6:31:GLN:HG2   | 1.70                     | 1.20              |
| 1:7:256:LEU:HD21 | 2:B8:31:GLN:HA    | 1.21                     | 1.19              |
| 1:19:243:ALA:HB2 | 3:E7:357:PRO:CD   | 1.72                     | 1.18              |
| 1:8:241:PHE:HE1  | 3:C1:356:ILE:CG2  | 1.56                     | 1.16              |
| 2:C6:407:TRP:CH2 | 3:C7:254:ALA:O    | 1.98                     | 1.16              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D0:279:GLU:OE2  | 4:p:197:LEU:O     | 1.62                     | 1.16              |
| 2:E0:71:GLU:OE2   | 3:E1:2:ARG:NH2    | 1.77                     | 1.16              |
| 3:B3:57:GLY:HA3   | 4:e:83:PRO:HB2    | 1.17                     | 1.16              |
| 5:k:27:ASP:OD2    | 4:m:23:LEU:CD2    | 1.93                     | 1.15              |
| 1:19:257:PRO:CG   | 2:E6:26:LEU:O     | 1.95                     | 1.15              |
| 1:19:257:PRO:HG2  | 2:E6:26:LEU:O     | 0.99                     | 1.14              |
| 2:E6:364:PRO:HB3  | 5:x:161:PHE:HE2   | 1.11                     | 1.14              |
| 1:15:256:LEU:HD11 | 2:D8:31:GLN:CA    | 1.77                     | 1.14              |
| 4:t:101:GLU:OE2   | 4:v:6:PHE:HB2     | 1.45                     | 1.14              |
| 2:A6:85:HIS:NE2   | 4:b:99:MET:HE1    | 1.61                     | 1.14              |
| 1:8:241:PHE:CE1   | 3:C1:356:ILE:HG23 | 1.83                     | 1.13              |
| 5:k:27:ASP:OD2    | 4:m:23:LEU:HD22   | 1.46                     | 1.13              |
| 1:19:241:PHE:CZ   | 3:E7:356:ILE:HG21 | 1.69                     | 1.12              |
| 5:k:27:ASP:CG     | 4:m:23:LEU:HD21   | 1.75                     | 1.11              |
| 1:8:241:PHE:CE1   | 3:C1:356:ILE:CG2  | 2.32                     | 1.11              |
| 2:A4:285:GLN:HB2  | 2:A8:57:GLY:H     | 1.00                     | 1.11              |
| 1:9:257:PRO:HG3   | 2:C2:26:LEU:HD12  | 1.25                     | 1.10              |
| 3:A1:219:THR:CA   | 2:A2:326:LYS:NZ   | 2.14                     | 1.10              |
| 1:6:256:LEU:HD11  | 2:B6:31:GLN:HG3   | 1.27                     | 1.10              |
| 2:C6:407:TRP:HZ3  | 3:C7:255:VAL:CA   | 1.64                     | 1.10              |
| 2:A2:282:TYR:O    | 2:A6:60:LYS:NZ    | 1.85                     | 1.10              |
| 2:C2:73:THR:OG1   | 3:C3:46:ARG:NH1   | 1.84                     | 1.09              |
| 1:0:243:ALA:HB1   | 3:A5:320:ARG:HD2  | 1.31                     | 1.09              |
| 1:9:243:ALA:HB2   | 3:C3:357:PRO:HD2  | 1.12                     | 1.09              |
| 2:A4:285:GLN:HB2  | 2:A8:57:GLY:N     | 1.68                     | 1.09              |
| 4:f:105:ASN:ND2   | 4:h:37:GLN:NE2    | 2.00                     | 1.09              |
| 3:C7:281:TYR:CD2  | 3:D1:87:PRO:HD3   | 1.86                     | 1.09              |
| 1:19:256:LEU:HD22 | 2:E6:31:GLN:HG2   | 1.16                     | 1.08              |
| 2:D8:285:GLN:HB2  | 2:E2:56:THR:HA    | 1.33                     | 1.08              |
| 2:E4:96:LYS:HD2   | 3:E5:1:MET:HA     | 1.12                     | 1.08              |
| 1:8:257:PRO:HG2   | 2:C0:29:GLY:HA2   | 1.19                     | 1.08              |
| 1:8:241:PHE:HE1   | 3:C1:356:ILE:HG23 | 1.06                     | 1.07              |
| 1:15:256:LEU:HD11 | 2:D8:31:GLN:HA    | 1.23                     | 1.07              |
| 2:D8:84:ARG:NH2   | 4:r:197:LEU:HD22  | 1.69                     | 1.07              |
| 4:d:71:LYS:HG3    | 4:f:39:PRO:HD3    | 1.37                     | 1.06              |
| 1:4:240:PRO:HB2   | 4:g:154:TYR:CD2   | 1.90                     | 1.06              |
| 1:6:256:LEU:CD1   | 2:B6:31:GLN:CG    | 2.29                     | 1.06              |
| 3:B5:57:GLY:HA3   | 4:f:83:PRO:HB2    | 1.37                     | 1.06              |
| 3:C7:281:TYR:HD2  | 3:D1:87:PRO:HD3   | 1.07                     | 1.05              |
| 1:2:240:PRO:CB    | 4:e:154:TYR:HB3   | 1.86                     | 1.05              |
| 1:19:241:PHE:CE1  | 3:E7:356:ILE:CG2  | 2.39                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:8:241:PHE:HZ    | 3:C1:356:ILE:HD12 | 1.19                     | 1.05              |
| 4:t:101:GLU:OE2   | 4:v:6:PHE:CB      | 2.03                     | 1.05              |
| 2:D0:285:GLN:HB3  | 2:D4:56:THR:HA    | 1.38                     | 1.05              |
| 1:9:241:PHE:HE1   | 3:C3:356:ILE:CG2  | 1.70                     | 1.05              |
| 3:B9:283:ALA:HA   | 3:C3:55:THR:HG23  | 1.36                     | 1.05              |
| 3:C9:220:PRO:HD2  | 2:D0:326:LYS:HG3  | 1.08                     | 1.05              |
| 1:4:247:TYR:HB3   | 2:B2:77:GLU:OE2   | 1.57                     | 1.04              |
| 1:9:257:PRO:HG3   | 2:C2:26:LEU:CD1   | 1.86                     | 1.04              |
| 3:C9:220:PRO:HD2  | 2:D0:326:LYS:CG   | 1.87                     | 1.04              |
| 2:D0:84:ARG:NH2   | 4:n:94:ASN:HD21   | 1.55                     | 1.04              |
| 1:6:256:LEU:HD11  | 2:B6:31:GLN:HG2   | 1.09                     | 1.04              |
| 2:C0:282:TYR:CD2  | 5:k:160:ARG:HD3   | 1.92                     | 1.04              |
| 3:A7:282:ARG:O    | 3:B1:55:THR:HG22  | 1.58                     | 1.04              |
| 2:B6:73:THR:HG22  | 3:B7:46:ARG:HE    | 1.17                     | 1.03              |
| 4:d:71:LYS:HD3    | 4:f:39:PRO:HG3    | 1.39                     | 1.03              |
| 2:C4:218:ASP:CG   | 4:m:194:ARG:HH22  | 1.65                     | 1.03              |
| 2:E0:176:GLN:OE1  | 3:E1:331:LEU:HD21 | 1.59                     | 1.03              |
| 2:E6:280:LYS:HZ3  | 2:F0:89:PRO:HB2   | 1.21                     | 1.02              |
| 2:F0:223:THR:HG23 | 2:F0:225:THR:HG22 | 1.39                     | 1.02              |
| 3:A9:39:ASP:HA    | 4:c:90:PRO:HG3    | 1.41                     | 1.02              |
| 4:u:59:ASN:ND2    | 5:w:100:CYS:CB    | 2.21                     | 1.02              |
| 1:11:244:GLN:H    | 3:D1:320:ARG:NH2  | 1.57                     | 1.01              |
| 1:4:247:TYR:CE1   | 2:B2:81:GLY:HA3   | 1.93                     | 1.01              |
| 1:14:256:LEU:HD11 | 2:D6:31:GLN:HE21  | 1.25                     | 1.01              |
| 1:6:256:LEU:HD21  | 2:B6:31:GLN:HA    | 1.38                     | 1.01              |
| 1:9:241:PHE:CE1   | 3:C3:356:ILE:CG2  | 2.43                     | 1.01              |
| 3:A1:219:THR:CA   | 2:A2:326:LYS:HZ2  | 1.69                     | 1.01              |
| 1:2:240:PRO:CG    | 4:e:154:TYR:HB3   | 1.90                     | 1.00              |
| 2:A0:282:TYR:HA   | 4:a:202:ARG:HH21  | 1.25                     | 1.00              |
| 2:D8:84:ARG:NH2   | 4:r:197:LEU:CD2   | 2.24                     | 1.00              |
| 1:13:244:GLN:CG   | 4:r:162:GLY:HA3   | 1.92                     | 1.00              |
| 2:D2:85:HIS:NE2   | 4:o:99:MET:SD     | 2.35                     | 0.99              |
| 2:A2:282:TYR:O    | 2:A6:60:LYS:CE    | 2.10                     | 0.99              |
| 3:C1:281:TYR:O    | 3:C5:54:ALA:HB1   | 1.62                     | 0.99              |
| 4:t:71:LYS:HE3    | 4:t:106:GLN:HG2   | 1.43                     | 0.99              |
| 3:B5:57:GLY:HA3   | 4:f:83:PRO:CB     | 1.93                     | 0.99              |
| 1:19:243:ALA:CB   | 3:E7:356:ILE:HA   | 1.93                     | 0.99              |
| 1:9:243:ALA:HB3   | 3:C3:356:ILE:HG23 | 1.40                     | 0.98              |
| 1:19:241:PHE:CE1  | 3:E7:356:ILE:HG23 | 1.98                     | 0.98              |
| 2:A4:210:TYR:HB3  | 3:A5:324:LYS:HE3  | 1.46                     | 0.98              |
| 2:D4:210:TYR:HB3  | 3:D5:324:LYS:HE2  | 1.46                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E6:364:PRO:HB3  | 5:x:161:PHE:CE2   | 1.97                     | 0.98              |
| 2:C2:84:ARG:NH2   | 4:j:197:LEU:HD11  | 1.78                     | 0.97              |
| 2:D4:97:GLU:HB2   | 2:D4:110:ILE:HD11 | 1.45                     | 0.97              |
| 4:b:97:ARG:HH22   | 4:d:7:ALA:HB2     | 1.29                     | 0.97              |
| 1:23:240:PRO:HB3  | 4:m:154:TYR:HB3   | 1.41                     | 0.97              |
| 1:19:243:ALA:HB1  | 3:E7:355:ASP:O    | 1.64                     | 0.97              |
| 2:A6:33:ASP:OD2   | 4:b:103:GLY:HA2   | 1.64                     | 0.97              |
| 3:A1:281:TYR:HD2  | 3:A5:87:PRO:HD3   | 1.27                     | 0.96              |
| 3:C9:220:PRO:CD   | 2:D0:326:LYS:HG3  | 1.94                     | 0.96              |
| 1:9:241:PHE:CE1   | 3:C3:356:ILE:HG23 | 1.99                     | 0.96              |
| 2:C6:407:TRP:HH2  | 3:C7:254:ALA:O    | 1.34                     | 0.96              |
| 1:19:256:LEU:HD22 | 2:E6:31:GLN:CG    | 1.95                     | 0.96              |
| 4:a:96:TYR:HH     | 4:c:6:PHE:HE2     | 1.01                     | 0.96              |
| 5:k:25:ARG:HG3    | 4:m:23:LEU:CD1    | 1.95                     | 0.96              |
| 1:8:241:PHE:CZ    | 3:C1:356:ILE:HD12 | 2.01                     | 0.96              |
| 1:21:256:LEU:HD21 | 2:F0:31:GLN:HG2   | 1.44                     | 0.96              |
| 5:k:27:ASP:CB     | 4:m:23:LEU:HD21   | 1.95                     | 0.96              |
| 3:D1:57:GLY:HA3   | 4:n:83:PRO:HB2    | 1.48                     | 0.95              |
| 3:F1:39:ASP:OD1   | 5:x:51:PRO:CG     | 2.13                     | 0.95              |
| 1:10:257:PRO:CG   | 2:C8:26:LEU:O     | 2.15                     | 0.95              |
| 3:D1:284:LEU:HB3  | 3:D5:55:THR:HG21  | 1.46                     | 0.95              |
| 3:D3:91:VAL:HG21  | 3:D3:116:VAL:HG22 | 1.48                     | 0.95              |
| 4:b:97:ARG:NH2    | 4:d:7:ALA:HB2     | 1.82                     | 0.94              |
| 1:8:257:PRO:CG    | 2:C0:29:GLY:HA2   | 1.96                     | 0.94              |
| 3:C7:281:TYR:HB3  | 3:D1:86:ARG:HD3   | 1.48                     | 0.94              |
| 2:C6:407:TRP:CZ3  | 3:C7:255:VAL:CA   | 2.45                     | 0.94              |
| 3:C9:220:PRO:HG2  | 2:D0:326:LYS:HZ2  | 1.30                     | 0.94              |
| 2:C2:84:ARG:HH22  | 4:j:197:LEU:HD11  | 1.29                     | 0.94              |
| 1:4:240:PRO:HB2   | 4:g:154:TYR:HD2   | 1.22                     | 0.94              |
| 2:B0:285:GLN:CD   | 2:B4:55:GLU:O     | 2.10                     | 0.94              |
| 3:C9:208:TYR:CD1  | 2:D0:326:LYS:HE2  | 2.03                     | 0.94              |
| 4:e:9:PRO:HB2     | 4:e:143:ILE:HG23  | 1.47                     | 0.94              |
| 1:10:241:PHE:CZ   | 3:C9:356:ILE:HG23 | 2.03                     | 0.94              |
| 3:B5:282:ARG:O    | 3:B9:55:THR:HG22  | 1.66                     | 0.93              |
| 2:C6:168:ASN:HD21 | 2:C6:194:LEU:HD11 | 1.31                     | 0.93              |
| 1:9:243:ALA:CB    | 3:C3:357:PRO:HD2  | 1.99                     | 0.93              |
| 2:D6:96:LYS:HE2   | 3:D7:129:CYS:SG   | 2.09                     | 0.93              |
| 3:D7:406:MET:HE2  | 3:D7:406:MET:HA   | 1.48                     | 0.93              |
| 3:C3:259:PRO:HG2  | 3:C3:311:LEU:HD21 | 1.50                     | 0.93              |
| 3:F1:267:LEU:HD21 | 3:F1:374:ILE:HD11 | 1.49                     | 0.93              |
| 1:16:247:TYR:HE2  | 2:E0:81:GLY:HA3   | 1.32                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D3:396:HIS:HE1  | 2:D4:261:PRO:O    | 1.52                     | 0.92              |
| 3:A7:321:MET:HE2  | 3:A7:326:VAL:HG22 | 1.49                     | 0.92              |
| 1:13:247:TYR:OH   | 2:D4:18:ASN:ND2   | 2.03                     | 0.92              |
| 1:9:243:ALA:HB2   | 3:C3:357:PRO:CD   | 1.98                     | 0.92              |
| 1:0:241:PHE:HZ    | 3:A5:356:ILE:HD12 | 1.32                     | 0.92              |
| 2:C8:292:THR:HG21 | 2:C8:331:ALA:HB1  | 1.51                     | 0.92              |
| 2:A4:210:TYR:HB3  | 3:A5:324:LYS:CE   | 2.00                     | 0.91              |
| 1:8:243:ALA:CB    | 3:C1:357:PRO:CD   | 2.34                     | 0.91              |
| 3:A1:219:THR:CG2  | 2:A2:324:VAL:HG21 | 2.00                     | 0.91              |
| 3:A1:218:THR:O    | 2:A2:326:LYS:HE3  | 1.68                     | 0.91              |
| 2:F0:407:TRP:CZ2  | 3:F1:258:ILE:HD11 | 2.06                     | 0.91              |
| 1:7:256:LEU:HD21  | 2:B8:31:GLN:CA    | 2.01                     | 0.91              |
| 2:D4:210:TYR:CE2  | 3:D5:327:ASP:OD2  | 2.24                     | 0.91              |
| 4:u:59:ASN:CG     | 5:w:100:CYS:HB2   | 1.93                     | 0.91              |
| 1:10:254:LYS:NZ   | 2:C8:22:GLU:HG2   | 1.86                     | 0.91              |
| 2:B0:73:THR:HA    | 3:B1:46:ARG:HH11  | 1.35                     | 0.91              |
| 2:E4:119:LEU:HD12 | 2:E4:156:ARG:HD3  | 1.53                     | 0.91              |
| 2:A6:222:PRO:HD2  | 3:A7:324:LYS:HB2  | 1.51                     | 0.90              |
| 1:9:243:ALA:HB1   | 3:C3:356:ILE:HA   | 1.53                     | 0.90              |
| 2:A8:285:GLN:HB2  | 2:B2:56:THR:HA    | 1.52                     | 0.90              |
| 3:B3:57:GLY:CA    | 4:e:83:PRO:HB2    | 2.02                     | 0.90              |
| 1:0:244:GLN:HB3   | 3:A5:320:ARG:HH21 | 1.37                     | 0.90              |
| 1:10:242:ASN:HD21 | 4:o:154:TYR:HB2   | 1.35                     | 0.90              |
| 2:E6:280:LYS:NZ   | 2:F0:89:PRO:HB2   | 1.87                     | 0.90              |
| 2:C6:176:GLN:OE1  | 3:C7:331:LEU:HD11 | 1.72                     | 0.89              |
| 1:4:240:PRO:CB    | 4:g:154:TYR:HB3   | 2.02                     | 0.89              |
| 3:C9:220:PRO:HG2  | 2:D0:326:LYS:NZ   | 1.86                     | 0.89              |
| 2:D0:84:ARG:HH21  | 4:n:94:ASN:HD21   | 1.19                     | 0.89              |
| 2:A4:79:ARG:HB3   | 2:A4:92:LEU:HD13  | 1.55                     | 0.89              |
| 3:C9:208:TYR:HD1  | 2:D0:326:LYS:HE2  | 1.36                     | 0.89              |
| 3:A1:219:THR:HA   | 2:A2:326:LYS:HZ1  | 1.31                     | 0.89              |
| 3:C1:117:LEU:HD13 | 3:C1:154:LYS:HG2  | 1.54                     | 0.89              |
| 2:C8:178:SER:HB2  | 3:C9:347:ASN:ND2  | 1.88                     | 0.89              |
| 2:C4:279:GLU:OE1  | 4:m:198:ARG:HA    | 1.72                     | 0.89              |
| 2:C6:282:TYR:HH   | 4:n:201:TRP:HH2   | 0.93                     | 0.89              |
| 2:C6:407:TRP:HZ3  | 3:C7:255:VAL:HA   | 1.09                     | 0.89              |
| 3:A1:219:THR:CB   | 2:A2:326:LYS:HZ1  | 1.85                     | 0.89              |
| 2:B0:100:ALA:HA   | 3:B1:252:LYS:HZ3  | 1.38                     | 0.89              |
| 2:E0:163:LYS:HE2  | 2:E0:163:LYS:HA   | 1.53                     | 0.89              |
| 3:E9:212:PHE:HE1  | 2:F0:326:LYS:HZ2  | 1.21                     | 0.88              |
| 1:20:256:LEU:HD11 | 2:E8:31:GLN:HG3   | 1.55                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:8:241:PHE:CE1   | 3:C1:356:ILE:HG21 | 2.09                     | 0.88              |
| 1:13:244:GLN:HG3  | 4:r:162:GLY:HA3   | 1.55                     | 0.88              |
| 2:D4:285:GLN:HG2  | 2:D8:55:GLU:O     | 1.71                     | 0.88              |
| 1:4:240:PRO:HB2   | 4:g:154:TYR:HB3   | 1.56                     | 0.88              |
| 3:C7:281:TYR:HD2  | 3:D1:87:PRO:CD    | 1.86                     | 0.88              |
| 2:A2:221:ARG:NE   | 3:A3:325:GLU:OE1  | 2.07                     | 0.88              |
| 4:f:105:ASN:HD21  | 4:h:37:GLN:HE22   | 0.93                     | 0.88              |
| 2:B4:285:GLN:CD   | 2:B8:55:GLU:O     | 2.17                     | 0.87              |
| 3:A9:220:PRO:HG2  | 2:B0:326:LYS:HE2  | 1.54                     | 0.87              |
| 1:0:244:GLN:HB3   | 3:A5:320:ARG:NH2  | 1.89                     | 0.87              |
| 1:18:243:ALA:HB2  | 3:E5:357:PRO:HD2  | 1.57                     | 0.87              |
| 1:5:255:PRO:HD3   | 4:h:3:GLN:NE2     | 1.89                     | 0.87              |
| 1:23:240:PRO:CB   | 4:m:154:TYR:HB3   | 2.03                     | 0.87              |
| 1:4:245:SER:HB2   | 3:B3:42:LEU:HD11  | 1.56                     | 0.87              |
| 2:A0:281:ALA:C    | 4:a:202:ARG:HH22  | 1.81                     | 0.87              |
| 3:B7:281:TYR:CE2  | 3:C1:87:PRO:HD3   | 2.09                     | 0.87              |
| 3:E9:219:THR:HB   | 2:F0:324:VAL:HG21 | 1.54                     | 0.87              |
| 2:A0:281:ALA:C    | 4:a:202:ARG:NH2   | 2.32                     | 0.87              |
| 2:A0:282:TYR:N    | 4:a:202:ARG:NH2   | 2.21                     | 0.87              |
| 1:2:257:PRO:HD3   | 2:A8:26:LEU:CD1   | 2.04                     | 0.86              |
| 2:C4:12:ALA:HB3   | 2:C4:140:ALA:HB2  | 1.56                     | 0.86              |
| 2:C8:178:SER:HB2  | 3:C9:347:ASN:HD21 | 1.38                     | 0.86              |
| 2:D4:218:ASP:OD1  | 4:r:198:ARG:NH1   | 2.09                     | 0.86              |
| 2:C8:282:TYR:HE1  | 4:o:201:TRP:HZ2   | 1.18                     | 0.86              |
| 5:k:27:ASP:CG     | 4:m:23:LEU:CD2    | 2.42                     | 0.86              |
| 3:C7:68:LEU:HD13  | 3:C7:93:GLY:HA3   | 1.57                     | 0.86              |
| 3:D5:135:ILE:HG13 | 3:D5:152:ILE:HD11 | 1.57                     | 0.86              |
| 4:b:97:ARG:CZ     | 4:d:6:PHE:HB3     | 2.05                     | 0.86              |
| 1:7:256:LEU:HD11  | 2:B8:31:GLN:HB3   | 1.55                     | 0.86              |
| 2:D0:84:ARG:NH2   | 4:n:94:ASN:ND2    | 2.24                     | 0.86              |
| 3:E5:281:TYR:CE2  | 3:E9:87:PRO:HD3   | 2.09                     | 0.86              |
| 4:j:59:ASN:ND2    | 5:l:100:CYS:CB    | 2.39                     | 0.86              |
| 2:D6:210:TYR:HE1  | 2:D6:227:LEU:HD11 | 1.41                     | 0.85              |
| 1:19:256:LEU:CD2  | 2:E6:31:GLN:HG2   | 2.04                     | 0.85              |
| 3:B3:16:ILE:HD11  | 3:B3:229:VAL:HG11 | 1.57                     | 0.85              |
| 2:D4:285:GLN:HB3  | 2:D8:56:THR:HA    | 1.56                     | 0.85              |
| 1:19:243:ALA:HB3  | 3:E7:356:ILE:HA   | 1.56                     | 0.85              |
| 2:A6:279:GLU:CD   | 4:d:198:ARG:HD3   | 2.00                     | 0.85              |
| 3:D9:260:PHE:HB3  | 3:D9:261:PRO:HD2  | 1.58                     | 0.85              |
| 4:t:106:GLN:HB3   | 4:v:39:PRO:HG3    | 1.56                     | 0.85              |
| 2:E8:210:TYR:HB3  | 3:E9:324:LYS:HD3  | 1.58                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B0:210:TYR:HB3  | 3:B1:324:LYS:HD2  | 1.58                     | 0.85              |
| 2:B6:73:THR:CG2   | 3:B7:46:ARG:HE    | 1.89                     | 0.85              |
| 2:C4:404:PHE:HE1  | 3:C5:255:VAL:O    | 1.58                     | 0.84              |
| 3:D3:220:PRO:HD2  | 2:D4:326:LYS:HD3  | 1.58                     | 0.84              |
| 2:A0:282:TYR:HA   | 4:a:202:ARG:NH2   | 1.92                     | 0.84              |
| 4:d:71:LYS:CG     | 4:f:39:PRO:HD3    | 2.07                     | 0.84              |
| 3:B5:99:ASN:HD22  | 3:B5:178:THR:HG23 | 1.42                     | 0.84              |
| 1:0:244:GLN:NE2   | 4:c:162:GLY:CA    | 2.38                     | 0.84              |
| 1:11:255:PRO:HG2  | 4:p:178:ARG:HH12  | 1.42                     | 0.84              |
| 2:C8:282:TYR:HE1  | 4:o:201:TRP:CZ2   | 1.95                     | 0.84              |
| 1:10:257:PRO:HG2  | 2:C8:26:LEU:O     | 1.77                     | 0.84              |
| 2:A2:282:TYR:O    | 2:A6:60:LYS:HE2   | 1.77                     | 0.84              |
| 1:11:240:PRO:HB3  | 4:p:154:TYR:HB3   | 1.60                     | 0.84              |
| 2:D2:292:THR:HG21 | 2:D2:331:ALA:HB1  | 1.59                     | 0.84              |
| 2:D4:274:PRO:HG3  | 2:D4:286:LEU:HD23 | 1.59                     | 0.84              |
| 2:E6:221:ARG:HB3  | 3:E7:322:SER:CB   | 2.08                     | 0.84              |
| 4:f:105:ASN:HD22  | 4:h:37:GLN:NE2    | 1.76                     | 0.84              |
| 3:D3:175:VAL:HG11 | 2:D4:333:ALA:HA   | 1.58                     | 0.84              |
| 4:u:59:ASN:CG     | 5:w:100:CYS:CB    | 2.51                     | 0.84              |
| 3:C7:291:GLN:NE2  | 3:D1:125:GLU:OE1  | 2.09                     | 0.84              |
| 3:E9:218:THR:O    | 2:F0:326:LYS:NZ   | 2.11                     | 0.84              |
| 2:C6:282:TYR:CD2  | 4:n:202:ARG:HD2   | 2.12                     | 0.83              |
| 4:c:97:ARG:HE     | 4:e:161:TYR:HE1   | 1.23                     | 0.83              |
| 2:A6:210:TYR:HB3  | 3:A7:324:LYS:HZ3  | 1.41                     | 0.83              |
| 2:E6:221:ARG:HG2  | 3:E7:322:SER:OG   | 1.77                     | 0.83              |
| 1:15:257:PRO:HG2  | 2:D8:26:LEU:HD23  | 1.59                     | 0.83              |
| 3:A9:39:ASP:CA    | 4:c:90:PRO:HG3    | 2.08                     | 0.83              |
| 1:16:247:TYR:CE2  | 2:E0:81:GLY:HA3   | 2.13                     | 0.83              |
| 3:B3:57:GLY:HA3   | 4:e:83:PRO:CB     | 2.04                     | 0.83              |
| 2:C6:222:PRO:HD2  | 3:C7:324:LYS:HG2  | 1.60                     | 0.83              |
| 1:5:253:ALA:HB1   | 2:B4:32:PRO:HG2   | 1.57                     | 0.83              |
| 1:15:256:LEU:HD11 | 2:D8:31:GLN:N     | 1.91                     | 0.83              |
| 1:2:240:PRO:HG3   | 4:e:154:TYR:HB3   | 1.59                     | 0.83              |
| 2:A2:210:TYR:HB3  | 3:A3:324:LYS:HE3  | 1.61                     | 0.83              |
| 2:F0:70:LEU:HD12  | 2:F0:99:ALA:HB2   | 1.59                     | 0.83              |
| 1:0:251:TYR:OH    | 2:A4:18:ASN:HB3   | 1.79                     | 0.82              |
| 1:9:243:ALA:CB    | 3:C3:356:ILE:HA   | 2.08                     | 0.82              |
| 2:A6:214:ARG:NH2  | 3:A7:324:LYS:HZ2  | 1.77                     | 0.82              |
| 2:E4:96:LYS:HD2   | 3:E5:1:MET:CA     | 2.03                     | 0.82              |
| 1:16:246:CYS:HA   | 3:E1:320:ARG:HH22 | 1.42                     | 0.82              |
| 1:21:241:PHE:HZ   | 3:F1:356:ILE:HG23 | 1.43                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:9:241:PHE:HE1   | 3:C3:356:ILE:HG23 | 1.34                     | 0.82              |
| 4:t:106:GLN:HB3   | 4:v:39:PRO:CG     | 2.07                     | 0.82              |
| 2:A0:282:TYR:CA   | 4:a:202:ARG:NH2   | 2.42                     | 0.82              |
| 2:B2:241:SER:HB2  | 2:B2:249:ASN:HB2  | 1.61                     | 0.82              |
| 1:4:248:ARG:HH22  | 2:B2:81:GLY:HA2   | 1.44                     | 0.82              |
| 2:C2:362:VAL:HG11 | 2:C2:370:LYS:HB3  | 1.60                     | 0.82              |
| 2:B6:73:THR:HG22  | 3:B7:46:ARG:NE    | 1.95                     | 0.82              |
| 2:C4:181:VAL:HG12 | 3:C5:256:ASN:HB2  | 1.58                     | 0.82              |
| 4:b:97:ARG:HH12   | 4:d:6:PHE:HB3     | 1.39                     | 0.82              |
| 4:e:63:ILE:HG22   | 4:g:16:ARG:CD     | 2.10                     | 0.82              |
| 4:g:105:ASN:HB2   | 4:i:39:PRO:HG2    | 1.60                     | 0.82              |
| 1:4:240:PRO:CG    | 4:g:154:TYR:O     | 2.27                     | 0.82              |
| 3:D5:7:VAL:HG11   | 3:D5:151:LEU:HD21 | 1.60                     | 0.82              |
| 2:B0:100:ALA:HA   | 3:B1:252:LYS:NZ   | 1.94                     | 0.82              |
| 2:B6:238:LEU:HD11 | 2:B6:378:ILE:HD11 | 1.62                     | 0.82              |
| 1:10:241:PHE:CE1  | 3:C9:356:ILE:HG23 | 2.15                     | 0.81              |
| 2:B2:179:THR:N    | 3:B3:347:ASN:HD21 | 1.76                     | 0.81              |
| 2:A6:214:ARG:HH21 | 3:A7:324:LYS:HZ2  | 1.27                     | 0.81              |
| 4:g:14:LYS:HB2    | 4:g:47:LEU:HD12   | 1.59                     | 0.81              |
| 1:16:246:CYS:CA   | 3:E1:320:ARG:HH22 | 1.93                     | 0.81              |
| 2:A0:282:TYR:CA   | 4:a:202:ARG:HH21  | 1.93                     | 0.81              |
| 3:C5:397:TRP:CH2  | 2:C6:260:VAL:HB   | 2.16                     | 0.81              |
| 3:A1:219:THR:HG23 | 2:A2:324:VAL:HG21 | 1.59                     | 0.81              |
| 2:F0:66:VAL:HG12  | 2:F0:91:GLN:HB2   | 1.62                     | 0.81              |
| 4:b:49:LEU:HD11   | 4:b:177:GLY:HA2   | 1.63                     | 0.81              |
| 4:e:63:ILE:CG2    | 4:g:16:ARG:CD     | 2.58                     | 0.81              |
| 4:a:97:ARG:HH22   | 4:c:7:ALA:CB      | 1.92                     | 0.81              |
| 4:j:59:ASN:ND2    | 5:l:100:CYS:HB3   | 1.95                     | 0.81              |
| 1:11:240:PRO:CB   | 4:p:154:TYR:HB3   | 2.11                     | 0.81              |
| 1:16:256:LEU:HD23 | 2:E0:31:GLN:HG2   | 1.63                     | 0.81              |
| 3:B3:282:ARG:O    | 3:B7:55:THR:CG2   | 2.28                     | 0.81              |
| 1:19:257:PRO:HD2  | 2:E6:29:GLY:HA2   | 1.61                     | 0.81              |
| 1:20:241:PHE:HE1  | 3:E9:356:ILE:HG21 | 1.45                     | 0.81              |
| 2:D4:177:VAL:CG2  | 3:D5:331:LEU:HD22 | 2.12                     | 0.80              |
| 1:4:247:TYR:CB    | 2:B2:77:GLU:OE2   | 2.29                     | 0.80              |
| 3:A1:281:TYR:CD2  | 3:A5:87:PRO:HD3   | 2.16                     | 0.80              |
| 3:E7:35:THR:HG22  | 4:v:83:PRO:HG3    | 1.60                     | 0.80              |
| 2:C0:176:GLN:O    | 3:C1:347:ASN:ND2  | 2.14                     | 0.80              |
| 2:C6:210:TYR:HB3  | 3:C7:324:LYS:HD2  | 1.62                     | 0.80              |
| 1:14:256:LEU:CD1  | 2:D6:31:GLN:HE21  | 1.95                     | 0.80              |
| 2:A8:136:LEU:HD13 | 2:A8:235:ILE:HD11 | 1.63                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:213:ARG:HH22 | 3:E7:297:LYS:HB2  | 1.45                     | 0.80              |
| 3:E9:317:PHE:HB3  | 3:E9:321:MET:HE3  | 1.63                     | 0.80              |
| 1:22:243:ALA:HB2  | 3:C7:357:PRO:HD2  | 1.64                     | 0.80              |
| 2:A6:214:ARG:HE   | 3:A7:324:LYS:NZ   | 1.80                     | 0.80              |
| 2:D4:105:ARG:HH12 | 3:D5:251:ARG:HD3  | 1.47                     | 0.80              |
| 2:F0:406:HIS:CD2  | 3:F1:261:PRO:HD3  | 2.16                     | 0.80              |
| 2:A6:279:GLU:OE2  | 4:d:198:ARG:HD3   | 1.82                     | 0.80              |
| 2:B0:285:GLN:HB3  | 2:B4:56:THR:HA    | 1.64                     | 0.80              |
| 4:c:9:PRO:HB2     | 4:c:143:ILE:HG23  | 1.62                     | 0.80              |
| 2:C6:181:VAL:HB   | 3:C7:256:ASN:OD1  | 1.80                     | 0.80              |
| 2:E0:292:THR:HG21 | 2:E0:331:ALA:HB1  | 1.62                     | 0.80              |
| 1:0:241:PHE:CZ    | 3:A5:356:ILE:HD12 | 2.16                     | 0.79              |
| 2:B4:234:VAL:HG21 | 2:B4:302:MET:HE1  | 1.64                     | 0.79              |
| 2:D8:407:TRP:CE2  | 3:D9:255:VAL:HA   | 2.16                     | 0.79              |
| 2:E6:221:ARG:HB3  | 3:E7:322:SER:HB2  | 1.65                     | 0.79              |
| 4:g:88:LEU:HD11   | 4:g:185:ILE:HD13  | 1.65                     | 0.79              |
| 2:B8:11:GLN:HE22  | 3:B9:246:LEU:HD12 | 1.48                     | 0.79              |
| 2:F0:407:TRP:HZ2  | 3:F1:258:ILE:HD11 | 1.45                     | 0.79              |
| 4:b:97:ARG:NH2    | 4:d:7:ALA:CB      | 2.44                     | 0.79              |
| 1:11:244:GLN:N    | 3:D1:320:ARG:NH2  | 2.31                     | 0.79              |
| 3:D7:135:ILE:HD11 | 3:D7:164:MET:HE3  | 1.65                     | 0.79              |
| 1:15:256:LEU:CD1  | 2:D8:31:GLN:HA    | 2.09                     | 0.79              |
| 1:7:256:LEU:HD11  | 2:B8:31:GLN:CB    | 2.12                     | 0.79              |
| 2:D2:12:ALA:HB3   | 2:D2:140:ALA:HB2  | 1.63                     | 0.79              |
| 2:D8:163:LYS:H    | 2:D8:163:LYS:HD2  | 1.48                     | 0.79              |
| 2:B2:11:GLN:HE22  | 3:B3:246:LEU:HD13 | 1.48                     | 0.79              |
| 2:D0:84:ARG:HH21  | 4:n:94:ASN:ND2    | 1.80                     | 0.79              |
| 1:8:243:ALA:HB3   | 3:C1:356:ILE:HG23 | 1.64                     | 0.78              |
| 3:A1:10:GLY:HA2   | 3:A1:143:THR:HG23 | 1.64                     | 0.78              |
| 2:C8:176:GLN:HB3  | 3:C9:331:LEU:HD22 | 1.65                     | 0.78              |
| 3:C9:391:ARG:O    | 2:D0:262:TYR:OH   | 2.00                     | 0.78              |
| 1:6:255:PRO:HD3   | 4:i:3:GLN:HE22    | 1.47                     | 0.78              |
| 2:C0:217:LEU:HD21 | 2:C0:275:ILE:HG13 | 1.64                     | 0.78              |
| 2:D0:285:GLN:HG2  | 2:D4:55:GLU:O     | 1.83                     | 0.78              |
| 3:D1:91:VAL:HG11  | 3:D1:116:VAL:HG22 | 1.65                     | 0.78              |
| 1:2:240:PRO:HB2   | 4:e:154:TYR:HB3   | 1.64                     | 0.78              |
| 1:22:243:ALA:CB   | 3:C7:357:PRO:HD2  | 2.13                     | 0.78              |
| 3:E9:208:TYR:CE1  | 2:F0:326:LYS:HB3  | 2.19                     | 0.78              |
| 4:n:9:PRO:HB2     | 4:n:143:ILE:HG23  | 1.66                     | 0.78              |
| 2:C4:218:ASP:CG   | 4:m:194:ARG:NH2   | 2.41                     | 0.78              |
| 1:21:238:THR:HG21 | 3:F1:29:GLY:HA2   | 1.66                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A8:210:TYR:CG   | 3:A9:324:LYS:HG3  | 2.18                     | 0.77              |
| 1:4:240:PRO:CB    | 4:g:154:TYR:HD2   | 1.97                     | 0.77              |
| 4:b:97:ARG:HH11   | 4:d:6:PHE:HB3     | 0.98                     | 0.77              |
| 5:l:15:ARG:HD3    | 5:l:93:CYS:HB3    | 1.65                     | 0.77              |
| 3:A1:379:LYS:HB2  | 3:A1:379:LYS:NZ   | 1.98                     | 0.77              |
| 2:A4:269:LEU:HB3  | 2:A4:301:MET:HE1  | 1.66                     | 0.77              |
| 3:D3:291:GLN:HG2  | 3:D7:122:LYS:NZ   | 2.00                     | 0.77              |
| 1:3:257:PRO:HG2   | 2:B0:26:LEU:O     | 1.83                     | 0.77              |
| 2:C6:407:TRP:HZ3  | 3:C7:255:VAL:C    | 1.91                     | 0.77              |
| 4:c:97:ARG:HG3    | 4:e:161:TYR:CZ    | 2.19                     | 0.77              |
| 3:B5:282:ARG:O    | 3:B9:55:THR:CG2   | 2.32                     | 0.77              |
| 3:B7:391:ARG:O    | 2:B8:262:TYR:OH   | 2.01                     | 0.77              |
| 2:C6:407:TRP:CZ3  | 3:C7:254:ALA:O    | 2.38                     | 0.77              |
| 2:D0:85:HIS:NE2   | 4:n:99:MET:SD     | 2.57                     | 0.77              |
| 2:D8:84:ARG:HH21  | 4:r:197:LEU:HD22  | 1.46                     | 0.77              |
| 1:5:248:ARG:HH12  | 3:B5:42:LEU:HD21  | 1.48                     | 0.77              |
| 3:B5:283:ALA:HA   | 3:B9:55:THR:HB    | 1.66                     | 0.77              |
| 3:D9:169:VAL:HG12 | 3:D9:202:ILE:HB   | 1.67                     | 0.77              |
| 2:A6:279:GLU:OE2  | 4:d:198:ARG:CD    | 2.33                     | 0.76              |
| 2:C6:6:SER:HA     | 2:C6:136:LEU:HB2  | 1.66                     | 0.76              |
| 1:0:244:GLN:HE22  | 4:c:162:GLY:HA3   | 1.43                     | 0.76              |
| 3:C7:2:ARG:NH1    | 3:C7:249:ASP:OD2  | 2.17                     | 0.76              |
| 1:11:250:GLU:OE1  | 2:D0:225:THR:HG21 | 1.84                     | 0.76              |
| 2:D0:285:GLN:HB3  | 2:D4:56:THR:CA    | 2.15                     | 0.76              |
| 4:a:97:ARG:HH22   | 4:c:7:ALA:HB3     | 1.50                     | 0.76              |
| 4:d:71:LYS:HD3    | 4:f:39:PRO:CG     | 2.13                     | 0.76              |
| 4:t:67:HIS:NE2    | 4:v:20:GLU:OE1    | 2.15                     | 0.76              |
| 1:4:247:TYR:HE1   | 2:B2:81:GLY:HA3   | 1.46                     | 0.76              |
| 2:C2:279:GLU:HG2  | 5:l:155:GLN:OE1   | 1.85                     | 0.76              |
| 2:C8:372:MET:HA   | 2:C8:372:MET:HE3  | 1.67                     | 0.76              |
| 2:D2:210:TYR:CG   | 3:D3:324:LYS:HD3  | 2.21                     | 0.76              |
| 1:10:244:GLN:HB2  | 3:C9:320:ARG:NH1  | 2.01                     | 0.76              |
| 1:4:240:PRO:HB2   | 4:g:154:TYR:CB    | 2.16                     | 0.76              |
| 1:6:247:TYR:HE2   | 2:B6:81:GLY:HA3   | 1.51                     | 0.76              |
| 3:B1:207:LEU:HB3  | 3:B1:225:LEU:HD22 | 1.68                     | 0.76              |
| 2:C6:176:GLN:OE1  | 3:C7:331:LEU:CD1  | 2.34                     | 0.76              |
| 1:1:254:LYS:HB3   | 2:A6:364:PRO:HB2  | 1.68                     | 0.76              |
| 2:A4:110:ILE:O    | 2:A4:110:ILE:HG13 | 1.85                     | 0.76              |
| 2:A4:222:PRO:HD2  | 3:A5:324:LYS:HB3  | 1.68                     | 0.76              |
| 3:B9:320:ARG:HH21 | 4:j:188:GLY:HA2   | 1.51                     | 0.75              |
| 3:C5:39:ASP:OD1   | 5:k:51:PRO:CG     | 2.27                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:10:241:PHE:HZ   | 3:C9:356:ILE:HG23 | 1.52                     | 0.75              |
| 2:D4:210:TYR:HB3  | 3:D5:324:LYS:CE   | 2.15                     | 0.75              |
| 3:E1:66:MET:HE2   | 3:E1:116:VAL:HG21 | 1.68                     | 0.75              |
| 1:8:243:ALA:HB2   | 3:C1:357:PRO:HD2  | 0.80                     | 0.75              |
| 4:s:9:PRO:HB2     | 4:s:143:ILE:HG23  | 1.66                     | 0.75              |
| 1:2:251:TYR:OH    | 2:A8:18:ASN:HB3   | 1.86                     | 0.75              |
| 3:A5:212:PHE:CG   | 2:A6:326:LYS:HE2  | 2.22                     | 0.75              |
| 2:D6:222:PRO:O    | 3:D7:324:LYS:NZ   | 2.19                     | 0.75              |
| 1:9:257:PRO:CG    | 2:C2:26:LEU:CD1   | 2.64                     | 0.75              |
| 3:B5:260:PHE:HB3  | 3:B5:261:PRO:HD2  | 1.68                     | 0.75              |
| 3:D9:155:VAL:HG13 | 3:D9:164:MET:HE1  | 1.67                     | 0.75              |
| 4:f:105:ASN:HD21  | 4:h:37:GLN:NE2    | 1.72                     | 0.75              |
| 1:7:255:PRO:HG3   | 4:j:3:GLN:NE2     | 2.00                     | 0.75              |
| 3:D9:66:MET:HG2   | 3:D9:147:MET:HE1  | 1.68                     | 0.75              |
| 2:A4:285:GLN:CB   | 2:A8:57:GLY:H     | 1.91                     | 0.75              |
| 3:D5:129:CYS:SG   | 3:D5:162:ARG:NH2  | 2.60                     | 0.75              |
| 4:f:70:GLY:HA3    | 4:h:38:LEU:O      | 1.85                     | 0.75              |
| 4:j:59:ASN:ND2    | 5:l:100:CYS:HB2   | 2.01                     | 0.75              |
| 3:A3:267:LEU:HD21 | 3:A3:371:SER:HB3  | 1.69                     | 0.74              |
| 2:C4:241:SER:HB2  | 2:C4:249:ASN:HB2  | 1.69                     | 0.74              |
| 2:A4:93:ILE:HD11  | 2:A4:118:SER:HB2  | 1.69                     | 0.74              |
| 3:B7:281:TYR:HE2  | 3:C1:87:PRO:HD3   | 1.51                     | 0.74              |
| 1:20:256:LEU:CD1  | 2:E8:31:GLN:HG3   | 2.17                     | 0.74              |
| 3:C9:139:LEU:HD13 | 3:C9:168:SER:HB2  | 1.69                     | 0.74              |
| 2:D4:210:TYR:HE2  | 3:D5:327:ASP:OD2  | 1.69                     | 0.74              |
| 2:D4:292:THR:HG21 | 2:D4:331:ALA:HB1  | 1.68                     | 0.74              |
| 3:D5:260:PHE:HB3  | 3:D5:261:PRO:HD2  | 1.68                     | 0.74              |
| 2:D8:79:ARG:CG    | 2:D8:92:LEU:HD12  | 2.18                     | 0.74              |
| 4:q:5:VAL:HG11    | 4:q:149:ARG:HD2   | 1.70                     | 0.74              |
| 1:9:241:PHE:CE1   | 3:C3:356:ILE:HG21 | 2.20                     | 0.74              |
| 2:A0:312:TYR:HE1  | 2:A0:379:SER:HB3  | 1.52                     | 0.74              |
| 3:B3:176:SER:CB   | 2:B4:349:THR:HG23 | 2.17                     | 0.74              |
| 3:D7:212:PHE:HE1  | 2:D8:326:LYS:HD3  | 1.53                     | 0.74              |
| 2:E0:96:LYS:HE2   | 3:E1:128:ASP:HB2  | 1.69                     | 0.74              |
| 1:5:256:LEU:HD13  | 2:B4:26:LEU:HD12  | 1.70                     | 0.74              |
| 1:9:254:LYS:HB3   | 1:9:255:PRO:HD2   | 1.68                     | 0.74              |
| 2:A8:210:TYR:HB3  | 3:A9:324:LYS:HE3  | 1.67                     | 0.74              |
| 3:A9:100:ASN:HB2  | 3:A9:103:LYS:HG2  | 1.70                     | 0.74              |
| 1:10:257:PRO:HG3  | 2:C8:26:LEU:O     | 1.85                     | 0.74              |
| 1:7:256:LEU:CD1   | 2:B8:31:GLN:HB3   | 2.17                     | 0.74              |
| 3:B1:49:VAL:HG21  | 3:B1:241:ARG:HG2  | 1.67                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D5:253:LEU:CD1  | 3:D5:316:MET:HE1  | 2.18                     | 0.74              |
| 2:D8:84:ARG:NH2   | 4:r:197:LEU:HD21  | 2.02                     | 0.74              |
| 3:D9:7:VAL:HG11   | 3:D9:151:LEU:CD2  | 2.17                     | 0.74              |
| 2:E4:151:CYS:SG   | 2:E4:193:SER:OG   | 2.44                     | 0.74              |
| 1:10:244:GLN:HB2  | 3:C9:320:ARG:HH12 | 1.51                     | 0.74              |
| 3:A9:10:GLY:HA2   | 3:A9:143:THR:HG23 | 1.69                     | 0.74              |
| 2:C8:279:GLU:OE2  | 4:o:198:ARG:HA    | 1.86                     | 0.74              |
| 3:D3:176:SER:HB3  | 2:D4:349:THR:HB   | 1.68                     | 0.74              |
| 3:B1:39:ASP:HA    | 4:d:90:PRO:HG3    | 1.69                     | 0.74              |
| 3:D3:175:VAL:HG11 | 2:D4:333:ALA:CA   | 2.17                     | 0.74              |
| 3:D7:391:ARG:O    | 2:D8:262:TYR:OH   | 2.05                     | 0.74              |
| 2:C4:398:MET:HE1  | 3:C5:345:ILE:HG23 | 1.69                     | 0.73              |
| 3:F1:311:LEU:HD12 | 3:F1:342:VAL:HG21 | 1.70                     | 0.73              |
| 1:2:247:TYR:HB3   | 2:A8:77:GLU:OE2   | 1.88                     | 0.73              |
| 2:A4:93:ILE:HG21  | 2:A4:117:LEU:HD22 | 1.69                     | 0.73              |
| 2:A4:241:SER:HB2  | 2:A4:249:ASN:HB2  | 1.69                     | 0.73              |
| 2:B0:174:SER:OG   | 2:B0:177:VAL:O    | 2.05                     | 0.73              |
| 3:C7:281:TYR:CB   | 3:D1:86:ARG:HD3   | 2.18                     | 0.73              |
| 5:l:17:GLN:HE22   | 5:l:22:VAL:HG23   | 1.53                     | 0.73              |
| 2:D4:66:VAL:HG21  | 2:D4:122:ILE:HD11 | 1.70                     | 0.73              |
| 2:E4:119:LEU:CD1  | 2:E4:156:ARG:HD3  | 2.18                     | 0.73              |
| 3:E5:281:TYR:CD2  | 3:E9:87:PRO:HD3   | 2.23                     | 0.73              |
| 5:l:131:LEU:HB3   | 5:l:144:MET:HB3   | 1.69                     | 0.73              |
| 1:5:242:ASN:OD1   | 4:h:154:TYR:HB2   | 1.87                     | 0.73              |
| 2:A8:183:GLU:HB2  | 2:A8:184:PRO:HD3  | 1.70                     | 0.73              |
| 2:B6:178:SER:HB3  | 3:B7:347:ASN:ND2  | 2.04                     | 0.73              |
| 4:c:22:ALA:HB1    | 4:c:38:LEU:CD2    | 2.19                     | 0.73              |
| 2:D6:210:TYR:CE1  | 2:D6:227:LEU:HD11 | 2.23                     | 0.73              |
| 2:D6:221:ARG:HA   | 3:D7:324:LYS:HE3  | 1.70                     | 0.73              |
| 2:F0:223:THR:CG2  | 2:F0:225:THR:HG22 | 2.17                     | 0.73              |
| 1:15:256:LEU:HD11 | 2:D8:30:ILE:C     | 2.13                     | 0.73              |
| 1:2:257:PRO:HD3   | 2:A8:26:LEU:HD12  | 1.69                     | 0.73              |
| 2:B8:282:TYR:HE2  | 2:C2:85:HIS:CG    | 2.06                     | 0.73              |
| 2:D4:215:ARG:HH12 | 2:D4:299:ALA:HB1  | 1.53                     | 0.73              |
| 1:18:243:ALA:CB   | 3:E5:357:PRO:HD2  | 2.17                     | 0.73              |
| 2:B0:221:ARG:HB2  | 3:B1:322:SER:OG   | 1.88                     | 0.73              |
| 2:C4:7:ILE:HG21   | 2:C4:153:LEU:HD23 | 1.70                     | 0.73              |
| 2:E4:274:PRO:HD3  | 2:E4:291:ILE:HD11 | 1.70                     | 0.73              |
| 3:E7:44:LEU:HD23  | 4:v:91:PHE:CE2    | 2.24                     | 0.73              |
| 2:C8:282:TYR:CE1  | 4:o:201:TRP:HZ2   | 2.06                     | 0.72              |
| 4:t:66:SER:C      | 4:v:23:LEU:HD11   | 2.13                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:11:244:GLN:H    | 3:D1:320:ARG:HH21 | 1.37                     | 0.72              |
| 2:C4:218:ASP:OD2  | 4:m:194:ARG:NH2   | 2.21                     | 0.72              |
| 3:C5:397:TRP:HH2  | 2:C6:260:VAL:HB   | 1.53                     | 0.72              |
| 2:D8:262:TYR:HB3  | 2:D8:263:PRO:HD2  | 1.71                     | 0.72              |
| 2:A8:210:TYR:HB3  | 3:A9:324:LYS:CE   | 2.20                     | 0.72              |
| 3:D5:117:LEU:HD22 | 3:D5:154:LYS:HD2  | 1.71                     | 0.72              |
| 3:F1:113:ILE:HG13 | 3:F1:150:LEU:HD22 | 1.71                     | 0.72              |
| 4:o:5:VAL:HG11    | 4:o:149:ARG:HE    | 1.55                     | 0.72              |
| 3:A9:39:ASP:HA    | 4:c:90:PRO:CG     | 2.19                     | 0.72              |
| 2:D4:96:LYS:NZ    | 3:D5:128:ASP:HB2  | 2.04                     | 0.72              |
| 4:p:18:ASN:HD21   | 4:p:46:ASP:H      | 1.36                     | 0.72              |
| 2:A6:214:ARG:NE   | 3:A7:324:LYS:HZ2  | 1.88                     | 0.72              |
| 2:A6:283:HIS:O    | 2:B0:56:THR:CB    | 2.37                     | 0.72              |
| 3:B9:181:GLU:HB2  | 3:B9:182:PRO:HD3  | 1.71                     | 0.72              |
| 2:E0:229:ARG:HH11 | 2:E0:229:ARG:HG3  | 1.55                     | 0.72              |
| 1:15:257:PRO:HD3  | 2:D8:26:LEU:HG    | 1.69                     | 0.72              |
| 3:A9:219:THR:HB   | 2:B0:324:VAL:HG21 | 1.72                     | 0.72              |
| 3:B3:176:SER:OG   | 2:B4:349:THR:HG23 | 1.89                     | 0.72              |
| 2:B4:282:TYR:HE2  | 2:B8:85:HIS:HB3   | 1.54                     | 0.72              |
| 3:D7:406:MET:HA   | 3:D7:406:MET:CE   | 2.18                     | 0.72              |
| 4:h:93:LEU:O      | 4:j:159:TYR:OH    | 2.05                     | 0.72              |
| 1:8:243:ALA:CB    | 3:C1:356:ILE:HA   | 2.20                     | 0.72              |
| 3:B9:283:ALA:HA   | 3:C3:55:THR:CG2   | 2.17                     | 0.72              |
| 3:C1:117:LEU:CD1  | 3:C1:154:LYS:HG2  | 2.19                     | 0.72              |
| 2:E4:223:THR:HG23 | 2:E4:225:THR:HG22 | 1.70                     | 0.72              |
| 1:2:251:TYR:CZ    | 2:A8:18:ASN:HB3   | 2.25                     | 0.72              |
| 1:5:256:LEU:HD21  | 2:B4:31:GLN:HA    | 1.72                     | 0.72              |
| 2:A6:214:ARG:CZ   | 3:A7:324:LYS:HZ2  | 2.02                     | 0.72              |
| 2:C4:2:ARG:CG     | 2:C4:2:ARG:HD3    | 2.13                     | 0.72              |
| 1:5:242:ASN:OD1   | 4:h:154:TYR:CB    | 2.37                     | 0.71              |
| 2:C0:84:ARG:HH22  | 4:i:197:LEU:HD11  | 0.78                     | 0.71              |
| 2:C4:222:PRO:HD2  | 3:C5:324:LYS:CB   | 2.19                     | 0.71              |
| 2:D0:370:LYS:HG2  | 4:p:203:ASN:HD21  | 1.54                     | 0.71              |
| 2:D2:215:ARG:HH12 | 2:D2:299:ALA:HB1  | 1.54                     | 0.71              |
| 2:E6:181:VAL:HG13 | 3:E7:350:LYS:NZ   | 2.05                     | 0.71              |
| 5:k:25:ARG:HG3    | 4:m:23:LEU:HD11   | 1.71                     | 0.71              |
| 1:12:257:PRO:HD3  | 2:D2:26:LEU:HD22  | 1.72                     | 0.71              |
| 1:9:255:PRO:HG2   | 2:C2:364:PRO:CG   | 2.20                     | 0.71              |
| 2:C0:10:GLY:HA2   | 2:C0:145:THR:HG23 | 1.70                     | 0.71              |
| 2:E6:222:PRO:HD2  | 3:E7:324:LYS:HB2  | 1.71                     | 0.71              |
| 5:x:39:ALA:HB3    | 5:x:73:TYR:HE1    | 1.55                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:10:242:ASN:HB2  | 4:o:153:GLU:OE2   | 1.90                     | 0.71              |
| 2:A8:181:VAL:HG21 | 3:A9:256:ASN:OD1  | 1.90                     | 0.71              |
| 2:D0:278:ALA:HB1  | 4:p:200:ASP:HB3   | 1.72                     | 0.71              |
| 4:v:14:LYS:HD2    | 4:v:47:LEU:HD23   | 1.72                     | 0.71              |
| 3:A5:284:LEU:CB   | 3:A9:55:THR:HG21  | 2.20                     | 0.71              |
| 3:B3:93:GLY:HA2   | 3:B3:112:LEU:HD21 | 1.72                     | 0.71              |
| 2:B8:250:VAL:HG23 | 2:B8:254:GLU:HG2  | 1.72                     | 0.71              |
| 3:D3:220:PRO:CD   | 2:D4:326:LYS:HD3  | 2.20                     | 0.71              |
| 1:0:244:GLN:H     | 3:A5:320:ARG:NE   | 1.88                     | 0.71              |
| 1:11:250:GLU:CD   | 2:D0:225:THR:HG21 | 2.14                     | 0.71              |
| 2:C0:223:THR:OG1  | 3:C1:245:GLN:OE1  | 2.08                     | 0.71              |
| 2:D6:12:ALA:HB3   | 2:D6:140:ALA:HB2  | 1.71                     | 0.71              |
| 4:d:71:LYS:HG3    | 4:f:39:PRO:CD     | 2.17                     | 0.71              |
| 4:e:63:ILE:HG21   | 4:g:16:ARG:HD3    | 1.70                     | 0.71              |
| 3:C5:219:THR:HB   | 2:C6:324:VAL:HG11 | 1.71                     | 0.71              |
| 4:d:105:ASN:HB3   | 4:f:41:ASN:HA     | 1.72                     | 0.71              |
| 1:16:246:CYS:HA   | 3:E1:320:ARG:NH2  | 2.05                     | 0.71              |
| 1:4:250:GLU:HG3   | 2:B2:225:THR:HG21 | 1.72                     | 0.71              |
| 3:C3:190:HIS:HB2  | 3:C3:414:ASN:HD21 | 1.56                     | 0.71              |
| 4:r:14:LYS:HB2    | 4:r:47:LEU:HD12   | 1.72                     | 0.71              |
| 3:B1:311:LEU:HD12 | 3:B1:342:VAL:HG11 | 1.72                     | 0.71              |
| 2:B4:269:LEU:HD21 | 2:B4:384:ILE:HD11 | 1.73                     | 0.71              |
| 2:C2:406:HIS:CD2  | 3:C3:261:PRO:HD3  | 2.26                     | 0.71              |
| 2:C4:2:ARG:HB3    | 2:C4:133:GLN:HE21 | 1.54                     | 0.71              |
| 3:D1:66:MET:HE2   | 3:D1:116:VAL:HG11 | 1.72                     | 0.71              |
| 4:b:97:ARG:HH11   | 4:d:6:PHE:CB      | 1.79                     | 0.71              |
| 2:C6:168:ASN:ND2  | 2:C6:194:LEU:HD11 | 2.06                     | 0.70              |
| 2:D8:84:ARG:HH22  | 4:r:197:LEU:HD21  | 1.56                     | 0.70              |
| 2:A4:282:TYR:HB2  | 4:c:202:ARG:HH21  | 1.55                     | 0.70              |
| 2:C6:407:TRP:CE3  | 3:C7:255:VAL:HA   | 2.25                     | 0.70              |
| 2:C4:404:PHE:CE1  | 3:C5:255:VAL:O    | 2.43                     | 0.70              |
| 2:E0:223:THR:HG23 | 2:E0:225:THR:HG22 | 1.73                     | 0.70              |
| 2:E2:96:LYS:HE3   | 3:E3:1:MET:N      | 2.07                     | 0.70              |
| 2:E6:84:ARG:NH2   | 4:v:197:LEU:HD21  | 2.05                     | 0.70              |
| 4:t:66:SER:O      | 4:v:23:LEU:HD11   | 1.91                     | 0.70              |
| 1:5:255:PRO:HD3   | 4:h:3:GLN:HE21    | 1.54                     | 0.70              |
| 3:A1:219:THR:CA   | 2:A2:326:LYS:HZ1  | 1.89                     | 0.70              |
| 3:B3:49:VAL:HG21  | 3:B3:241:ARG:HG2  | 1.74                     | 0.70              |
| 3:C3:259:PRO:HG2  | 3:C3:311:LEU:CD2  | 2.20                     | 0.70              |
| 2:D0:85:HIS:CD2   | 4:n:99:MET:SD     | 2.85                     | 0.70              |
| 4:a:191:GLU:HB2   | 4:a:195:ALA:HB2   | 1.71                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:20:243:ALA:HB2  | 3:E9:357:PRO:HD2  | 1.72                     | 0.70              |
| 1:4:240:PRO:CB    | 4:g:154:TYR:O     | 2.39                     | 0.70              |
| 2:A4:93:ILE:CD1   | 2:A4:118:SER:HB2  | 2.22                     | 0.70              |
| 3:A7:66:MET:HE1   | 3:A7:147:MET:HE1  | 1.73                     | 0.70              |
| 3:A9:220:PRO:HG2  | 2:B0:326:LYS:CE   | 2.21                     | 0.70              |
| 3:A9:259:PRO:HG2  | 3:A9:311:LEU:HD21 | 1.74                     | 0.70              |
| 3:B3:56:GLY:O     | 4:e:83:PRO:HG2    | 1.91                     | 0.70              |
| 2:B6:84:ARG:NH1   | 4:g:197:LEU:HD21  | 2.06                     | 0.70              |
| 4:h:14:LYS:HD3    | 4:h:47:LEU:HD12   | 1.74                     | 0.70              |
| 2:A0:221:ARG:HG3  | 3:A1:325:GLU:HB3  | 1.74                     | 0.70              |
| 3:B1:163:ILE:HD13 | 3:B1:250:LEU:HB3  | 1.74                     | 0.70              |
| 2:C6:276:ILE:HD12 | 2:C6:281:ALA:HA   | 1.74                     | 0.70              |
| 3:D7:91:VAL:HG11  | 3:D7:116:VAL:HB   | 1.72                     | 0.70              |
| 1:10:241:PHE:HZ   | 3:C9:356:ILE:HD12 | 1.57                     | 0.70              |
| 1:13:253:ALA:CB   | 2:D4:32:PRO:HG3   | 2.22                     | 0.70              |
| 1:15:257:PRO:CD   | 2:D8:26:LEU:HG    | 2.21                     | 0.70              |
| 1:2:244:GLN:HE21  | 4:e:162:GLY:HA3   | 1.57                     | 0.70              |
| 3:A3:135:ILE:HG21 | 3:A3:152:ILE:HD11 | 1.73                     | 0.70              |
| 3:B3:282:ARG:O    | 3:B7:55:THR:HG22  | 1.89                     | 0.70              |
| 2:C4:222:PRO:HD2  | 3:C5:324:LYS:HB3  | 1.74                     | 0.70              |
| 1:8:239:LEU:O     | 3:C1:359:LYS:HE3  | 1.90                     | 0.70              |
| 1:10:242:ASN:ND2  | 4:o:154:TYR:HB2   | 2.07                     | 0.69              |
| 2:A6:214:ARG:HE   | 3:A7:324:LYS:HZ2  | 1.37                     | 0.69              |
| 2:E8:80:THR:HA    | 2:E8:84:ARG:HE    | 1.57                     | 0.69              |
| 1:15:257:PRO:HG2  | 2:D8:26:LEU:CD2   | 2.22                     | 0.69              |
| 1:6:256:LEU:CD1   | 2:B6:31:GLN:HG3   | 2.08                     | 0.69              |
| 2:A0:79:ARG:HG3   | 2:A0:92:LEU:HD22  | 1.74                     | 0.69              |
| 2:A0:279:GLU:OE2  | 4:a:198:ARG:HD3   | 1.92                     | 0.69              |
| 3:C5:57:GLY:HA3   | 5:k:44:SER:OG     | 1.91                     | 0.69              |
| 2:D6:223:THR:OG1  | 3:D7:323:THR:HG23 | 1.92                     | 0.69              |
| 4:f:9:PRO:HB2     | 4:f:143:ILE:HG23  | 1.75                     | 0.69              |
| 1:4:248:ARG:NH2   | 2:B2:81:GLY:HA2   | 2.06                     | 0.69              |
| 3:C5:12:CYS:HB3   | 3:C5:138:SER:HB3  | 1.73                     | 0.69              |
| 2:D0:107:HIS:HE2  | 2:D0:151:CYS:HG   | 1.37                     | 0.69              |
| 2:D4:176:GLN:CD   | 3:D5:331:LEU:HD21 | 2.17                     | 0.69              |
| 3:D7:66:MET:HE2   | 3:D7:116:VAL:HG21 | 1.73                     | 0.69              |
| 2:E0:298:PRO:HG3  | 2:E0:308:ARG:HH22 | 1.57                     | 0.69              |
| 2:E6:181:VAL:HG13 | 3:E7:350:LYS:HZ1  | 1.54                     | 0.69              |
| 4:o:53:GLY:HA2    | 4:o:62:VAL:HG21   | 1.74                     | 0.69              |
| 3:C7:97:ALA:HB3   | 3:C7:143:THR:HG22 | 1.75                     | 0.69              |
| 3:D3:397:TRP:CZ2  | 2:D4:256:GLN:O    | 2.46                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:q:9:PRO:HB2     | 4:q:143:ILE:HG23  | 1.74                     | 0.69              |
| 2:C8:323:VAL:HG13 | 2:C8:355:ILE:HG23 | 1.75                     | 0.69              |
| 1:2:240:PRO:HB2   | 4:e:154:TYR:CB    | 2.22                     | 0.69              |
| 1:2:257:PRO:HG2   | 2:A8:26:LEU:O     | 1.91                     | 0.69              |
| 4:e:100:ASN:HB3   | 4:g:6:PHE:CE1     | 2.28                     | 0.69              |
| 3:A1:222:TYR:HB2  | 2:A2:325:PRO:HG2  | 1.75                     | 0.69              |
| 2:C2:84:ARG:CZ    | 4:j:197:LEU:HD11  | 2.22                     | 0.69              |
| 2:C8:281:ALA:HB3  | 4:o:202:ARG:HH21  | 1.58                     | 0.69              |
| 2:D0:283:HIS:HA   | 2:D4:60:LYS:HZ3   | 1.58                     | 0.69              |
| 3:D3:391:ARG:O    | 2:D4:262:TYR:OH   | 2.11                     | 0.69              |
| 2:D6:176:GLN:O    | 3:D7:347:ASN:ND2  | 2.26                     | 0.69              |
| 2:F0:176:GLN:CG   | 3:F1:331:LEU:HD21 | 2.23                     | 0.69              |
| 3:D5:107:THR:HG21 | 3:D5:401:GLU:HB2  | 1.74                     | 0.69              |
| 2:D6:220:GLU:O    | 3:D7:324:LYS:HE3  | 1.93                     | 0.69              |
| 3:F1:2:ARG:NH2    | 3:F1:249:ASP:OD2  | 2.25                     | 0.69              |
| 4:a:117:ARG:NH1   | 4:a:118:ASP:OD1   | 2.26                     | 0.69              |
| 1:10:241:PHE:CE1  | 3:C9:356:ILE:CG2  | 2.76                     | 0.69              |
| 1:11:255:PRO:HG2  | 4:p:178:ARG:NH1   | 2.07                     | 0.69              |
| 3:C1:113:ILE:HG21 | 3:C1:154:LYS:HD2  | 1.74                     | 0.69              |
| 3:C9:397:TRP:CD1  | 2:D0:257:THR:HG1  | 2.11                     | 0.69              |
| 1:6:256:LEU:CG    | 2:B6:31:GLN:HG2   | 2.22                     | 0.68              |
| 3:E7:163:ILE:HD13 | 3:E7:250:LEU:HB3  | 1.74                     | 0.68              |
| 4:e:53:GLY:HA2    | 4:e:62:VAL:HG21   | 1.75                     | 0.68              |
| 3:B5:99:ASN:ND2   | 3:B5:178:THR:HG23 | 2.08                     | 0.68              |
| 2:C4:209:ILE:HG23 | 2:C4:227:LEU:HD22 | 1.75                     | 0.68              |
| 2:D4:262:TYR:HB2  | 2:D4:265:ILE:HD12 | 1.74                     | 0.68              |
| 1:11:255:PRO:CG   | 4:p:178:ARG:NH1   | 2.56                     | 0.68              |
| 1:15:256:LEU:CD1  | 2:D8:30:ILE:C     | 2.66                     | 0.68              |
| 2:D0:204:LEU:HD13 | 2:D0:231:ILE:HD12 | 1.76                     | 0.68              |
| 4:c:111:ILE:HD13  | 4:c:132:LEU:HB2   | 1.74                     | 0.68              |
| 4:s:97:ARG:NH1    | 4:u:161:TYR:CE1   | 2.61                     | 0.68              |
| 4:t:9:PRO:HB2     | 4:t:143:ILE:HG23  | 1.75                     | 0.68              |
| 1:4:240:PRO:HB2   | 4:g:154:TYR:CG    | 2.29                     | 0.68              |
| 4:g:151:MET:HE1   | 4:g:158:THR:HG21  | 1.75                     | 0.68              |
| 1:10:244:GLN:OE1  | 4:o:162:GLY:HA3   | 1.93                     | 0.68              |
| 2:A2:398:MET:CE   | 3:A3:345:ILE:HG23 | 2.24                     | 0.68              |
| 2:A6:222:PRO:HD2  | 3:A7:324:LYS:CB   | 2.21                     | 0.68              |
| 2:B2:53:PHE:HB3   | 2:B2:61:HIS:HB3   | 1.75                     | 0.68              |
| 3:B3:176:SER:HB2  | 2:B4:349:THR:HG23 | 1.74                     | 0.68              |
| 2:C8:276:ILE:HG23 | 2:C8:280:LYS:HB2  | 1.75                     | 0.68              |
| 3:C9:66:MET:HE1   | 3:C9:151:LEU:HD22 | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D0:107:HIS:NE2  | 2:D0:151:CYS:SG   | 2.66                     | 0.68              |
| 1:11:244:GLN:H    | 3:D1:320:ARG:HH22 | 1.37                     | 0.68              |
| 1:16:256:LEU:CD2  | 2:E0:31:GLN:HG2   | 2.24                     | 0.68              |
| 3:B3:219:THR:HB   | 2:B4:324:VAL:HG21 | 1.74                     | 0.68              |
| 2:E6:221:ARG:CB   | 3:E7:322:SER:HB2  | 2.23                     | 0.68              |
| 1:3:257:PRO:CG    | 2:B0:26:LEU:O     | 2.42                     | 0.68              |
| 2:D4:12:ALA:HB3   | 2:D4:140:ALA:HB2  | 1.76                     | 0.68              |
| 1:9:244:GLN:H     | 3:C3:320:ARG:HD2  | 1.57                     | 0.68              |
| 2:C4:279:GLU:OE2  | 4:m:197:LEU:O     | 2.11                     | 0.68              |
| 4:j:9:PRO:HB2     | 4:j:143:ILE:HG23  | 1.74                     | 0.68              |
| 1:0:244:GLN:HE22  | 4:c:162:GLY:CA    | 2.02                     | 0.68              |
| 1:11:244:GLN:N    | 3:D1:320:ARG:HH22 | 1.92                     | 0.68              |
| 3:A9:248:SER:HA   | 3:A9:252:LYS:HG2  | 1.76                     | 0.68              |
| 3:B3:375:GLN:NE2  | 3:B3:423:GLN:OE1  | 2.27                     | 0.68              |
| 3:B9:200:GLN:HB2  | 3:B9:268:ILE:HD11 | 1.76                     | 0.68              |
| 2:D4:210:TYR:HB3  | 3:D5:324:LYS:HD3  | 1.75                     | 0.68              |
| 3:F1:10:GLY:HA2   | 3:F1:143:THR:HG23 | 1.75                     | 0.68              |
| 3:A5:287:PRO:HA   | 3:A5:329:GLN:HE22 | 1.59                     | 0.68              |
| 3:B3:396:HIS:HA   | 3:B3:399:THR:HG22 | 1.74                     | 0.68              |
| 2:A8:288:VAL:HG21 | 2:A8:323:VAL:HG13 | 1.76                     | 0.67              |
| 2:D0:8:HIS:CD2    | 2:D0:17:GLY:HA3   | 2.29                     | 0.67              |
| 4:g:119:ARG:NH1   | 4:g:137:GLU:OE1   | 2.26                     | 0.67              |
| 4:m:96:TYR:HA     | 4:m:108:ILE:HD11  | 1.77                     | 0.67              |
| 4:t:8:SER:OG      | 4:t:11:ASN:ND2    | 2.27                     | 0.67              |
| 3:B3:91:VAL:HG21  | 3:B3:116:VAL:HG22 | 1.77                     | 0.67              |
| 2:E6:174:SER:OG   | 2:E6:177:VAL:O    | 2.09                     | 0.67              |
| 1:8:243:ALA:HB1   | 3:C1:356:ILE:HA   | 1.76                     | 0.67              |
| 3:A7:207:LEU:HB3  | 3:A7:225:LEU:HD12 | 1.76                     | 0.67              |
| 3:A1:42:LEU:HD21  | 3:A1:243:PRO:HD2  | 1.76                     | 0.67              |
| 2:E6:84:ARG:HH21  | 4:v:197:LEU:HD11  | 1.58                     | 0.67              |
| 1:17:246:CYS:HB2  | 3:E3:320:ARG:HH21 | 1.60                     | 0.67              |
| 2:A2:377:MET:HE2  | 2:A2:379:SER:HB2  | 1.76                     | 0.67              |
| 3:D1:98:GLY:H     | 3:D1:103:LYS:HD3  | 1.59                     | 0.67              |
| 4:a:96:TYR:HA     | 4:a:108:ILE:HD11  | 1.77                     | 0.67              |
| 5:x:40:LYS:HZ3    | 5:x:76:LEU:HB3    | 1.60                     | 0.67              |
| 1:14:256:LEU:HD11 | 2:D6:31:GLN:NE2   | 2.04                     | 0.67              |
| 2:A0:222:PRO:HD2  | 3:A1:324:LYS:CB   | 2.25                     | 0.67              |
| 2:A4:82:THR:HA    | 4:a:98:THR:HG23   | 1.76                     | 0.67              |
| 2:A6:177:VAL:HG23 | 3:A7:331:LEU:HD22 | 1.75                     | 0.67              |
| 2:D0:174:SER:OG   | 2:D0:177:VAL:O    | 2.13                     | 0.67              |
| 3:D3:155:VAL:HG13 | 3:D3:164:MET:HE2  | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D3:220:PRO:HG2  | 2:D4:326:LYS:HD3  | 1.76                     | 0.67              |
| 4:a:78:ALA:HA     | 4:a:167:VAL:HG23  | 1.75                     | 0.67              |
| 5:k:25:ARG:HG3    | 4:m:23:LEU:HD12   | 1.77                     | 0.67              |
| 1:11:255:PRO:CG   | 4:p:178:ARG:HH12  | 2.06                     | 0.67              |
| 1:15:257:PRO:HD2  | 2:D8:26:LEU:O     | 1.95                     | 0.67              |
| 3:A1:412:GLU:OE2  | 3:A1:416:ASN:ND2  | 2.27                     | 0.67              |
| 2:B0:285:GLN:OE1  | 2:B4:55:GLU:O     | 2.12                     | 0.67              |
| 2:C8:105:ARG:HH12 | 3:C9:251:ARG:HG2  | 1.60                     | 0.67              |
| 3:D9:14:ASN:HD22  | 3:D9:72:THR:HG23  | 1.60                     | 0.67              |
| 3:E7:44:LEU:HD23  | 4:v:91:PHE:HE2    | 1.58                     | 0.67              |
| 4:c:22:ALA:HB1    | 4:c:38:LEU:HD21   | 1.74                     | 0.67              |
| 4:e:63:ILE:HG22   | 4:g:16:ARG:NE     | 2.09                     | 0.67              |
| 3:B3:130:LEU:HD23 | 3:B3:130:LEU:H    | 1.59                     | 0.67              |
| 1:4:240:PRO:CG    | 4:g:154:TYR:HB3   | 2.25                     | 0.67              |
| 3:B3:95:THR:OG1   | 3:B3:108:GLU:OE2  | 2.10                     | 0.67              |
| 3:B5:324:LYS:HA   | 3:B5:327:ASP:HB2  | 1.77                     | 0.67              |
| 2:B8:250:VAL:HG21 | 2:B8:318:MET:HE1  | 1.77                     | 0.67              |
| 3:D1:67:ASP:OD2   | 3:D1:72:THR:OG1   | 2.13                     | 0.67              |
| 2:E2:96:LYS:HE3   | 3:E3:1:MET:H1     | 1.58                     | 0.67              |
| 2:E6:223:THR:HG23 | 2:E6:225:THR:HG22 | 1.77                     | 0.67              |
| 2:B4:285:GLN:NE2  | 2:B8:55:GLU:O     | 2.28                     | 0.67              |
| 3:B5:56:GLY:O     | 4:f:83:PRO:HG2    | 1.95                     | 0.67              |
| 3:B9:318:ARG:HD2  | 3:B9:358:PRO:HD3  | 1.76                     | 0.67              |
| 3:D3:293:MET:SD   | 3:D3:365:VAL:HG11 | 2.35                     | 0.67              |
| 2:E6:221:ARG:HG2  | 3:E7:322:SER:CB   | 2.25                     | 0.67              |
| 4:m:172:VAL:HG23  | 4:m:180:ALA:HB3   | 1.76                     | 0.67              |
| 3:E5:274:THR:HG21 | 3:E5:282:ARG:HD2  | 1.76                     | 0.66              |
| 2:E6:283:HIS:NE2  | 2:F0:85:HIS:HB3   | 2.10                     | 0.66              |
| 2:A8:282:TYR:OH   | 2:B2:33:ASP:OD1   | 2.12                     | 0.66              |
| 3:B3:336:LYS:HE2  | 3:B3:336:LYS:HA   | 1.77                     | 0.66              |
| 3:D7:135:ILE:CD1  | 3:D7:164:MET:HE3  | 2.26                     | 0.66              |
| 3:E1:248:SER:HA   | 3:E1:252:LYS:HG3  | 1.77                     | 0.66              |
| 3:E9:267:LEU:HD21 | 3:E9:374:ILE:HD11 | 1.77                     | 0.66              |
| 4:n:117:ARG:NH1   | 4:n:118:ASP:OD1   | 2.29                     | 0.66              |
| 1:9:241:PHE:CZ    | 3:C3:356:ILE:CG2  | 2.78                     | 0.66              |
| 2:B0:2:ARG:HB2    | 2:B0:133:GLN:HE22 | 1.59                     | 0.66              |
| 2:B4:178:SER:OG   | 3:B5:347:ASN:ND2  | 2.28                     | 0.66              |
| 2:C2:221:ARG:HB3  | 3:C3:322:SER:CB   | 2.25                     | 0.66              |
| 3:C5:207:LEU:HB3  | 3:C5:225:LEU:HD12 | 1.77                     | 0.66              |
| 3:C5:293:MET:HE1  | 3:C5:365:VAL:HG11 | 1.77                     | 0.66              |
| 2:D4:177:VAL:HG23 | 3:D5:331:LEU:HD22 | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D8:407:TRP:CZ2  | 3:D9:255:VAL:HA   | 2.31                     | 0.66              |
| 3:E5:172:SER:HB2  | 3:E5:205:GLU:HG2  | 1.77                     | 0.66              |
| 4:q:37:GLN:NE2    | 4:q:41:ASN:OD1    | 2.28                     | 0.66              |
| 1:8:255:PRO:HG2   | 2:C0:364:PRO:HG2  | 1.77                     | 0.66              |
| 2:A4:104:ALA:HB2  | 2:A4:413:MET:HE3  | 1.78                     | 0.66              |
| 3:B3:10:GLY:HA2   | 3:B3:143:THR:HG23 | 1.76                     | 0.66              |
| 3:C3:267:LEU:HD11 | 3:C3:374:ILE:HD13 | 1.78                     | 0.66              |
| 3:D3:175:VAL:CG1  | 2:D4:333:ALA:HA   | 2.25                     | 0.66              |
| 3:D9:102:ALA:HB2  | 3:D9:403:MET:HE2  | 1.77                     | 0.66              |
| 2:E6:221:ARG:HB3  | 3:E7:322:SER:HB3  | 1.76                     | 0.66              |
| 2:E6:339:ARG:NH2  | 2:E6:342:GLN:OE1  | 2.29                     | 0.66              |
| 4:d:71:LYS:CG     | 4:f:39:PRO:CD     | 2.73                     | 0.66              |
| 4:e:63:ILE:CG2    | 4:g:16:ARG:HD2    | 2.26                     | 0.66              |
| 1:0:243:ALA:CB    | 3:A5:320:ARG:HD2  | 2.19                     | 0.66              |
| 1:6:255:PRO:HD3   | 4:i:3:GLN:NE2     | 2.11                     | 0.66              |
| 3:B7:274:THR:HG21 | 3:B7:282:ARG:HD2  | 1.76                     | 0.66              |
| 4:t:96:TYR:CE2    | 4:v:6:PHE:HE2     | 2.13                     | 0.66              |
| 4:t:198:ARG:HG2   | 4:t:198:ARG:HH11  | 1.61                     | 0.66              |
| 3:B9:282:ARG:O    | 3:C3:55:THR:OG1   | 2.11                     | 0.66              |
| 3:C1:166:THR:HB   | 3:C1:199:VAL:HG12 | 1.78                     | 0.66              |
| 3:E5:12:CYS:HB3   | 3:E5:138:SER:HB2  | 1.76                     | 0.66              |
| 3:A5:172:SER:HB3  | 3:A5:205:GLU:HG2  | 1.77                     | 0.66              |
| 3:D3:44:LEU:O     | 3:D3:44:LEU:HD23  | 1.95                     | 0.66              |
| 2:E8:180:ALA:HB3  | 2:E8:183:GLU:HG2  | 1.78                     | 0.66              |
| 5:k:27:ASP:HB3    | 4:m:23:LEU:HD21   | 1.78                     | 0.66              |
| 1:10:257:PRO:HD3  | 2:C8:26:LEU:HD22  | 1.78                     | 0.66              |
| 1:2:257:PRO:HD3   | 2:A8:26:LEU:HD11  | 1.76                     | 0.66              |
| 3:A7:57:GLY:HA3   | 4:b:83:PRO:HB2    | 1.78                     | 0.66              |
| 2:C2:250:VAL:HG23 | 2:C2:352:LYS:HZ3  | 1.60                     | 0.66              |
| 3:D9:10:GLY:HA2   | 3:D9:143:THR:HG23 | 1.78                     | 0.66              |
| 2:E6:221:ARG:CG   | 3:E7:322:SER:CB   | 2.74                     | 0.66              |
| 1:1:239:LEU:HD22  | 3:A7:359:LYS:HB3  | 1.76                     | 0.66              |
| 3:A1:130:LEU:H    | 3:A1:162:ARG:HH12 | 1.42                     | 0.66              |
| 2:B0:285:GLN:NE2  | 2:B4:55:GLU:O     | 2.28                     | 0.66              |
| 2:B8:224:TYR:HB2  | 3:B9:245:GLN:NE2  | 2.11                     | 0.66              |
| 4:c:185:ILE:HG22  | 4:c:186:CYS:SG    | 2.36                     | 0.66              |
| 4:e:67:HIS:NE2    | 4:g:20:GLU:HB3    | 2.11                     | 0.66              |
| 4:r:111:ILE:HD13  | 4:r:132:LEU:HB2   | 1.77                     | 0.66              |
| 1:19:250:GLU:HG3  | 2:E6:225:THR:HG21 | 1.78                     | 0.65              |
| 1:2:244:GLN:HE21  | 4:e:162:GLY:CA    | 2.09                     | 0.65              |
| 2:A0:73:THR:HA    | 3:A1:46:ARG:HH11  | 1.60                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B6:285:GLN:HB3  | 2:C0:56:THR:HA    | 1.77                     | 0.65              |
| 3:C1:249:ASP:H    | 3:C1:252:LYS:HB2  | 1.61                     | 0.65              |
| 2:D0:142:GLY:HA3  | 2:D0:183:GLU:HG2  | 1.78                     | 0.65              |
| 1:17:244:GLN:HE22 | 4:v:162:GLY:HA3   | 1.61                     | 0.65              |
| 3:A1:205:GLU:HA   | 3:A1:208:TYR:HD2  | 1.61                     | 0.65              |
| 2:B2:177:VAL:CG1  | 3:B3:331:LEU:HD22 | 2.26                     | 0.65              |
| 3:B5:257:LEU:HD21 | 3:B5:314:SER:HB2  | 1.79                     | 0.65              |
| 2:B8:195:LEU:HD21 | 2:B8:264:ARG:HE   | 1.61                     | 0.65              |
| 3:C9:220:PRO:O    | 2:D0:326:LYS:HE3  | 1.96                     | 0.65              |
| 1:13:251:TYR:CE2  | 2:D4:18:ASN:HB3   | 2.32                     | 0.65              |
| 1:9:241:PHE:CZ    | 3:C3:356:ILE:HG21 | 2.31                     | 0.65              |
| 3:A5:27:GLU:HA    | 3:A5:359:LYS:HD2  | 1.77                     | 0.65              |
| 2:C0:220:GLU:HG3  | 2:C0:220:GLU:O    | 1.94                     | 0.65              |
| 2:C0:274:PRO:HG3  | 2:C0:286:LEU:HD13 | 1.77                     | 0.65              |
| 2:C4:6:SER:HA     | 2:C4:136:LEU:HB2  | 1.78                     | 0.65              |
| 2:D8:259:LEU:HD11 | 2:D8:316:CYS:HB2  | 1.77                     | 0.65              |
| 4:f:105:ASN:HD22  | 4:h:37:GLN:HE22   | 1.27                     | 0.65              |
| 5:l:103:LYS:HA    | 5:l:106:ILE:HG12  | 1.77                     | 0.65              |
| 4:s:146:ARG:HD3   | 4:s:156:VAL:HG21  | 1.78                     | 0.65              |
| 1:2:240:PRO:CB    | 4:e:154:TYR:CB    | 2.72                     | 0.65              |
| 2:A0:142:GLY:O    | 2:A0:186:ASN:ND2  | 2.29                     | 0.65              |
| 3:A9:283:ALA:HB2  | 3:B3:53:GLU:O     | 1.97                     | 0.65              |
| 4:h:10:LEU:HD21   | 4:h:49:LEU:CD1    | 2.25                     | 0.65              |
| 3:A7:132:GLY:HA3  | 3:A7:163:ILE:HG22 | 1.78                     | 0.65              |
| 3:B5:57:GLY:CA    | 4:f:83:PRO:HB2    | 2.20                     | 0.65              |
| 2:B8:241:SER:OG   | 2:B8:250:VAL:O    | 2.14                     | 0.65              |
| 2:C4:175:PRO:HG3  | 2:C4:304:LYS:HG2  | 1.78                     | 0.65              |
| 3:D7:68:LEU:HB3   | 3:D7:96:GLY:HA2   | 1.78                     | 0.65              |
| 4:i:37:GLN:NE2    | 4:i:41:ASN:OD1    | 2.29                     | 0.65              |
| 4:r:154:TYR:HE1   | 4:r:158:THR:HG22  | 1.62                     | 0.65              |
| 4:t:8:SER:HB2     | 4:t:147:HIS:HA    | 1.78                     | 0.65              |
| 2:C4:310:GLY:HA3  | 2:C4:383:ALA:HB2  | 1.78                     | 0.65              |
| 2:D0:137:MET:HE1  | 2:D0:154:LEU:HD11 | 1.79                     | 0.65              |
| 2:D0:229:ARG:HH11 | 2:D0:229:ARG:HG3  | 1.60                     | 0.65              |
| 3:E9:208:TYR:CD1  | 2:F0:326:LYS:HB3  | 2.31                     | 0.65              |
| 1:8:239:LEU:O     | 3:C1:359:LYS:CE   | 2.45                     | 0.65              |
| 2:B4:223:THR:HG23 | 2:B4:225:THR:HG22 | 1.77                     | 0.65              |
| 3:C5:354:CYS:SG   | 3:C5:355:ASP:N    | 2.68                     | 0.65              |
| 2:E6:133:GLN:HG3  | 2:E6:252:VAL:HG22 | 1.79                     | 0.65              |
| 3:A3:7:VAL:HB     | 3:A3:135:ILE:HG22 | 1.79                     | 0.65              |
| 3:A3:308:GLY:HA3  | 3:A3:373:ALA:HB2  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B0:11:GLN:NE2   | 3:B1:245:GLN:O    | 2.30                     | 0.65              |
| 2:B8:269:LEU:HD12 | 2:B8:303:ALA:HB3  | 1.78                     | 0.65              |
| 2:C6:282:TYR:CZ   | 4:n:201:TRP:CZ2   | 2.85                     | 0.65              |
| 2:D6:33:ASP:O     | 2:D6:60:LYS:NZ    | 2.30                     | 0.65              |
| 1:11:239:LEU:HG   | 1:11:240:PRO:HD2  | 1.78                     | 0.65              |
| 3:A7:321:MET:HE2  | 3:A7:326:VAL:CG2  | 2.26                     | 0.65              |
| 3:D5:239:CYS:SG   | 3:D5:247:ASN:HB3  | 2.36                     | 0.65              |
| 4:t:101:GLU:CD    | 4:v:6:PHE:HB2     | 2.18                     | 0.65              |
| 2:A6:282:TYR:CZ   | 4:d:201:TRP:HZ2   | 2.15                     | 0.65              |
| 3:A9:256:ASN:HB2  | 3:A9:350:LYS:HE3  | 1.79                     | 0.65              |
| 3:B3:404:ASP:OD2  | 3:B3:406:MET:HG2  | 1.96                     | 0.65              |
| 3:E9:256:ASN:HD21 | 3:E9:350:LYS:HG2  | 1.60                     | 0.65              |
| 5:k:27:ASP:O      | 4:m:38:LEU:HB3    | 1.97                     | 0.65              |
| 3:A1:117:LEU:HD13 | 3:A1:154:LYS:NZ   | 2.12                     | 0.64              |
| 2:D6:27:GLU:OE1   | 2:D6:243:ARG:NH1  | 2.30                     | 0.64              |
| 2:E8:84:ARG:NH1   | 5:w:155:GLN:HE21  | 1.95                     | 0.64              |
| 4:r:53:GLY:HA2    | 4:r:62:VAL:HG21   | 1.77                     | 0.64              |
| 3:C5:1:MET:N      | 3:C5:128:ASP:OD2  | 2.29                     | 0.64              |
| 2:D2:221:ARG:NH2  | 4:q:190:GLU:O     | 2.30                     | 0.64              |
| 2:E6:218:ASP:O    | 5:x:156:ARG:NH1   | 2.30                     | 0.64              |
| 4:g:115:LEU:HD23  | 4:g:152:LYS:HG3   | 1.79                     | 0.64              |
| 5:w:40:LYS:NZ     | 5:w:113:ASN:OD1   | 2.30                     | 0.64              |
| 1:10:241:PHE:CZ   | 3:C9:356:ILE:CG2  | 2.81                     | 0.64              |
| 1:5:253:ALA:CB    | 2:B4:32:PRO:HG2   | 2.28                     | 0.64              |
| 2:C6:282:TYR:CZ   | 4:n:201:TRP:CH2   | 2.85                     | 0.64              |
| 2:E4:107:HIS:HE2  | 2:E4:151:CYS:HG   | 1.37                     | 0.64              |
| 2:E8:377:MET:HE2  | 2:E8:379:SER:HB3  | 1.80                     | 0.64              |
| 3:E9:221:THR:HA   | 2:F0:325:PRO:CD   | 2.27                     | 0.64              |
| 4:d:14:LYS:HD3    | 4:d:47:LEU:HD23   | 1.79                     | 0.64              |
| 4:m:92:LEU:HD21   | 4:m:110:ILE:HD13  | 1.78                     | 0.64              |
| 3:A9:68:LEU:HB3   | 3:A9:96:GLY:HA2   | 1.80                     | 0.64              |
| 2:B0:73:THR:HA    | 3:B1:46:ARG:NH1   | 2.10                     | 0.64              |
| 2:D8:79:ARG:HG3   | 2:D8:92:LEU:HD12  | 1.78                     | 0.64              |
| 2:E8:84:ARG:CZ    | 5:w:155:GLN:HE21  | 2.11                     | 0.64              |
| 1:19:243:ALA:HB2  | 3:E7:357:PRO:HD2  | 0.81                     | 0.64              |
| 3:A5:284:LEU:HB2  | 3:A9:55:THR:HG21  | 1.78                     | 0.64              |
| 2:B2:282:TYR:OH   | 2:B6:33:ASP:OD1   | 2.13                     | 0.64              |
| 3:C3:30:ILE:HD11  | 3:C3:47:ILE:HD11  | 1.80                     | 0.64              |
| 3:D1:66:MET:CE    | 3:D1:116:VAL:HG11 | 2.27                     | 0.64              |
| 3:D3:56:GLY:O     | 4:o:83:PRO:HB2    | 1.98                     | 0.64              |
| 3:D3:396:HIS:CE1  | 2:D4:261:PRO:O    | 2.43                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D4:96:LYS:CE    | 3:D5:128:ASP:HB2  | 2.27                     | 0.64              |
| 4:r:100:ASN:HB3   | 4:t:6:PHE:CE1     | 2.31                     | 0.64              |
| 3:B3:212:PHE:CZ   | 2:B4:326:LYS:HG2  | 2.33                     | 0.64              |
| 3:C1:164:MET:HB2  | 3:C1:197:ASP:H    | 1.60                     | 0.64              |
| 2:C2:406:HIS:CE1  | 3:C3:261:PRO:HB3  | 2.32                     | 0.64              |
| 2:D0:230:LEU:HD23 | 2:D0:368:LEU:HD21 | 1.80                     | 0.64              |
| 4:m:14:LYS:HB2    | 4:m:47:LEU:HD22   | 1.79                     | 0.64              |
| 2:C2:202:VAL:HG22 | 2:C2:268:MET:HG3  | 1.78                     | 0.64              |
| 3:C5:294:PHE:O    | 3:C5:306:ARG:NH2  | 2.27                     | 0.64              |
| 2:D0:285:GLN:CB   | 2:D4:56:THR:HA    | 2.22                     | 0.64              |
| 2:D4:221:ARG:HG2  | 3:D5:322:SER:HB2  | 1.79                     | 0.64              |
| 2:E6:221:ARG:CG   | 3:E7:322:SER:HB2  | 2.28                     | 0.64              |
| 1:13:247:TYR:CE2  | 2:D4:77:GLU:HB3   | 2.31                     | 0.64              |
| 1:23:240:PRO:HB3  | 4:m:154:TYR:CB    | 2.21                     | 0.64              |
| 2:A6:168:ASN:HD22 | 2:A6:194:LEU:HD11 | 1.63                     | 0.64              |
| 3:B1:293:MET:HE2  | 3:B1:365:VAL:HG11 | 1.78                     | 0.64              |
| 3:C5:97:ALA:HB3   | 3:C5:143:THR:HB   | 1.80                     | 0.64              |
| 2:E4:68:LEU:HD11  | 2:E4:118:SER:HB2  | 1.79                     | 0.64              |
| 2:A8:22:GLU:OE2   | 2:A8:229:ARG:NH1  | 2.30                     | 0.64              |
| 3:C3:166:THR:HB   | 3:C3:199:VAL:HG22 | 1.79                     | 0.64              |
| 2:C8:85:HIS:NE2   | 4:m:99:MET:SD     | 2.71                     | 0.64              |
| 2:E0:96:LYS:HZ1   | 3:E1:129:CYS:N    | 1.96                     | 0.64              |
| 3:A3:186:THR:HG23 | 3:A3:415:MET:HG3  | 1.79                     | 0.64              |
| 2:D4:210:TYR:HB3  | 3:D5:324:LYS:CD   | 2.28                     | 0.64              |
| 3:D5:192:LEU:HD21 | 3:D5:199:VAL:HG11 | 1.80                     | 0.64              |
| 3:E3:2:ARG:HD2    | 3:E3:240:LEU:HD23 | 1.79                     | 0.64              |
| 3:A7:27:GLU:OE2   | 3:A7:241:ARG:NH2  | 2.31                     | 0.63              |
| 3:B9:267:LEU:HD23 | 3:B9:374:ILE:HD11 | 1.80                     | 0.63              |
| 3:C5:257:LEU:HD11 | 3:C5:314:SER:HB3  | 1.80                     | 0.63              |
| 3:E1:176:SER:HB3  | 2:E2:351:PHE:HB2  | 1.79                     | 0.63              |
| 4:s:67:HIS:O      | 4:s:71:LYS:NZ     | 2.30                     | 0.63              |
| 2:A6:214:ARG:NE   | 3:A7:324:LYS:NZ   | 2.45                     | 0.63              |
| 2:B0:82:THR:HG23  | 4:d:101:GLU:OE2   | 1.98                     | 0.63              |
| 3:B3:336:LYS:HA   | 3:B3:336:LYS:CE   | 2.29                     | 0.63              |
| 3:B7:256:ASN:O    | 3:B7:256:ASN:ND2  | 2.32                     | 0.63              |
| 2:C0:285:GLN:HB2  | 2:C4:56:THR:HA    | 1.80                     | 0.63              |
| 2:C4:31:GLN:HE22  | 5:k:65:GLU:H      | 1.45                     | 0.63              |
| 2:C8:221:ARG:HH21 | 4:o:191:GLU:HB3   | 1.63                     | 0.63              |
| 3:C9:317:PHE:HB3  | 3:C9:321:MET:HE1  | 1.80                     | 0.63              |
| 2:E2:259:LEU:HD21 | 2:E2:316:CYS:HB2  | 1.80                     | 0.63              |
| 3:E9:221:THR:HA   | 2:F0:325:PRO:HD2  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:12:246:CYS:HB2  | 3:D3:355:ASP:OD2  | 1.97                     | 0.63              |
| 1:20:253:ALA:HB1  | 2:E8:32:PRO:HG2   | 1.79                     | 0.63              |
| 1:23:240:PRO:CB   | 4:m:154:TYR:CB    | 2.74                     | 0.63              |
| 2:A6:137:MET:HB3  | 2:A6:168:ASN:HA   | 1.80                     | 0.63              |
| 2:C2:399:TYR:O    | 2:C2:402:ARG:NH2  | 2.30                     | 0.63              |
| 2:C4:204:LEU:HD22 | 2:C4:302:MET:SD   | 2.38                     | 0.63              |
| 2:C6:136:LEU:HD22 | 2:C6:167:LEU:HD23 | 1.79                     | 0.63              |
| 2:D0:230:LEU:CD2  | 2:D0:368:LEU:HD21 | 2.28                     | 0.63              |
| 4:r:15:ARG:HG2    | 4:r:45:MET:HE1    | 1.80                     | 0.63              |
| 4:u:59:ASN:HD21   | 5:w:100:CYS:CB    | 2.09                     | 0.63              |
| 2:B2:179:THR:N    | 3:B3:347:ASN:ND2  | 2.46                     | 0.63              |
| 4:t:22:ALA:HB1    | 4:t:38:LEU:CD2    | 2.28                     | 0.63              |
| 1:16:256:LEU:HD23 | 2:E0:31:GLN:CG    | 2.28                     | 0.63              |
| 2:A6:22:GLU:OE2   | 2:A6:229:ARG:NH1  | 2.32                     | 0.63              |
| 2:B0:241:SER:HB2  | 2:B0:249:ASN:HB2  | 1.80                     | 0.63              |
| 3:B1:57:GLY:HA3   | 4:d:83:PRO:HB2    | 1.79                     | 0.63              |
| 3:B9:332:ASN:OD1  | 3:B9:336:LYS:NZ   | 2.32                     | 0.63              |
| 2:C6:135:PHE:HD2  | 2:C6:166:LYS:HG2  | 1.64                     | 0.63              |
| 2:D8:79:ARG:HG2   | 2:D8:92:LEU:HD12  | 1.81                     | 0.63              |
| 4:f:96:TYR:HA     | 4:f:108:ILE:HD11  | 1.81                     | 0.63              |
| 2:A2:218:ASP:OD1  | 4:b:198:ARG:NH1   | 2.31                     | 0.63              |
| 3:A5:132:GLY:HA3  | 3:A5:163:ILE:HG22 | 1.79                     | 0.63              |
| 2:C4:7:ILE:HG21   | 2:C4:153:LEU:CD2  | 2.27                     | 0.63              |
| 2:C4:151:CYS:SG   | 2:C4:193:SER:OG   | 2.53                     | 0.63              |
| 3:E5:57:GLY:HA3   | 4:u:83:PRO:HB2    | 1.79                     | 0.63              |
| 3:F1:239:CYS:SG   | 3:F1:248:SER:N    | 2.69                     | 0.63              |
| 5:k:65:GLU:HA     | 4:m:42:TYR:CE2    | 2.33                     | 0.63              |
| 4:s:84:LYS:HD2    | 4:s:186:CYS:SG    | 2.38                     | 0.63              |
| 2:A0:222:PRO:HD2  | 3:A1:324:LYS:HB3  | 1.80                     | 0.63              |
| 3:A1:207:LEU:HB3  | 3:A1:225:LEU:HD22 | 1.81                     | 0.63              |
| 3:A3:7:VAL:HG11   | 3:A3:151:LEU:HD21 | 1.81                     | 0.63              |
| 2:C6:244:PHE:HB2  | 2:C6:356:ASN:HD21 | 1.64                     | 0.63              |
| 2:D0:90:GLU:HG3   | 2:D0:121:ARG:HD3  | 1.81                     | 0.63              |
| 2:B4:285:GLN:HB3  | 2:B8:57:GLY:H     | 1.63                     | 0.63              |
| 2:C6:339:ARG:O    | 2:C6:342:GLN:NE2  | 2.32                     | 0.63              |
| 3:D1:390:ARG:HG2  | 3:D1:390:ARG:HH21 | 1.63                     | 0.63              |
| 3:D3:49:VAL:HG21  | 3:D3:241:ARG:HG2  | 1.81                     | 0.63              |
| 3:D7:153:SER:HB2  | 3:D7:191:GLN:HE22 | 1.63                     | 0.63              |
| 4:e:63:ILE:CG2    | 4:g:16:ARG:HD3    | 2.27                     | 0.63              |
| 2:C2:10:GLY:HA2   | 2:C2:145:THR:HG23 | 1.81                     | 0.63              |
| 2:D2:210:TYR:CD1  | 3:D3:324:LYS:HD3  | 2.34                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D6:85:HIS:NE2   | 4:q:99:MET:HG2    | 2.14                     | 0.63              |
| 2:E4:369:ALA:HB1  | 5:w:161:PHE:CE1   | 2.33                     | 0.63              |
| 2:E6:221:ARG:CB   | 3:E7:322:SER:CB   | 2.77                     | 0.63              |
| 2:E8:292:THR:HG21 | 2:E8:331:ALA:HB1  | 1.80                     | 0.63              |
| 3:A3:174:LYS:NZ   | 3:A3:205:GLU:OE1  | 2.32                     | 0.62              |
| 2:B4:254:GLU:OE1  | 2:B4:352:LYS:NZ   | 2.32                     | 0.62              |
| 3:C1:221:THR:HG22 | 3:C1:223:GLY:H    | 1.64                     | 0.62              |
| 3:C3:306:ARG:HA   | 3:C3:340:TYR:HE1  | 1.64                     | 0.62              |
| 2:E4:238:LEU:HD11 | 2:E4:378:ILE:HG13 | 1.80                     | 0.62              |
| 2:B2:174:SER:OG   | 2:B2:177:VAL:O    | 2.17                     | 0.62              |
| 3:C3:337:ASN:HB3  | 3:C3:340:TYR:HB2  | 1.79                     | 0.62              |
| 3:C5:248:SER:HA   | 3:C5:252:LYS:HE3  | 1.80                     | 0.62              |
| 2:C6:36:MET:HG2   | 2:C6:36:MET:O     | 2.00                     | 0.62              |
| 2:D0:221:ARG:HB3  | 3:D1:322:SER:HB2  | 1.80                     | 0.62              |
| 2:D4:177:VAL:HG22 | 3:D5:331:LEU:HD22 | 1.81                     | 0.62              |
| 2:E6:364:PRO:CB   | 5:x:161:PHE:CE2   | 2.80                     | 0.62              |
| 3:A3:329:GLN:HA   | 3:A3:332:ASN:HB2  | 1.80                     | 0.62              |
| 3:A5:313:ALA:HB3  | 3:A5:349:MET:HG2  | 1.80                     | 0.62              |
| 2:A8:262:TYR:HB3  | 2:A8:263:PRO:HD2  | 1.81                     | 0.62              |
| 2:B8:76:ASP:HA    | 2:B8:79:ARG:HD2   | 1.80                     | 0.62              |
| 2:C2:221:ARG:HB3  | 3:C3:322:SER:HB3  | 1.81                     | 0.62              |
| 4:e:63:ILE:HG21   | 4:g:16:ARG:CD     | 2.27                     | 0.62              |
| 4:t:19:GLU:HB3    | 4:t:40:PRO:HD2    | 1.80                     | 0.62              |
| 1:5:256:LEU:HD23  | 2:B4:31:GLN:CG    | 2.30                     | 0.62              |
| 3:B3:219:THR:HB   | 2:B4:324:VAL:HG11 | 1.81                     | 0.62              |
| 2:B4:174:SER:OG   | 2:B4:177:VAL:O    | 2.17                     | 0.62              |
| 3:B5:64:ILE:HD11  | 3:B5:123:GLU:HG3  | 1.80                     | 0.62              |
| 2:D2:177:VAL:HG11 | 3:D3:327:ASP:HB3  | 1.82                     | 0.62              |
| 2:E2:184:PRO:HA   | 2:E2:391:MET:HE1  | 1.79                     | 0.62              |
| 2:F0:407:TRP:HE1  | 3:F1:258:ILE:HG13 | 1.64                     | 0.62              |
| 4:a:97:ARG:NH2    | 4:c:7:ALA:HB3     | 2.13                     | 0.62              |
| 1:14:240:PRO:HB3  | 4:s:154:TYR:CD2   | 2.35                     | 0.62              |
| 1:9:242:ASN:O     | 3:C3:362:LYS:NZ   | 2.33                     | 0.62              |
| 3:A3:6:HIS:NE2    | 3:A3:8:GLN:OE1    | 2.32                     | 0.62              |
| 2:B2:11:GLN:HE22  | 3:B3:246:LEU:CD1  | 2.13                     | 0.62              |
| 3:B9:11:GLN:HA    | 3:B9:72:THR:HG21  | 1.81                     | 0.62              |
| 3:C3:165:GLU:OE2  | 3:C3:200:GLN:NE2  | 2.33                     | 0.62              |
| 2:A4:282:TYR:HB2  | 4:c:202:ARG:NH2   | 2.14                     | 0.62              |
| 2:A8:106:GLY:HA3  | 2:A8:148:GLY:HA3  | 1.81                     | 0.62              |
| 2:C2:76:ASP:OD2   | 3:C3:46:ARG:NH2   | 2.30                     | 0.62              |
| 3:C9:323:THR:HA   | 3:C9:326:VAL:HG12 | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E0:96:LYS:HE2   | 3:E1:128:ASP:CG   | 2.25                     | 0.62              |
| 1:4:240:PRO:HG2   | 4:g:154:TYR:HB3   | 1.81                     | 0.62              |
| 3:A5:212:PHE:CB   | 2:A6:326:LYS:HE2  | 2.29                     | 0.62              |
| 2:B6:50:ASN:O     | 2:B6:64:ARG:NH2   | 2.32                     | 0.62              |
| 3:D5:7:VAL:HG11   | 3:D5:151:LEU:CD2  | 2.28                     | 0.62              |
| 2:D6:221:ARG:HA   | 3:D7:324:LYS:CE   | 2.29                     | 0.62              |
| 3:D7:281:TYR:CE1  | 3:E1:58:ARG:CZ    | 2.82                     | 0.62              |
| 2:D8:30:ILE:HG22  | 2:D8:36:MET:HB3   | 1.82                     | 0.62              |
| 3:A1:113:ILE:HG13 | 3:A1:117:LEU:HD12 | 1.82                     | 0.62              |
| 2:A2:221:ARG:HB2  | 3:A3:322:SER:OG   | 2.00                     | 0.62              |
| 3:A5:179:VAL:HB   | 2:A6:351:PHE:O    | 2.00                     | 0.62              |
| 2:B0:11:GLN:HE22  | 3:B1:246:LEU:HA   | 1.64                     | 0.62              |
| 2:B6:282:TYR:HE2  | 2:C0:85:HIS:HB3   | 1.65                     | 0.62              |
| 2:C0:84:ARG:NH2   | 4:i:197:LEU:CD1   | 2.25                     | 0.62              |
| 3:C9:16:ILE:HD11  | 3:C9:229:VAL:HG21 | 1.82                     | 0.62              |
| 2:F0:176:GLN:HG3  | 3:F1:331:LEU:HD21 | 1.82                     | 0.62              |
| 4:f:18:ASN:HD21   | 4:f:46:ASP:H      | 1.47                     | 0.62              |
| 1:10:244:GLN:H    | 3:C9:320:ARG:NH1  | 1.98                     | 0.62              |
| 2:A0:3:GLU:OE2    | 2:A0:64:ARG:NH1   | 2.33                     | 0.62              |
| 2:B8:11:GLN:NE2   | 3:B9:246:LEU:HD12 | 2.14                     | 0.62              |
| 3:C1:362:LYS:HE2  | 5:k:126:THR:HB    | 1.81                     | 0.62              |
| 3:C3:293:MET:HE1  | 3:C3:365:VAL:HG21 | 1.82                     | 0.62              |
| 2:D0:221:ARG:HB3  | 3:D1:322:SER:CB   | 2.30                     | 0.62              |
| 2:D0:292:THR:HG21 | 2:D0:331:ALA:HB1  | 1.80                     | 0.62              |
| 3:D7:169:VAL:HG12 | 3:D7:202:ILE:HB   | 1.81                     | 0.62              |
| 3:E9:57:GLY:HA3   | 5:w:44:SER:OG     | 2.00                     | 0.62              |
| 4:r:101:GLU:HG3   | 4:t:6:PHE:HB2     | 1.81                     | 0.62              |
| 1:2:240:PRO:CG    | 4:e:154:TYR:CB    | 2.73                     | 0.62              |
| 2:B2:177:VAL:HG13 | 3:B3:331:LEU:HD22 | 1.81                     | 0.62              |
| 3:B7:281:TYR:HD2  | 3:C1:87:PRO:HD2   | 1.64                     | 0.62              |
| 2:C0:399:TYR:O    | 2:C0:402:ARG:NH2  | 2.32                     | 0.62              |
| 3:C1:280:GLN:O    | 3:C5:58:ARG:HD3   | 1.99                     | 0.62              |
| 3:C7:135:ILE:HB   | 3:C7:166:THR:HG22 | 1.81                     | 0.62              |
| 2:C8:181:VAL:HG12 | 3:C9:256:ASN:OD1  | 2.00                     | 0.62              |
| 2:D6:30:ILE:HG22  | 2:D6:36:MET:HB3   | 1.82                     | 0.62              |
| 2:E8:274:PRO:HB2  | 2:E8:276:ILE:HG12 | 1.82                     | 0.62              |
| 2:F0:218:ASP:OD2  | 2:F0:280:LYS:NZ   | 2.31                     | 0.62              |
| 5:k:100:CYS:SG    | 5:k:104:LYS:NZ    | 2.73                     | 0.62              |
| 1:10:254:LYS:HZ2  | 2:C8:22:GLU:HG2   | 1.65                     | 0.61              |
| 1:11:255:PRO:HD2  | 2:D0:364:PRO:CB   | 2.29                     | 0.61              |
| 2:A0:290:GLU:HB2  | 2:A4:124:LYS:HE2  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:286:LEU:O    | 2:B2:373:ARG:NH1  | 2.29                     | 0.61              |
| 2:C6:31:GLN:NE2   | 2:C6:33:ASP:OD2   | 2.33                     | 0.61              |
| 3:C9:245:GLN:HB2  | 3:C9:353:VAL:HG13 | 1.82                     | 0.61              |
| 3:D9:6:HIS:HE1    | 3:D9:8:GLN:HE21   | 1.47                     | 0.61              |
| 4:j:59:ASN:HD22   | 5:l:100:CYS:CB    | 2.13                     | 0.61              |
| 1:8:241:PHE:CZ    | 3:C1:356:ILE:CG2  | 2.81                     | 0.61              |
| 2:A6:80:THR:HA    | 2:A6:84:ARG:HH21  | 1.63                     | 0.61              |
| 3:C3:249:ASP:H    | 3:C3:252:LYS:HB2  | 1.65                     | 0.61              |
| 2:D2:178:SER:OG   | 3:D3:347:ASN:ND2  | 2.27                     | 0.61              |
| 3:D3:219:THR:HA   | 2:D4:326:LYS:HE2  | 1.80                     | 0.61              |
| 4:f:198:ARG:HG3   | 4:f:198:ARG:HH11  | 1.65                     | 0.61              |
| 1:15:244:GLN:NE2  | 4:t:163:SER:O     | 2.32                     | 0.61              |
| 2:A2:259:LEU:HD21 | 2:A2:316:CYS:HB2  | 1.83                     | 0.61              |
| 3:B7:281:TYR:CD2  | 3:C1:87:PRO:CD    | 2.83                     | 0.61              |
| 3:B9:39:ASP:HA    | 4:h:90:PRO:HG3    | 1.82                     | 0.61              |
| 3:E7:332:ASN:OD1  | 3:E7:336:LYS:NZ   | 2.32                     | 0.61              |
| 4:b:97:ARG:HH22   | 4:d:7:ALA:CB      | 2.08                     | 0.61              |
| 4:p:18:ASN:HD22   | 4:p:45:MET:HG2    | 1.65                     | 0.61              |
| 4:v:191:GLU:OE1   | 4:v:198:ARG:NH2   | 2.33                     | 0.61              |
| 2:A2:282:TYR:CD1  | 4:b:202:ARG:HD3   | 2.35                     | 0.61              |
| 2:D2:136:LEU:HD23 | 2:D2:235:ILE:HD11 | 1.81                     | 0.61              |
| 3:D5:253:LEU:HD12 | 3:D5:316:MET:HE1  | 1.82                     | 0.61              |
| 3:F1:244:GLY:HA2  | 3:F1:355:ASP:HB2  | 1.82                     | 0.61              |
| 4:c:112:PHE:CG    | 4:c:129:MET:HE1   | 2.35                     | 0.61              |
| 4:t:5:VAL:HG11    | 4:t:149:ARG:HD3   | 1.83                     | 0.61              |
| 2:A2:91:GLN:HA    | 2:A2:121:ARG:HH12 | 1.65                     | 0.61              |
| 2:A6:282:TYR:CE2  | 4:d:201:TRP:HZ2   | 2.19                     | 0.61              |
| 3:C7:1:MET:N      | 3:C7:128:ASP:OD2  | 2.33                     | 0.61              |
| 3:C7:165:GLU:OE2  | 3:C7:200:GLN:NE2  | 2.33                     | 0.61              |
| 2:C8:50:ASN:O     | 2:C8:64:ARG:NH2   | 2.32                     | 0.61              |
| 2:D0:206:ASN:HD22 | 2:D0:227:LEU:HD23 | 1.65                     | 0.61              |
| 2:E0:96:LYS:HE2   | 3:E1:128:ASP:CB   | 2.29                     | 0.61              |
| 4:s:67:HIS:CE1    | 4:u:20:GLU:OE1    | 2.54                     | 0.61              |
| 3:A5:284:LEU:HB3  | 3:A9:55:THR:HG21  | 1.81                     | 0.61              |
| 2:A8:209:ILE:HA   | 2:A8:212:ILE:HG22 | 1.81                     | 0.61              |
| 3:C9:397:TRP:CZ2  | 2:D0:256:GLN:O    | 2.53                     | 0.61              |
| 3:D3:291:GLN:CG   | 3:D7:122:LYS:NZ   | 2.63                     | 0.61              |
| 4:c:7:ALA:O       | 4:c:161:TYR:OH    | 2.17                     | 0.61              |
| 4:c:15:ARG:HG2    | 4:c:45:MET:HE1    | 1.82                     | 0.61              |
| 3:A7:107:THR:OG1  | 3:A7:108:GLU:OE1  | 2.18                     | 0.61              |
| 2:C2:73:THR:OG1   | 3:C3:46:ARG:CZ    | 2.48                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D0:223:THR:HG23 | 2:D0:225:THR:HG22 | 1.82                     | 0.61              |
| 2:D0:370:LYS:HD3  | 4:p:203:ASN:OD1   | 2.01                     | 0.61              |
| 3:D3:248:SER:HA   | 3:D3:252:LYS:HD3  | 1.81                     | 0.61              |
| 3:D3:397:TRP:CE2  | 2:D4:256:GLN:O    | 2.54                     | 0.61              |
| 3:D7:49:VAL:HG21  | 3:D7:241:ARG:HG2  | 1.83                     | 0.61              |
| 2:D8:238:LEU:HD11 | 2:D8:255:PHE:HE2  | 1.65                     | 0.61              |
| 2:E4:398:MET:HA   | 2:E4:398:MET:HE3  | 1.83                     | 0.61              |
| 4:n:184:PRO:HB3   | 4:n:189:LEU:HB2   | 1.82                     | 0.61              |
| 1:0:244:GLN:HE21  | 4:c:162:GLY:HA3   | 1.57                     | 0.61              |
| 1:16:256:LEU:HD11 | 2:E0:30:ILE:O     | 2.00                     | 0.61              |
| 1:5:240:PRO:HB3   | 4:h:154:TYR:HD2   | 1.65                     | 0.61              |
| 3:D7:139:LEU:HA   | 3:D7:145:SER:HB2  | 1.83                     | 0.61              |
| 4:m:171:ILE:HD11  | 4:m:179:GLU:HB2   | 1.83                     | 0.61              |
| 4:t:198:ARG:HG2   | 4:t:198:ARG:NH1   | 2.14                     | 0.61              |
| 3:A1:130:LEU:O    | 3:A1:162:ARG:NH1  | 2.34                     | 0.61              |
| 2:A6:214:ARG:HH21 | 3:A7:324:LYS:NZ   | 1.99                     | 0.61              |
| 3:A7:27:GLU:HA    | 3:A7:359:LYS:HD2  | 1.82                     | 0.61              |
| 3:C3:20:PHE:HD2   | 3:C3:233:MET:HE3  | 1.66                     | 0.61              |
| 2:C4:31:GLN:NE2   | 5:k:65:GLU:H      | 1.99                     | 0.61              |
| 3:C5:133:PHE:HB2  | 3:C5:164:MET:HB3  | 1.83                     | 0.61              |
| 2:D2:407:TRP:CE2  | 3:D3:255:VAL:HA   | 2.35                     | 0.61              |
| 2:D8:36:MET:HG2   | 2:D8:61:HIS:NE2   | 2.16                     | 0.61              |
| 1:11:244:GLN:O    | 3:D1:355:ASP:OD2  | 2.19                     | 0.61              |
| 1:9:257:PRO:CG    | 2:C2:26:LEU:HD13  | 2.29                     | 0.61              |
| 2:A0:222:PRO:HD2  | 3:A1:324:LYS:HG2  | 1.83                     | 0.61              |
| 2:C4:271:SER:HB3  | 2:C4:377:MET:HB3  | 1.82                     | 0.61              |
| 3:C9:354:CYS:SG   | 3:C9:355:ASP:N    | 2.65                     | 0.61              |
| 3:D3:220:PRO:HD2  | 2:D4:326:LYS:CD   | 2.30                     | 0.61              |
| 4:q:14:LYS:HD3    | 4:q:47:LEU:HD12   | 1.83                     | 0.61              |
| 4:t:72:SER:HB3    | 4:t:108:ILE:HG22  | 1.81                     | 0.61              |
| 2:A2:204:LEU:CD2  | 2:A2:231:ILE:HD12 | 2.31                     | 0.60              |
| 2:A2:204:LEU:HD23 | 2:A2:231:ILE:HD12 | 1.82                     | 0.60              |
| 3:B7:281:TYR:CD2  | 3:C1:87:PRO:HD3   | 2.35                     | 0.60              |
| 3:B7:325:GLU:HA   | 3:B7:328:GLU:HG3  | 1.83                     | 0.60              |
| 3:C9:232:ALA:HB1  | 3:C9:268:ILE:HG12 | 1.83                     | 0.60              |
| 3:E5:248:SER:HA   | 3:E5:252:LYS:HG2  | 1.83                     | 0.60              |
| 2:E6:26:LEU:HD13  | 2:E6:363:VAL:HG12 | 1.82                     | 0.60              |
| 3:E9:175:VAL:HG23 | 2:F0:332:VAL:HG11 | 1.82                     | 0.60              |
| 1:13:253:ALA:HB2  | 2:D4:32:PRO:HG3   | 1.83                     | 0.60              |
| 2:A8:285:GLN:OE1  | 2:B2:57:GLY:HA2   | 2.00                     | 0.60              |
| 3:C9:7:VAL:HB     | 3:C9:135:ILE:HG12 | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D1:390:ARG:HG2  | 3:D1:390:ARG:NH2  | 2.16                     | 0.60              |
| 3:D3:238:CYS:SG   | 3:D3:318:ARG:NE   | 2.73                     | 0.60              |
| 2:E4:119:LEU:HD12 | 2:E4:156:ARG:CD   | 2.28                     | 0.60              |
| 4:m:10:LEU:HG     | 4:m:143:ILE:HG22  | 1.83                     | 0.60              |
| 1:8:243:ALA:CB    | 3:C1:357:PRO:HD3  | 2.31                     | 0.60              |
| 3:A5:221:THR:HG23 | 3:A5:223:GLY:H    | 1.66                     | 0.60              |
| 2:B6:213:CYS:HA   | 2:B6:217:LEU:HD13 | 1.82                     | 0.60              |
| 2:C2:394:LYS:HG2  | 3:C3:346:PRO:HG3  | 1.83                     | 0.60              |
| 3:C7:291:GLN:HE22 | 3:D1:125:GLU:CD   | 2.08                     | 0.60              |
| 3:D3:220:PRO:CG   | 2:D4:326:LYS:HD3  | 2.31                     | 0.60              |
| 3:E1:198:GLU:HB2  | 3:E1:266:PHE:HE2  | 1.66                     | 0.60              |
| 3:E9:10:GLY:HA2   | 3:E9:143:THR:HG23 | 1.82                     | 0.60              |
| 4:j:151:MET:HE2   | 4:j:154:TYR:HA    | 1.82                     | 0.60              |
| 3:B1:135:ILE:HB   | 3:B1:166:THR:HG22 | 1.82                     | 0.60              |
| 2:C0:223:THR:HG23 | 2:C0:225:THR:HG22 | 1.83                     | 0.60              |
| 2:D0:50:ASN:O     | 2:D0:64:ARG:NH2   | 2.32                     | 0.60              |
| 2:D4:221:ARG:CG   | 3:D5:322:SER:HB2  | 2.32                     | 0.60              |
| 3:D9:12:CYS:SG    | 3:D9:13:GLY:N     | 2.74                     | 0.60              |
| 2:E4:283:HIS:NE2  | 2:E8:85:HIS:O     | 2.35                     | 0.60              |
| 5:w:17:GLN:NE2    | 5:w:20:ASN:OD1    | 2.33                     | 0.60              |
| 1:5:256:LEU:CD1   | 2:B4:26:LEU:HD12  | 2.31                     | 0.60              |
| 2:A8:285:GLN:CB   | 2:B2:56:THR:HA    | 2.30                     | 0.60              |
| 2:B6:230:LEU:HD21 | 2:B6:368:LEU:HD11 | 1.84                     | 0.60              |
| 3:D3:68:LEU:HB3   | 3:D3:96:GLY:HA2   | 1.83                     | 0.60              |
| 3:D9:291:GLN:NE2  | 3:E3:122:LYS:HD2  | 2.15                     | 0.60              |
| 2:E6:280:LYS:HE2  | 2:F0:89:PRO:HD2   | 1.84                     | 0.60              |
| 4:c:53:GLY:HA2    | 4:c:62:VAL:HG21   | 1.82                     | 0.60              |
| 1:5:248:ARG:NH2   | 2:B4:77:GLU:HB2   | 2.17                     | 0.60              |
| 3:A9:167:PHE:CE2  | 3:A9:233:MET:HG2  | 2.36                     | 0.60              |
| 2:B4:223:THR:CG2  | 2:B4:225:THR:HG22 | 2.31                     | 0.60              |
| 2:C4:387:VAL:HA   | 2:C4:390:ARG:HH21 | 1.65                     | 0.60              |
| 3:C5:179:VAL:HG22 | 2:C6:258:ASN:OD1  | 2.01                     | 0.60              |
| 2:D2:328:VAL:HG21 | 2:D2:355:ILE:HD11 | 1.83                     | 0.60              |
| 3:E9:212:PHE:HE1  | 2:F0:326:LYS:NZ   | 1.98                     | 0.60              |
| 2:A2:207:GLU:HG3  | 2:A2:304:LYS:HE3  | 1.84                     | 0.60              |
| 3:C9:67:ASP:OD2   | 3:C9:72:THR:OG1   | 2.20                     | 0.60              |
| 3:D1:39:ASP:HA    | 4:n:90:PRO:HG3    | 1.84                     | 0.60              |
| 2:D4:97:GLU:HB2   | 2:D4:110:ILE:CD1  | 2.26                     | 0.60              |
| 3:E5:113:ILE:HD11 | 3:E5:147:MET:HG3  | 1.83                     | 0.60              |
| 4:d:106:GLN:NE2   | 4:f:6:PHE:HZ      | 1.99                     | 0.60              |
| 5:l:144:MET:HE1   | 5:l:156:ARG:HB3   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:v:85:CYS:SG     | 4:v:167:VAL:HG22  | 2.41                     | 0.60              |
| 3:A7:117:LEU:HA   | 3:A7:120:VAL:HG12 | 1.84                     | 0.60              |
| 3:B1:135:ILE:HG13 | 3:B1:152:ILE:HG12 | 1.84                     | 0.60              |
| 3:D3:202:ILE:HD11 | 3:D3:268:ILE:HD12 | 1.84                     | 0.60              |
| 3:D7:281:TYR:HE1  | 3:E1:58:ARG:NH2   | 2.00                     | 0.60              |
| 3:E7:100:ASN:HB3  | 3:E7:103:LYS:HG2  | 1.84                     | 0.60              |
| 4:j:191:GLU:OE1   | 4:j:194:ARG:NH2   | 2.35                     | 0.60              |
| 1:13:244:GLN:HG2  | 4:r:162:GLY:HA3   | 1.79                     | 0.60              |
| 3:B9:57:GLY:HA3   | 4:h:83:PRO:HB2    | 1.83                     | 0.60              |
| 4:g:129:MET:HE2   | 4:g:131:TRP:HE1   | 1.66                     | 0.60              |
| 4:o:14:LYS:HB2    | 4:o:47:LEU:HD22   | 1.84                     | 0.60              |
| 1:17:253:ALA:CB   | 2:E2:32:PRO:HG2   | 2.32                     | 0.60              |
| 1:5:248:ARG:HH21  | 2:B4:77:GLU:HB2   | 1.67                     | 0.60              |
| 2:A6:279:GLU:OE1  | 4:d:198:ARG:HD3   | 2.02                     | 0.60              |
| 2:A8:208:ALA:HB2  | 2:A8:304:LYS:HB2  | 1.84                     | 0.60              |
| 2:B0:73:THR:CB    | 3:B1:46:ARG:HE    | 2.14                     | 0.60              |
| 3:B5:281:TYR:O    | 3:B9:54:ALA:HB1   | 2.01                     | 0.60              |
| 2:B6:396:ASP:OD2  | 2:B6:422:ARG:NH2  | 2.35                     | 0.60              |
| 2:C6:319:TYR:CD1  | 2:C6:375:VAL:HG22 | 2.37                     | 0.60              |
| 3:D3:175:VAL:HG12 | 2:D4:336:LYS:HG3  | 1.83                     | 0.60              |
| 3:D5:209:ASP:OD1  | 3:D5:213:ARG:NH1  | 2.35                     | 0.60              |
| 2:E6:101:ASN:HB3  | 2:E6:182:VAL:HG11 | 1.84                     | 0.60              |
| 2:E6:282:TYR:CD2  | 5:x:160:ARG:HD3   | 2.37                     | 0.60              |
| 4:f:14:LYS:HG2    | 4:f:45:MET:HE3    | 1.84                     | 0.60              |
| 1:21:238:THR:CG2  | 3:F1:29:GLY:HA2   | 2.30                     | 0.59              |
| 2:A6:241:SER:OG   | 2:A6:250:VAL:O    | 2.19                     | 0.59              |
| 2:C2:283:HIS:NE2  | 2:C6:85:HIS:HB3   | 2.17                     | 0.59              |
| 2:C4:221:ARG:NH2  | 4:m:190:GLU:HB3   | 2.17                     | 0.59              |
| 4:t:22:ALA:HB1    | 4:t:38:LEU:HD21   | 1.84                     | 0.59              |
| 2:A0:88:HIS:HB3   | 2:A0:91:GLN:HB2   | 1.84                     | 0.59              |
| 2:A0:309:HIS:NE2  | 2:A0:386:GLU:OE2  | 2.32                     | 0.59              |
| 2:A2:26:LEU:HD22  | 2:A2:364:PRO:HD3  | 1.83                     | 0.59              |
| 3:C7:354:CYS:SG   | 3:C7:355:ASP:N    | 2.75                     | 0.59              |
| 3:E3:248:SER:HA   | 3:E3:252:LYS:HG2  | 1.84                     | 0.59              |
| 2:E4:229:ARG:HD2  | 2:E4:363:VAL:HG21 | 1.82                     | 0.59              |
| 4:e:73:VAL:HG12   | 4:e:109:GLU:HB3   | 1.84                     | 0.59              |
| 4:s:67:HIS:NE2    | 4:u:20:GLU:OE1    | 2.35                     | 0.59              |
| 3:A9:107:THR:OG1  | 3:A9:108:GLU:OE1  | 2.20                     | 0.59              |
| 2:C4:70:LEU:HD13  | 2:C4:95:GLY:HA3   | 1.84                     | 0.59              |
| 3:C7:139:LEU:HD13 | 3:C7:168:SER:HB2  | 1.82                     | 0.59              |
| 3:E5:105:HIS:HD2  | 3:E5:150:LEU:HD22 | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A1:140:GLY:O    | 3:A1:184:ASN:ND2  | 2.33                     | 0.59              |
| 2:A2:282:TYR:HD1  | 4:b:202:ARG:HD3   | 1.67                     | 0.59              |
| 2:A4:191:THR:HA   | 2:A4:194:LEU:HG   | 1.84                     | 0.59              |
| 3:B5:57:GLY:CA    | 4:f:83:PRO:CB     | 2.75                     | 0.59              |
| 2:B6:282:TYR:CE2  | 2:C0:85:HIS:ND1   | 2.71                     | 0.59              |
| 3:E3:215:LEU:HD21 | 3:E3:273:LEU:HD22 | 1.84                     | 0.59              |
| 2:E6:71:GLU:HB2   | 2:E6:98:ASP:HB3   | 1.84                     | 0.59              |
| 2:E8:269:LEU:HD21 | 2:E8:384:ILE:HD11 | 1.83                     | 0.59              |
| 4:b:145:LYS:HE2   | 4:b:150:VAL:HG23  | 1.84                     | 0.59              |
| 4:d:172:VAL:HG23  | 4:d:180:ALA:HB3   | 1.84                     | 0.59              |
| 3:A7:33:THR:O     | 3:A7:58:ARG:NH2   | 2.35                     | 0.59              |
| 2:C4:2:ARG:CG     | 2:C4:2:ARG:HD2    | 2.14                     | 0.59              |
| 2:C6:282:TYR:CD2  | 4:n:202:ARG:CD    | 2.86                     | 0.59              |
| 2:D0:335:ILE:HG23 | 2:D0:341:ILE:HD13 | 1.84                     | 0.59              |
| 2:F0:269:LEU:HD11 | 2:F0:384:ILE:HD11 | 1.84                     | 0.59              |
| 4:e:14:LYS:HB2    | 4:e:47:LEU:HD22   | 1.84                     | 0.59              |
| 3:A3:249:ASP:H    | 3:A3:252:LYS:HB2  | 1.65                     | 0.59              |
| 3:B1:238:CYS:SG   | 3:B1:241:ARG:NH2  | 2.76                     | 0.59              |
| 2:C6:304:LYS:O    | 2:C6:304:LYS:HD3  | 2.03                     | 0.59              |
| 2:D2:250:VAL:CG1  | 2:D2:318:MET:HE1  | 2.32                     | 0.59              |
| 3:D9:311:LEU:HD12 | 3:D9:342:VAL:HG11 | 1.83                     | 0.59              |
| 2:E8:311:LYS:HE2  | 2:E8:344:VAL:HA   | 1.85                     | 0.59              |
| 1:22:247:TYR:OH   | 2:C6:18:ASN:HB2   | 2.03                     | 0.59              |
| 1:5:240:PRO:HB2   | 4:h:154:TYR:HB3   | 1.85                     | 0.59              |
| 2:A0:290:GLU:HB3  | 2:A4:124:LYS:NZ   | 2.17                     | 0.59              |
| 2:A2:195:LEU:HD21 | 2:A2:264:ARG:HE   | 1.66                     | 0.59              |
| 3:A9:27:GLU:OE2   | 3:A9:241:ARG:NH1  | 2.35                     | 0.59              |
| 2:B8:109:THR:HG22 | 2:B8:110:ILE:HG23 | 1.84                     | 0.59              |
| 2:C2:51:THR:HG23  | 2:C2:52:PHE:HD1   | 1.66                     | 0.59              |
| 3:C5:117:LEU:HD11 | 3:C5:154:LYS:HB3  | 1.85                     | 0.59              |
| 3:C7:178:THR:OG1  | 3:C7:181:GLU:OE2  | 2.21                     | 0.59              |
| 3:A1:282:ARG:HA   | 3:A5:86:ARG:NH1   | 2.18                     | 0.59              |
| 3:A5:397:TRP:CH2  | 2:A6:256:GLN:HB3  | 2.38                     | 0.59              |
| 2:A6:254:GLU:O    | 2:A6:258:ASN:ND2  | 2.36                     | 0.59              |
| 2:C0:280:LYS:HA   | 2:C4:89:PRO:HG2   | 1.84                     | 0.59              |
| 3:D1:283:ALA:HB2  | 3:D5:53:GLU:O     | 2.03                     | 0.59              |
| 2:D4:210:TYR:CG   | 3:D5:324:LYS:HD3  | 2.38                     | 0.59              |
| 3:D9:139:LEU:HD12 | 3:D9:170:PHE:HE1  | 1.66                     | 0.59              |
| 2:E0:163:LYS:HE2  | 2:E0:163:LYS:CA   | 2.31                     | 0.59              |
| 2:E2:88:HIS:HB3   | 2:E2:91:GLN:HG2   | 1.84                     | 0.59              |
| 3:E5:256:ASN:HD21 | 3:E5:350:LYS:HG2  | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:35:THR:CG2   | 4:v:83:PRO:HG3    | 2.31                     | 0.59              |
| 3:E9:113:ILE:HA   | 3:E9:116:VAL:HG12 | 1.85                     | 0.59              |
| 5:w:38:PHE:HE2    | 5:w:132:ILE:HD12  | 1.68                     | 0.59              |
| 2:B0:53:PHE:HB3   | 2:B0:61:HIS:HB3   | 1.83                     | 0.59              |
| 3:B5:334:GLN:HE21 | 3:B5:349:MET:HG2  | 1.67                     | 0.59              |
| 3:C3:68:LEU:HD12  | 3:C3:143:THR:HG22 | 1.85                     | 0.59              |
| 3:D1:281:TYR:HD2  | 3:D5:87:PRO:HD3   | 1.67                     | 0.59              |
| 2:D2:182:VAL:HG11 | 3:D3:255:VAL:HG12 | 1.84                     | 0.59              |
| 2:D4:221:ARG:HG3  | 3:D5:322:SER:CB   | 2.32                     | 0.59              |
| 3:D5:248:SER:HA   | 3:D5:252:LYS:HG2  | 1.84                     | 0.59              |
| 2:E2:76:ASP:OD1   | 2:E2:79:ARG:NH2   | 2.35                     | 0.59              |
| 4:i:96:TYR:HA     | 4:i:108:ILE:HD11  | 1.85                     | 0.59              |
| 1:23:257:PRO:CG   | 2:C4:26:LEU:HD12  | 2.32                     | 0.59              |
| 2:A0:132:LEU:HG   | 2:A0:164:LYS:HE2  | 1.85                     | 0.59              |
| 2:B0:222:PRO:HD2  | 3:B1:324:LYS:HB3  | 1.85                     | 0.59              |
| 2:C0:84:ARG:HH21  | 4:i:197:LEU:HD11  | 1.57                     | 0.59              |
| 3:C9:7:VAL:CG1    | 3:C9:66:MET:HE3   | 2.32                     | 0.59              |
| 2:E0:229:ARG:HG3  | 2:E0:229:ARG:NH1  | 2.18                     | 0.59              |
| 4:u:14:LYS:NZ     | 4:u:45:MET:SD     | 2.73                     | 0.59              |
| 2:A6:214:ARG:HE   | 3:A7:324:LYS:CE   | 2.16                     | 0.58              |
| 2:A8:285:GLN:OE1  | 2:B2:57:GLY:CA    | 2.51                     | 0.58              |
| 2:B2:177:VAL:HG12 | 3:B3:331:LEU:HB2  | 1.83                     | 0.58              |
| 3:B9:272:PRO:HG3  | 3:B9:284:LEU:HD11 | 1.84                     | 0.58              |
| 2:C0:33:ASP:O     | 2:C0:60:LYS:NZ    | 2.35                     | 0.58              |
| 3:C1:248:SER:HA   | 3:C1:252:LYS:HG3  | 1.85                     | 0.58              |
| 3:C5:135:ILE:HG12 | 3:C5:166:THR:HG22 | 1.85                     | 0.58              |
| 2:C8:168:ASN:ND2  | 2:C8:170:CYS:SG   | 2.76                     | 0.58              |
| 2:D2:217:LEU:HD11 | 2:D2:275:ILE:HG22 | 1.85                     | 0.58              |
| 2:D4:90:GLU:HB3   | 2:D4:121:ARG:HD3  | 1.85                     | 0.58              |
| 4:m:64:PRO:HD2    | 4:m:67:HIS:CE1    | 2.37                     | 0.58              |
| 4:u:130:PRO:HB3   | 5:w:107:GLU:OE2   | 2.02                     | 0.58              |
| 2:A0:229:ARG:HD3  | 2:A0:363:VAL:HG21 | 1.85                     | 0.58              |
| 3:A9:263:LEU:H    | 3:A9:263:LEU:HD23 | 1.67                     | 0.58              |
| 3:B1:237:THR:HG22 | 3:B1:250:LEU:HD11 | 1.84                     | 0.58              |
| 3:C1:253:LEU:HD11 | 3:C1:368:VAL:HG21 | 1.85                     | 0.58              |
| 5:w:15:ARG:NH1    | 5:w:91:PRO:O      | 2.32                     | 0.58              |
| 1:15:253:ALA:HB2  | 2:D8:82:THR:CG2   | 2.33                     | 0.58              |
| 3:B1:171:PRO:O    | 3:B1:380:ARG:NH1  | 2.34                     | 0.58              |
| 2:B6:329:ASN:HA   | 2:B6:332:VAL:HG12 | 1.83                     | 0.58              |
| 2:C8:392:ASP:OD1  | 2:C8:422:ARG:NE   | 2.35                     | 0.58              |
| 3:D3:107:THR:HG21 | 3:D3:401:GLU:HB2  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D6:286:LEU:O    | 2:D6:373:ARG:NH1  | 2.32                     | 0.58              |
| 4:q:14:LYS:HB2    | 4:q:47:LEU:HD12   | 1.85                     | 0.58              |
| 1:21:256:LEU:HD21 | 2:F0:31:GLN:CG    | 2.27                     | 0.58              |
| 3:A9:73:MET:HG2   | 3:A9:92:PHE:CE1   | 2.37                     | 0.58              |
| 2:B2:406:HIS:HA   | 2:B2:409:VAL:HG12 | 1.85                     | 0.58              |
| 2:C2:259:LEU:HD21 | 2:C2:316:CYS:HB2  | 1.84                     | 0.58              |
| 3:C9:12:CYS:HB3   | 3:C9:138:SER:HB2  | 1.85                     | 0.58              |
| 3:D9:284:LEU:H    | 3:E3:55:THR:HB    | 1.66                     | 0.58              |
| 3:E9:305:PRO:HB2  | 3:E9:310:TYR:HE1  | 1.68                     | 0.58              |
| 4:f:14:LYS:HB2    | 4:f:47:LEU:HD12   | 1.84                     | 0.58              |
| 1:10:254:LYS:NZ   | 2:C8:22:GLU:CG    | 2.65                     | 0.58              |
| 1:22:241:PHE:CZ   | 3:C7:356:ILE:HG23 | 2.39                     | 0.58              |
| 2:A6:119:LEU:HD13 | 2:A6:122:ILE:HD11 | 1.85                     | 0.58              |
| 3:A9:282:ARG:O    | 3:B3:55:THR:HG22  | 2.03                     | 0.58              |
| 2:B2:107:HIS:HE2  | 2:B2:151:CYS:HG   | 1.49                     | 0.58              |
| 2:D2:69:ASP:OD1   | 2:D2:70:LEU:N     | 2.36                     | 0.58              |
| 2:E4:338:LYS:HZ3  | 2:E4:340:THR:HG22 | 1.68                     | 0.58              |
| 3:F1:248:SER:OG   | 3:F1:350:LYS:NZ   | 2.37                     | 0.58              |
| 1:2:245:SER:OG    | 2:A8:77:GLU:OE2   | 2.20                     | 0.58              |
| 3:A3:207:LEU:HB3  | 3:A3:225:LEU:HD22 | 1.85                     | 0.58              |
| 3:A3:330:MET:HA   | 3:A3:330:MET:HE3  | 1.86                     | 0.58              |
| 3:A9:220:PRO:HD2  | 2:B0:326:LYS:HB2  | 1.85                     | 0.58              |
| 2:B2:240:ALA:HB1  | 2:B2:356:ASN:HD22 | 1.68                     | 0.58              |
| 3:B9:320:ARG:NH2  | 4:j:188:GLY:HA2   | 2.16                     | 0.58              |
| 2:C6:282:TYR:HB2  | 4:n:202:ARG:HD2   | 1.85                     | 0.58              |
| 2:D2:407:TRP:CE3  | 3:D3:255:VAL:HG22 | 2.38                     | 0.58              |
| 4:e:152:LYS:NZ    | 4:e:152:LYS:HB3   | 2.19                     | 0.58              |
| 4:f:117:ARG:HH12  | 4:f:152:LYS:HE2   | 1.68                     | 0.58              |
| 4:n:97:ARG:O      | 4:n:101:GLU:HB3   | 2.04                     | 0.58              |
| 3:A3:117:LEU:HA   | 3:A3:120:VAL:HG12 | 1.86                     | 0.58              |
| 3:A5:212:PHE:HB2  | 2:A6:326:LYS:HE2  | 1.85                     | 0.58              |
| 2:C8:386:GLU:OE1  | 2:C8:390:ARG:NH1  | 2.37                     | 0.58              |
| 2:D2:262:TYR:HB3  | 2:D2:263:PRO:HD2  | 1.85                     | 0.58              |
| 2:D6:138:PHE:HZ   | 2:D6:235:ILE:HD12 | 1.68                     | 0.58              |
| 2:D8:276:ILE:HD12 | 2:D8:281:ALA:HA   | 1.86                     | 0.58              |
| 3:E9:398:TYR:HB3  | 3:E9:403:MET:HG3  | 1.84                     | 0.58              |
| 4:t:66:SER:CB     | 4:v:23:LEU:HD13   | 2.34                     | 0.58              |
| 3:A1:49:VAL:HG11  | 3:A1:241:ARG:HG2  | 1.86                     | 0.58              |
| 3:A3:7:VAL:HG11   | 3:A3:151:LEU:CD2  | 2.34                     | 0.58              |
| 2:C0:202:VAL:HA   | 2:C0:268:MET:HB2  | 1.86                     | 0.58              |
| 2:C8:174:SER:OG   | 2:C8:177:VAL:O    | 2.22                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D7:334:GLN:HE21 | 3:D7:349:MET:HG2  | 1.68                     | 0.58              |
| 2:E4:71:GLU:HB3   | 2:E4:98:ASP:HB2   | 1.85                     | 0.58              |
| 1:7:255:PRO:HG3   | 4:j:3:GLN:HE22    | 1.69                     | 0.58              |
| 3:A9:207:LEU:HB3  | 3:A9:225:LEU:HD22 | 1.86                     | 0.58              |
| 2:B4:262:TYR:HB3  | 2:B4:263:PRO:HD2  | 1.86                     | 0.58              |
| 2:B8:175:PRO:HB3  | 2:B8:390:ARG:HH21 | 1.69                     | 0.58              |
| 2:E2:223:THR:HG23 | 2:E2:225:THR:HG22 | 1.84                     | 0.58              |
| 3:E5:186:THR:HG22 | 3:E5:415:MET:HE1  | 1.86                     | 0.58              |
| 4:c:119:ARG:HH22  | 4:c:137:GLU:HB3   | 1.69                     | 0.58              |
| 5:l:18:GLN:HG2    | 4:n:146:ARG:HH11  | 1.69                     | 0.58              |
| 1:0:247:TYR:OH    | 2:A4:81:GLY:HA3   | 2.04                     | 0.58              |
| 1:4:240:PRO:HG3   | 4:g:154:TYR:O     | 2.04                     | 0.58              |
| 1:7:253:ALA:HB2   | 2:B8:82:THR:HG21  | 1.86                     | 0.58              |
| 3:A1:219:THR:HA   | 2:A2:326:LYS:HZ2  | 0.75                     | 0.58              |
| 2:A8:151:CYS:SG   | 2:A8:193:SER:OG   | 2.57                     | 0.58              |
| 3:C3:163:ILE:HD13 | 3:C3:250:LEU:HB3  | 1.86                     | 0.58              |
| 3:D9:296:ALA:HB2  | 3:D9:305:PRO:HD2  | 1.86                     | 0.58              |
| 2:E4:422:ARG:HH12 | 2:E4:426:ALA:HB2  | 1.68                     | 0.58              |
| 3:F1:238:CYS:SG   | 3:F1:239:CYS:N    | 2.77                     | 0.58              |
| 4:c:8:SER:OG      | 4:c:11:ASN:OD1    | 2.21                     | 0.58              |
| 4:e:100:ASN:HB3   | 4:g:6:PHE:CD1     | 2.39                     | 0.58              |
| 1:3:248:ARG:NH2   | 2:B0:82:THR:OG1   | 2.37                     | 0.57              |
| 2:A0:382:THR:HG22 | 2:A0:382:THR:O    | 2.04                     | 0.57              |
| 2:A2:253:THR:O    | 2:A2:256:GLN:NE2  | 2.37                     | 0.57              |
| 3:A7:67:ASP:OD1   | 3:A7:73:MET:HE1   | 2.04                     | 0.57              |
| 2:C6:204:LEU:HD13 | 2:C6:231:ILE:HD12 | 1.84                     | 0.57              |
| 2:D8:222:PRO:HD2  | 3:D9:324:LYS:HD3  | 1.86                     | 0.57              |
| 2:E8:178:SER:HB3  | 2:E8:183:GLU:HG3  | 1.86                     | 0.57              |
| 2:E8:191:THR:HG23 | 2:E8:425:LEU:HD21 | 1.86                     | 0.57              |
| 4:a:169:SER:HA    | 4:a:185:ILE:HD11  | 1.85                     | 0.57              |
| 4:c:97:ARG:CG     | 4:e:161:TYR:OH    | 2.52                     | 0.57              |
| 4:d:38:LEU:HD23   | 4:d:38:LEU:H      | 1.70                     | 0.57              |
| 4:h:97:ARG:N      | 4:j:159:TYR:OH    | 2.36                     | 0.57              |
| 1:11:244:GLN:HB2  | 3:D1:320:ARG:NH2  | 2.19                     | 0.57              |
| 2:B8:240:ALA:HB1  | 2:B8:356:ASN:HD22 | 1.69                     | 0.57              |
| 2:D4:66:VAL:CG2   | 2:D4:122:ILE:HD11 | 2.33                     | 0.57              |
| 2:E0:259:LEU:HD21 | 2:E0:316:CYS:HB2  | 1.84                     | 0.57              |
| 3:E7:293:MET:HE2  | 3:E7:367:PHE:HB2  | 1.86                     | 0.57              |
| 4:j:59:ASN:HD22   | 5:l:100:CYS:HB2   | 1.68                     | 0.57              |
| 1:15:253:ALA:HB2  | 2:D8:82:THR:HG21  | 1.86                     | 0.57              |
| 2:B6:53:PHE:HB3   | 2:B6:61:HIS:HB3   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C4:221:ARG:HB3  | 3:C5:322:SER:CB   | 2.35                     | 0.57              |
| 2:C6:176:GLN:HB3  | 3:C7:331:LEU:HD22 | 1.85                     | 0.57              |
| 3:D5:274:THR:OG1  | 3:D5:279:GLN:OE1  | 2.23                     | 0.57              |
| 3:E3:180:VAL:O    | 3:E3:184:ASN:ND2  | 2.38                     | 0.57              |
| 2:E4:107:HIS:NE2  | 2:E4:151:CYS:SG   | 2.66                     | 0.57              |
| 2:E6:65:CYS:SG    | 2:E6:66:VAL:N     | 2.77                     | 0.57              |
| 4:q:9:PRO:HA      | 4:q:12:VAL:HG22   | 1.85                     | 0.57              |
| 2:A0:174:SER:OG   | 2:A0:177:VAL:O    | 2.21                     | 0.57              |
| 3:A5:180:VAL:O    | 3:A5:184:ASN:ND2  | 2.38                     | 0.57              |
| 2:C0:176:GLN:HB3  | 3:C1:331:LEU:HD21 | 1.86                     | 0.57              |
| 2:D0:241:SER:HB2  | 2:D0:249:ASN:HB2  | 1.86                     | 0.57              |
| 2:D6:370:LYS:NZ   | 4:s:202:ARG:HH12  | 2.02                     | 0.57              |
| 4:c:14:LYS:HB3    | 4:c:47:LEU:HD13   | 1.87                     | 0.57              |
| 4:e:95:TYR:CE2    | 4:e:99:MET:HE1    | 2.39                     | 0.57              |
| 4:h:119:ARG:NH1   | 4:h:137:GLU:OE1   | 2.33                     | 0.57              |
| 1:10:241:PHE:HE1  | 3:C9:356:ILE:CG2  | 2.18                     | 0.57              |
| 3:A5:252:LYS:CE   | 3:A5:252:LYS:CG   | 2.79                     | 0.57              |
| 2:A8:285:GLN:HB2  | 2:B2:56:THR:CA    | 2.30                     | 0.57              |
| 2:A8:285:GLN:HG3  | 2:A8:286:LEU:H    | 1.69                     | 0.57              |
| 3:C3:105:HIS:HE1  | 3:C3:191:GLN:HE22 | 1.51                     | 0.57              |
| 3:C3:200:GLN:HB3  | 3:C3:266:PHE:HB2  | 1.86                     | 0.57              |
| 2:C6:407:TRP:CH2  | 3:C7:258:ILE:HB   | 2.39                     | 0.57              |
| 1:21:250:GLU:OE1  | 2:F0:225:THR:HG21 | 2.05                     | 0.57              |
| 3:A7:190:HIS:HB2  | 3:A7:414:ASN:HD22 | 1.70                     | 0.57              |
| 2:A8:102:ASN:HB2  | 2:A8:105:ARG:HB2  | 1.86                     | 0.57              |
| 2:B6:230:LEU:CD2  | 2:B6:368:LEU:HD11 | 2.35                     | 0.57              |
| 2:C4:288:VAL:HA   | 2:C4:291:ILE:HG12 | 1.86                     | 0.57              |
| 2:C6:236:SER:O    | 2:C6:243:ARG:NH2  | 2.37                     | 0.57              |
| 3:D5:64:ILE:HD11  | 3:D5:123:GLU:HG3  | 1.85                     | 0.57              |
| 3:E7:389:PHE:HE1  | 3:E7:395:LEU:HD11 | 1.69                     | 0.57              |
| 1:21:241:PHE:HZ   | 3:F1:356:ILE:CG2  | 2.14                     | 0.57              |
| 1:7:253:ALA:HB1   | 4:h:102:GLY:HA2   | 1.87                     | 0.57              |
| 3:B5:396:HIS:HA   | 3:B5:399:THR:HG22 | 1.87                     | 0.57              |
| 2:C0:282:TYR:HB3  | 5:k:160:ARG:NH1   | 2.20                     | 0.57              |
| 2:C6:282:TYR:HD2  | 4:n:202:ARG:CD    | 2.18                     | 0.57              |
| 2:C8:281:ALA:HB3  | 4:o:202:ARG:NH2   | 2.19                     | 0.57              |
| 2:D4:96:LYS:HE2   | 3:D5:128:ASP:HB2  | 1.86                     | 0.57              |
| 4:f:12:VAL:HG12   | 4:f:15:ARG:HH22   | 1.69                     | 0.57              |
| 4:g:25:GLN:HE22   | 4:g:36:ILE:HG12   | 1.69                     | 0.57              |
| 3:B5:218:THR:HG23 | 3:B5:219:THR:HG23 | 1.87                     | 0.57              |
| 2:C2:269:LEU:HB3  | 2:C2:301:MET:HE2  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C8:262:TYR:HB3  | 2:C8:263:PRO:HD2  | 1.87                     | 0.57              |
| 3:C9:208:TYR:HD1  | 2:D0:326:LYS:CE   | 2.14                     | 0.57              |
| 3:D5:155:VAL:HG13 | 3:D5:164:MET:CE   | 2.35                     | 0.57              |
| 3:D5:274:THR:HG21 | 3:D5:282:ARG:HD3  | 1.86                     | 0.57              |
| 3:D7:213:ARG:HB3  | 3:D7:297:LYS:HD2  | 1.87                     | 0.57              |
| 3:D9:97:ALA:HA    | 3:D9:103:LYS:HE2  | 1.85                     | 0.57              |
| 3:E5:113:ILE:HA   | 3:E5:116:VAL:HG12 | 1.86                     | 0.57              |
| 3:E7:284:LEU:HB3  | 3:E7:362:LYS:HE3  | 1.87                     | 0.57              |
| 4:a:96:TYR:OH     | 4:c:6:PHE:HE2     | 1.78                     | 0.57              |
| 2:A6:296:PHE:CE2  | 2:A6:335:ILE:HG21 | 2.40                     | 0.57              |
| 3:A7:281:TYR:OH   | 3:B1:83:GLN:O     | 2.18                     | 0.57              |
| 3:B7:212:PHE:HD1  | 2:B8:326:LYS:HD3  | 1.69                     | 0.57              |
| 2:C2:168:ASN:HD22 | 2:C2:198:THR:HG21 | 1.70                     | 0.57              |
| 3:C5:207:LEU:HG   | 3:C5:228:LEU:HD11 | 1.86                     | 0.57              |
| 3:D9:6:HIS:CE1    | 3:D9:8:GLN:HE21   | 2.22                     | 0.57              |
| 3:D9:139:LEU:HD11 | 3:D9:192:LEU:HD13 | 1.87                     | 0.57              |
| 3:E5:169:VAL:HG12 | 3:E5:202:ILE:HB   | 1.86                     | 0.57              |
| 3:E5:172:SER:OG   | 3:E5:175:VAL:O    | 2.22                     | 0.57              |
| 4:d:89:LEU:HB3    | 4:d:90:PRO:HD3    | 1.87                     | 0.57              |
| 4:m:117:ARG:NH1   | 4:m:118:ASP:OD1   | 2.38                     | 0.57              |
| 4:r:14:LYS:HD3    | 4:r:47:LEU:HB2    | 1.87                     | 0.57              |
| 2:B6:213:CYS:SG   | 2:B6:222:PRO:HG3  | 2.45                     | 0.57              |
| 2:B6:262:TYR:HB2  | 2:B6:265:ILE:HD12 | 1.87                     | 0.57              |
| 2:C2:210:TYR:HE2  | 3:C3:327:ASP:OD2  | 1.88                     | 0.57              |
| 2:C8:397:LEU:HB3  | 3:C9:344:TRP:O    | 2.04                     | 0.57              |
| 2:D8:69:ASP:OD1   | 2:D8:70:LEU:N     | 2.37                     | 0.57              |
| 2:E8:210:TYR:CB   | 3:E9:324:LYS:HD3  | 2.31                     | 0.57              |
| 3:F1:210:ILE:HD11 | 3:F1:298:ASN:HA   | 1.87                     | 0.57              |
| 5:k:91:PRO:HB3    | 4:m:159:TYR:HD2   | 1.70                     | 0.57              |
| 4:t:75:LEU:HD23   | 4:t:111:ILE:HB    | 1.87                     | 0.57              |
| 4:u:14:LYS:HD2    | 4:u:47:LEU:HD23   | 1.86                     | 0.57              |
| 2:B0:108:TYR:HE2  | 2:B0:413:MET:HB3  | 1.70                     | 0.56              |
| 3:B5:132:GLY:HA3  | 3:B5:163:ILE:HG22 | 1.87                     | 0.56              |
| 3:B9:267:LEU:CD2  | 3:B9:374:ILE:HD11 | 2.35                     | 0.56              |
| 2:C2:84:ARG:HH22  | 4:j:197:LEU:CD1   | 2.11                     | 0.56              |
| 2:C8:176:GLN:HB3  | 3:C9:331:LEU:CD2  | 2.33                     | 0.56              |
| 3:E3:385:PHE:HE2  | 3:E3:412:GLU:HB3  | 1.69                     | 0.56              |
| 2:E8:2:ARG:HE     | 2:E8:133:GLN:HE21 | 1.53                     | 0.56              |
| 3:E9:139:LEU:HD12 | 3:E9:170:PHE:HE1  | 1.70                     | 0.56              |
| 4:m:9:PRO:HA      | 4:m:12:VAL:HG22   | 1.87                     | 0.56              |
| 2:A0:56:THR:HA    | 3:F1:283:ALA:HB2  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A2:66:VAL:HG21  | 2:A2:122:ILE:HD11 | 1.85                     | 0.56              |
| 3:A5:318:ARG:HD3  | 3:A5:358:PRO:HD3  | 1.87                     | 0.56              |
| 3:B5:27:GLU:OE1   | 3:B5:318:ARG:NH2  | 2.34                     | 0.56              |
| 2:B8:175:PRO:HB3  | 2:B8:390:ARG:NH2  | 2.20                     | 0.56              |
| 2:B8:406:HIS:HA   | 2:B8:409:VAL:HG12 | 1.87                     | 0.56              |
| 2:C4:71:GLU:HG2   | 2:C4:73:THR:HG22  | 1.88                     | 0.56              |
| 2:C6:12:ALA:HB3   | 2:C6:140:ALA:HB2  | 1.86                     | 0.56              |
| 3:C7:281:TYR:CD2  | 3:D1:87:PRO:CD    | 2.71                     | 0.56              |
| 3:C9:66:MET:HE2   | 3:C9:116:VAL:HG21 | 1.88                     | 0.56              |
| 2:D0:309:HIS:NE2  | 2:D0:386:GLU:OE1  | 2.31                     | 0.56              |
| 2:D8:12:ALA:HB3   | 2:D8:140:ALA:HB2  | 1.87                     | 0.56              |
| 4:a:200:ASP:OD2   | 4:a:203:ASN:ND2   | 2.35                     | 0.56              |
| 1:4:240:PRO:HG2   | 4:g:154:TYR:C     | 2.31                     | 0.56              |
| 1:5:242:ASN:CG    | 4:h:154:TYR:HB2   | 2.29                     | 0.56              |
| 1:8:241:PHE:CZ    | 3:C1:356:ILE:HG21 | 2.38                     | 0.56              |
| 1:9:257:PRO:HG2   | 2:C2:26:LEU:O     | 2.06                     | 0.56              |
| 3:A5:27:GLU:OE1   | 3:A5:241:ARG:NH2  | 2.38                     | 0.56              |
| 2:A6:323:VAL:HG13 | 2:A6:355:ILE:HG23 | 1.87                     | 0.56              |
| 2:B2:262:TYR:HB3  | 2:B2:263:PRO:HD2  | 1.86                     | 0.56              |
| 2:B4:56:THR:O     | 2:B4:60:LYS:HB3   | 2.05                     | 0.56              |
| 2:B4:66:VAL:HG21  | 2:B4:122:ILE:HD11 | 1.87                     | 0.56              |
| 3:B9:358:PRO:HG2  | 3:B9:361:LEU:HD12 | 1.86                     | 0.56              |
| 2:C2:255:PHE:HB3  | 2:C2:259:LEU:HD12 | 1.87                     | 0.56              |
| 2:C6:121:ARG:HH12 | 2:C6:124:LYS:HE3  | 1.71                     | 0.56              |
| 2:C6:282:TYR:CD2  | 4:n:202:ARG:HG2   | 2.40                     | 0.56              |
| 2:C6:282:TYR:OH   | 4:n:201:TRP:CH2   | 2.52                     | 0.56              |
| 3:C7:12:CYS:HB3   | 3:C7:138:SER:HB3  | 1.87                     | 0.56              |
| 2:D0:104:ALA:HB2  | 2:D0:413:MET:HE3  | 1.86                     | 0.56              |
| 3:D3:129:CYS:SG   | 3:D3:162:ARG:NH2  | 2.78                     | 0.56              |
| 2:D4:262:TYR:HB3  | 2:D4:263:PRO:HD2  | 1.87                     | 0.56              |
| 3:D9:283:ALA:HB2  | 3:E3:54:ALA:HA    | 1.85                     | 0.56              |
| 3:D9:313:ALA:HB3  | 3:D9:349:MET:HG2  | 1.88                     | 0.56              |
| 2:E2:281:ALA:HB3  | 4:v:202:ARG:NH2   | 2.19                     | 0.56              |
| 3:E3:238:CYS:SG   | 3:E3:318:ARG:NE   | 2.78                     | 0.56              |
| 2:E6:76:ASP:OD1   | 2:E6:79:ARG:NH2   | 2.38                     | 0.56              |
| 4:a:112:PHE:HB2   | 4:a:131:TRP:HE1   | 1.70                     | 0.56              |
| 4:c:78:ALA:HB3    | 4:c:112:PHE:HE1   | 1.69                     | 0.56              |
| 4:t:106:GLN:HB3   | 4:v:39:PRO:HG2    | 1.86                     | 0.56              |
| 1:0:244:GLN:H     | 3:A5:320:ARG:CZ   | 2.17                     | 0.56              |
| 1:9:257:PRO:HG2   | 2:C2:26:LEU:HA    | 1.87                     | 0.56              |
| 2:A2:285:GLN:OE1  | 2:A6:57:GLY:O     | 2.23                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C1:317:PHE:HB3  | 3:C1:321:MET:HE1  | 1.88                     | 0.56              |
| 2:C2:76:ASP:HA    | 2:C2:79:ARG:HD2   | 1.87                     | 0.56              |
| 2:C6:309:HIS:NE2  | 2:C6:386:GLU:OE1  | 2.38                     | 0.56              |
| 3:C9:309:ARG:H    | 3:C9:372:THR:HG22 | 1.71                     | 0.56              |
| 3:D1:386:THR:O    | 3:D1:390:ARG:HG3  | 2.05                     | 0.56              |
| 2:D4:178:SER:H    | 3:D5:347:ASN:ND2  | 2.03                     | 0.56              |
| 2:D4:274:PRO:HG3  | 2:D4:286:LEU:CD2  | 2.32                     | 0.56              |
| 3:E1:311:LEU:HD12 | 3:E1:342:VAL:HG11 | 1.87                     | 0.56              |
| 3:E5:267:LEU:HD12 | 3:E5:301:CYS:HB3  | 1.87                     | 0.56              |
| 2:E8:181:VAL:HG11 | 2:E8:404:PHE:CE1  | 2.40                     | 0.56              |
| 1:0:251:TYR:HE2   | 2:A4:18:ASN:O     | 1.87                     | 0.56              |
| 2:A6:33:ASP:OD1   | 4:b:102:GLY:O     | 2.23                     | 0.56              |
| 3:A9:219:THR:C    | 2:B0:324:VAL:HG11 | 2.31                     | 0.56              |
| 3:B3:3:GLU:HA     | 3:B3:49:VAL:HA    | 1.88                     | 0.56              |
| 2:C2:215:ARG:NH2  | 2:C2:297:GLU:OE2  | 2.39                     | 0.56              |
| 2:C2:267:PHE:O    | 2:C2:380:ASN:ND2  | 2.39                     | 0.56              |
| 2:E0:221:ARG:HG3  | 3:E1:322:SER:OG   | 2.06                     | 0.56              |
| 3:E3:100:ASN:HB3  | 3:E3:103:LYS:HG2  | 1.88                     | 0.56              |
| 2:F0:80:THR:HA    | 2:F0:84:ARG:HE    | 1.69                     | 0.56              |
| 4:b:106:GLN:NE2   | 4:b:108:ILE:O     | 2.39                     | 0.56              |
| 2:A4:164:LYS:NZ   | 2:A4:165:SER:O    | 2.38                     | 0.56              |
| 2:A6:279:GLU:OE2  | 4:d:198:ARG:HD2   | 2.05                     | 0.56              |
| 3:A7:303:SER:HB3  | 3:A7:377:MET:HE3  | 1.87                     | 0.56              |
| 3:B7:7:VAL:HB     | 3:B7:135:ILE:HG12 | 1.87                     | 0.56              |
| 3:B7:95:THR:OG1   | 3:B7:108:GLU:OE2  | 2.16                     | 0.56              |
| 3:D3:176:SER:CB   | 2:D4:349:THR:HB   | 2.36                     | 0.56              |
| 4:b:97:ARG:HH12   | 4:d:6:PHE:HD2     | 1.52                     | 0.56              |
| 4:c:14:LYS:HD2    | 4:c:47:LEU:HD22   | 1.88                     | 0.56              |
| 4:u:59:ASN:CG     | 5:w:100:CYS:HB3   | 2.28                     | 0.56              |
| 2:B0:212:ILE:HG12 | 2:B0:275:ILE:HD11 | 1.87                     | 0.56              |
| 3:B3:152:ILE:HG12 | 3:B3:164:MET:HE1  | 1.88                     | 0.56              |
| 3:B7:293:MET:HE3  | 3:B7:367:PHE:HB2  | 1.88                     | 0.56              |
| 2:C4:277:SER:OG   | 2:C4:278:ALA:N    | 2.37                     | 0.56              |
| 3:D5:95:THR:OG1   | 3:D5:108:GLU:OE2  | 2.22                     | 0.56              |
| 2:E4:272:TYR:HB3  | 2:E4:275:ILE:HD11 | 1.88                     | 0.56              |
| 2:E6:283:HIS:HA   | 2:F0:60:LYS:HE2   | 1.87                     | 0.56              |
| 3:E7:236:VAL:HA   | 3:E7:316:MET:HE1  | 1.86                     | 0.56              |
| 2:E8:298:PRO:HA   | 2:E8:301:MET:HE3  | 1.87                     | 0.56              |
| 2:F0:271:SER:HB2  | 2:F0:377:MET:HB3  | 1.87                     | 0.56              |
| 5:k:39:ALA:O      | 5:k:75:SER:HA     | 2.05                     | 0.56              |
| 1:0:243:ALA:HA    | 3:A5:320:ARG:NH1  | 2.21                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:247:TYR:CD2  | 2:D4:77:GLU:HB3   | 2.40                     | 0.56              |
| 1:13:248:ARG:NH2  | 3:D5:42:LEU:HD21  | 2.20                     | 0.56              |
| 2:A2:324:VAL:HG11 | 2:A2:326:LYS:HZ3  | 1.71                     | 0.56              |
| 3:A5:33:THR:O     | 3:A5:58:ARG:NH2   | 2.39                     | 0.56              |
| 3:A7:139:LEU:HD12 | 3:A7:170:PHE:HE1  | 1.71                     | 0.56              |
| 2:A8:221:ARG:HB3  | 3:A9:322:SER:HB2  | 1.87                     | 0.56              |
| 3:C9:244:GLY:HA2  | 3:C9:355:ASP:HB2  | 1.87                     | 0.56              |
| 2:D0:397:LEU:HB3  | 3:D1:344:TRP:O    | 2.05                     | 0.56              |
| 3:D5:201:VAL:HG11 | 3:D5:377:MET:HE1  | 1.86                     | 0.56              |
| 2:E6:100:ALA:HA   | 3:E7:252:LYS:HD2  | 1.87                     | 0.56              |
| 3:D7:249:ASP:OD1  | 3:D7:250:LEU:N    | 2.38                     | 0.56              |
| 2:E0:176:GLN:HB3  | 3:E1:331:LEU:HD22 | 1.88                     | 0.56              |
| 3:E1:12:CYS:HB3   | 3:E1:138:SER:HB2  | 1.88                     | 0.56              |
| 2:E4:319:TYR:HB3  | 2:E4:323:VAL:HG21 | 1.87                     | 0.56              |
| 3:E9:239:CYS:SG   | 3:E9:248:SER:N    | 2.76                     | 0.56              |
| 4:h:78:ALA:HB3    | 4:h:112:PHE:HE1   | 1.71                     | 0.56              |
| 4:s:8:SER:OG      | 4:s:11:ASN:OD1    | 2.24                     | 0.56              |
| 5:w:34:VAL:HA     | 5:w:70:GLU:O      | 2.06                     | 0.56              |
| 2:A0:282:TYR:CZ   | 4:a:201:TRP:CZ2   | 2.93                     | 0.56              |
| 2:B2:107:HIS:NE2  | 2:B2:151:CYS:SG   | 2.77                     | 0.56              |
| 2:B2:269:LEU:HD11 | 2:B2:384:ILE:HD11 | 1.87                     | 0.56              |
| 2:B4:283:HIS:C    | 2:B8:56:THR:CB    | 2.73                     | 0.56              |
| 3:C3:73:MET:HB3   | 3:C3:77:ARG:HH22  | 1.70                     | 0.56              |
| 2:C4:309:HIS:NE2  | 2:C4:386:GLU:OE1  | 2.39                     | 0.56              |
| 2:C4:339:ARG:O    | 2:C4:342:GLN:NE2  | 2.39                     | 0.56              |
| 3:D1:192:LEU:HD21 | 3:D1:199:VAL:HG11 | 1.87                     | 0.56              |
| 3:D1:228:LEU:HG   | 3:D1:300:MET:HE2  | 1.88                     | 0.56              |
| 3:D5:274:THR:CG2  | 3:D5:282:ARG:HD3  | 2.36                     | 0.56              |
| 3:E1:99:ASN:HD21  | 2:E2:258:ASN:HD21 | 1.53                     | 0.56              |
| 4:p:71:LYS:HD3    | 4:r:39:PRO:HG3    | 1.86                     | 0.56              |
| 1:9:255:PRO:HG2   | 2:C2:364:PRO:HG2  | 1.88                     | 0.55              |
| 2:A4:278:ALA:HB1  | 4:c:202:ARG:HH12  | 1.71                     | 0.55              |
| 3:A5:208:TYR:HB3  | 2:A6:326:LYS:HD2  | 1.87                     | 0.55              |
| 2:A6:282:TYR:CE2  | 4:d:201:TRP:CZ2   | 2.94                     | 0.55              |
| 2:C2:202:VAL:HA   | 2:C2:268:MET:HB2  | 1.87                     | 0.55              |
| 2:C8:12:ALA:HB3   | 2:C8:140:ALA:HB2  | 1.87                     | 0.55              |
| 3:D5:49:VAL:HG21  | 3:D5:241:ARG:HG2  | 1.87                     | 0.55              |
| 3:D7:274:THR:HG21 | 3:D7:282:ARG:HD2  | 1.88                     | 0.55              |
| 4:j:181:GLN:NE2   | 4:j:198:ARG:O     | 2.39                     | 0.55              |
| 1:10:242:ASN:CB   | 4:o:153:GLU:OE2   | 2.54                     | 0.55              |
| 3:A1:12:CYS:HB3   | 3:A1:138:SER:HB2  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A1:289:LEU:HD21 | 3:A1:365:VAL:HG11 | 1.87                     | 0.55              |
| 2:A6:109:THR:HG21 | 2:A6:411:GLU:HB2  | 1.87                     | 0.55              |
| 2:A8:85:HIS:CE1   | 4:c:99:MET:HG3    | 2.41                     | 0.55              |
| 3:A9:39:ASP:CB    | 4:c:90:PRO:HG3    | 2.36                     | 0.55              |
| 3:B3:208:TYR:CE1  | 3:B3:225:LEU:HD11 | 2.41                     | 0.55              |
| 2:B4:285:GLN:HB3  | 2:B8:57:GLY:N     | 2.22                     | 0.55              |
| 2:B6:274:PRO:HG3  | 2:B6:286:LEU:HD12 | 1.87                     | 0.55              |
| 2:D0:103:PHE:HD2  | 2:D0:413:MET:HE1  | 1.70                     | 0.55              |
| 2:D2:259:LEU:HD13 | 2:D2:268:MET:HE2  | 1.87                     | 0.55              |
| 3:D3:101:TRP:NE1  | 3:D3:145:SER:O    | 2.39                     | 0.55              |
| 3:D5:276:ARG:NH2  | 3:D5:279:GLN:HG3  | 2.20                     | 0.55              |
| 2:E0:244:PHE:HB2  | 2:E0:356:ASN:HD21 | 1.70                     | 0.55              |
| 4:a:113:VAL:HG22  | 4:a:134:ILE:HD12  | 1.88                     | 0.55              |
| 4:c:97:ARG:HG3    | 4:e:161:TYR:CE1   | 2.40                     | 0.55              |
| 4:f:142:GLU:OE2   | 4:f:146:ARG:NE    | 2.40                     | 0.55              |
| 1:16:256:LEU:HD21 | 2:E0:31:GLN:HA    | 1.89                     | 0.55              |
| 2:A2:356:ASN:OD1  | 2:A2:358:GLN:NE2  | 2.39                     | 0.55              |
| 2:A6:282:TYR:CZ   | 4:d:201:TRP:CZ2   | 2.95                     | 0.55              |
| 3:B5:16:ILE:HD11  | 3:B5:229:VAL:HG11 | 1.89                     | 0.55              |
| 2:B8:73:THR:HG23  | 3:B9:46:ARG:NH1   | 2.22                     | 0.55              |
| 2:C6:34:GLY:O     | 2:C6:61:HIS:N     | 2.39                     | 0.55              |
| 3:D3:117:LEU:HA   | 3:D3:120:VAL:HG12 | 1.89                     | 0.55              |
| 3:D7:324:LYS:O    | 3:D7:327:ASP:N    | 2.39                     | 0.55              |
| 2:E0:73:THR:HB    | 3:E1:46:ARG:HH22  | 1.71                     | 0.55              |
| 3:E5:10:GLY:HA2   | 3:E5:143:THR:HG23 | 1.86                     | 0.55              |
| 3:E5:334:GLN:OE1  | 3:E5:348:ASN:ND2  | 2.38                     | 0.55              |
| 2:E6:282:TYR:CG   | 5:x:160:ARG:CD    | 2.89                     | 0.55              |
| 5:k:68:VAL:HG13   | 5:k:69:ILE:HG23   | 1.88                     | 0.55              |
| 4:q:8:SER:OG      | 4:q:11:ASN:OD1    | 2.23                     | 0.55              |
| 3:A5:179:VAL:HG23 | 2:A6:349:THR:O    | 2.06                     | 0.55              |
| 3:A7:128:ASP:OD1  | 3:A7:128:ASP:N    | 2.39                     | 0.55              |
| 2:B0:221:ARG:HB2  | 3:B1:322:SER:CB   | 2.36                     | 0.55              |
| 3:B3:200:GLN:HB3  | 3:B3:268:ILE:HD11 | 1.88                     | 0.55              |
| 2:C0:207:GLU:HA   | 2:C0:210:TYR:HB2  | 1.88                     | 0.55              |
| 2:C0:210:TYR:HB3  | 3:C1:324:LYS:HE3  | 1.86                     | 0.55              |
| 2:C2:404:PHE:CD1  | 3:C3:259:PRO:HA   | 2.41                     | 0.55              |
| 3:C5:167:PHE:CD2  | 3:C5:233:MET:HG2  | 2.41                     | 0.55              |
| 2:C6:10:GLY:HA2   | 2:C6:145:THR:HG23 | 1.88                     | 0.55              |
| 2:D0:34:GLY:O     | 2:D0:61:HIS:N     | 2.39                     | 0.55              |
| 3:D1:152:ILE:HD13 | 3:D1:166:THR:HG21 | 1.89                     | 0.55              |
| 2:D4:221:ARG:HG3  | 3:D5:322:SER:HB3  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E6:283:HIS:CG   | 2:F0:60:LYS:HE2   | 2.41                     | 0.55              |
| 4:d:126:ARG:NH1   | 4:d:133:SER:OG    | 2.40                     | 0.55              |
| 4:e:101:GLU:HG3   | 4:g:6:PHE:HB2     | 1.88                     | 0.55              |
| 1:2:240:PRO:HG3   | 4:e:154:TYR:CB    | 2.34                     | 0.55              |
| 1:2:257:PRO:CD    | 2:A8:26:LEU:HD12  | 2.36                     | 0.55              |
| 2:A0:115:VAL:HG21 | 2:A0:152:LEU:HD22 | 1.89                     | 0.55              |
| 2:B2:120:ASP:OD1  | 2:B2:123:ARG:NH2  | 2.39                     | 0.55              |
| 2:B8:53:PHE:HB3   | 2:B8:61:HIS:HB3   | 1.88                     | 0.55              |
| 3:C3:68:LEU:HA    | 3:C3:93:GLY:HA3   | 1.88                     | 0.55              |
| 3:C5:107:THR:OG1  | 3:C5:401:GLU:OE2  | 2.23                     | 0.55              |
| 2:D2:30:ILE:HG22  | 2:D2:36:MET:HB3   | 1.89                     | 0.55              |
| 2:D4:36:MET:HE3   | 2:D4:61:HIS:NE2   | 2.22                     | 0.55              |
| 3:D9:68:LEU:HD23  | 3:D9:112:LEU:HD13 | 1.89                     | 0.55              |
| 2:E0:276:ILE:HG23 | 2:E0:280:LYS:HB2  | 1.89                     | 0.55              |
| 3:F1:100:ASN:HB3  | 3:F1:103:LYS:HG2  | 1.89                     | 0.55              |
| 4:f:56:LYS:HD3    | 4:f:60:ASN:OD1    | 2.06                     | 0.55              |
| 1:20:241:PHE:CE1  | 3:E9:356:ILE:HG21 | 2.34                     | 0.55              |
| 1:8:239:LEU:O     | 3:C1:359:LYS:NZ   | 2.39                     | 0.55              |
| 3:A1:193:VAL:HG12 | 3:A1:265:PHE:HE2  | 1.72                     | 0.55              |
| 3:A5:94:GLN:O     | 2:A6:2:ARG:NH2    | 2.40                     | 0.55              |
| 3:A7:200:GLN:HB3  | 3:A7:268:ILE:HD11 | 1.89                     | 0.55              |
| 3:B5:14:ASN:HD21  | 3:B5:73:MET:HE3   | 1.72                     | 0.55              |
| 2:B6:250:VAL:HG13 | 2:B6:318:MET:HE1  | 1.88                     | 0.55              |
| 2:D4:52:PHE:HD2   | 2:D4:243:ARG:HD3  | 1.71                     | 0.55              |
| 3:A7:253:LEU:HD21 | 3:A7:316:MET:SD   | 2.47                     | 0.55              |
| 3:A7:259:PRO:HG2  | 3:A7:311:LEU:HD21 | 1.88                     | 0.55              |
| 3:A7:282:ARG:O    | 3:B1:55:THR:CG2   | 2.45                     | 0.55              |
| 3:B3:372:THR:HG21 | 3:B3:426:GLN:HB3  | 1.88                     | 0.55              |
| 2:B4:282:TYR:OH   | 2:B8:33:ASP:OD1   | 2.19                     | 0.55              |
| 2:C6:271:SER:HB3  | 2:C6:377:MET:HB3  | 1.89                     | 0.55              |
| 3:C9:2:ARG:HB3    | 3:C9:131:GLN:HB2  | 1.88                     | 0.55              |
| 2:D6:222:PRO:HD2  | 3:D7:324:LYS:HZ2  | 1.71                     | 0.55              |
| 3:D7:282:ARG:O    | 3:E1:55:THR:HG22  | 2.06                     | 0.55              |
| 3:E1:10:GLY:O     | 3:E1:14:ASN:ND2   | 2.39                     | 0.55              |
| 3:F1:49:VAL:HG11  | 3:F1:241:ARG:HG2  | 1.89                     | 0.55              |
| 4:d:96:TYR:HA     | 4:d:108:ILE:HD11  | 1.89                     | 0.55              |
| 4:d:97:ARG:O      | 4:d:101:GLU:HB3   | 2.07                     | 0.55              |
| 5:k:65:GLU:HA     | 4:m:42:TYR:HE2    | 1.71                     | 0.55              |
| 2:A4:79:ARG:HB3   | 2:A4:92:LEU:CD1   | 2.32                     | 0.55              |
| 3:A5:257:LEU:HD21 | 3:A5:314:SER:HB2  | 1.87                     | 0.55              |
| 2:C2:282:TYR:CE2  | 5:l:160:ARG:NH2   | 2.75                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C5:329:GLN:OE1  | 3:C5:332:ASN:ND2  | 2.33                     | 0.55              |
| 2:D8:2:ARG:HG3    | 2:D8:51:THR:HG22  | 1.88                     | 0.55              |
| 3:F1:183:TYR:OH   | 3:F1:388:MET:O    | 2.22                     | 0.55              |
| 4:v:71:LYS:NZ     | 4:v:106:GLN:HG3   | 2.21                     | 0.55              |
| 2:A6:210:TYR:C    | 3:A7:324:LYS:NZ   | 2.65                     | 0.55              |
| 3:A9:292:GLN:O    | 3:A9:298:ASN:ND2  | 2.40                     | 0.55              |
| 2:C4:206:ASN:HA   | 2:C4:209:ILE:HG22 | 1.87                     | 0.55              |
| 2:C6:298:PRO:HA   | 2:C6:301:MET:HE1  | 1.89                     | 0.55              |
| 2:D2:203:MET:HE2  | 2:D2:267:PHE:HB3  | 1.89                     | 0.55              |
| 3:D5:321:MET:CE   | 3:D5:353:VAL:HG22 | 2.37                     | 0.55              |
| 3:D7:322:SER:OG   | 3:D7:325:GLU:OE2  | 2.24                     | 0.55              |
| 2:E8:101:ASN:HB3  | 2:E8:182:VAL:HG21 | 1.87                     | 0.55              |
| 4:n:149:ARG:HE    | 4:n:164:ARG:HB2   | 1.72                     | 0.55              |
| 4:o:53:GLY:HA2    | 4:o:62:VAL:CG2    | 2.36                     | 0.55              |
| 4:q:75:LEU:HD23   | 4:q:111:ILE:HB    | 1.89                     | 0.55              |
| 4:t:15:ARG:O      | 4:t:19:GLU:HG3    | 2.07                     | 0.55              |
| 2:A2:126:ALA:HB1  | 2:A2:132:LEU:HD22 | 1.89                     | 0.55              |
| 3:A3:207:LEU:HD11 | 3:A3:300:MET:HE2  | 1.89                     | 0.55              |
| 3:A9:11:GLN:HB2   | 3:A9:72:THR:HG21  | 1.89                     | 0.55              |
| 3:B9:33:THR:HG23  | 3:B9:35:THR:HG23  | 1.88                     | 0.55              |
| 3:C1:220:PRO:HG2  | 2:C2:326:LYS:HB2  | 1.89                     | 0.55              |
| 3:C5:68:LEU:HD12  | 3:C5:97:ALA:HB2   | 1.87                     | 0.55              |
| 3:C5:350:LYS:NZ   | 3:C5:352:SER:OG   | 2.40                     | 0.55              |
| 3:D3:21:TRP:HA    | 3:D3:24:ILE:HG22  | 1.88                     | 0.55              |
| 3:D3:291:GLN:HG2  | 3:D7:122:LYS:HZ3  | 1.69                     | 0.55              |
| 3:D7:212:PHE:HE1  | 2:D8:326:LYS:CD   | 2.18                     | 0.55              |
| 3:F1:7:VAL:HB     | 3:F1:135:ILE:HG12 | 1.89                     | 0.55              |
| 3:F1:117:LEU:HA   | 3:F1:120:VAL:HG12 | 1.88                     | 0.55              |
| 1:7:253:ALA:HB2   | 2:B8:82:THR:CG2   | 2.37                     | 0.54              |
| 2:A0:356:ASN:OD1  | 2:A0:358:GLN:NE2  | 2.40                     | 0.54              |
| 3:A7:73:MET:HG3   | 3:A7:90:PHE:HD2   | 1.72                     | 0.54              |
| 2:D6:11:GLN:NE2   | 2:D6:15:GLN:OE1   | 2.39                     | 0.54              |
| 3:F1:358:PRO:HG2  | 3:F1:361:LEU:HB3  | 1.88                     | 0.54              |
| 4:a:97:ARG:HH22   | 4:c:7:ALA:HB2     | 1.70                     | 0.54              |
| 4:j:57:ASN:OD1    | 4:j:61:THR:OG1    | 2.25                     | 0.54              |
| 4:r:146:ARG:HG3   | 4:r:146:ARG:NH1   | 2.20                     | 0.54              |
| 4:t:14:LYS:HD3    | 4:t:47:LEU:HD22   | 1.89                     | 0.54              |
| 2:A8:33:ASP:O     | 2:A8:60:LYS:NZ    | 2.40                     | 0.54              |
| 3:B1:68:LEU:HB3   | 3:B1:96:GLY:HA2   | 1.89                     | 0.54              |
| 2:B6:241:SER:HB2  | 2:B6:249:ASN:HB2  | 1.89                     | 0.54              |
| 2:B8:262:TYR:HB3  | 2:B8:263:PRO:HD2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B9:274:THR:HG21 | 3:B9:279:GLN:HA   | 1.88                     | 0.54              |
| 3:C1:165:GLU:OE2  | 3:C1:200:GLN:NE2  | 2.40                     | 0.54              |
| 3:D9:135:ILE:HG22 | 3:D9:137:HIS:HD2  | 1.72                     | 0.54              |
| 2:E0:102:ASN:HB3  | 2:E0:105:ARG:HB3  | 1.89                     | 0.54              |
| 2:E2:319:TYR:HB3  | 2:E2:323:VAL:HG21 | 1.90                     | 0.54              |
| 3:E7:309:ARG:H    | 3:E7:372:THR:HG22 | 1.72                     | 0.54              |
| 4:e:8:SER:HB2     | 4:e:147:HIS:HA    | 1.89                     | 0.54              |
| 4:e:71:LYS:HG2    | 4:g:39:PRO:HG3    | 1.89                     | 0.54              |
| 4:n:97:ARG:HD2    | 4:p:161:TYR:CZ    | 2.42                     | 0.54              |
| 1:2:244:GLN:HG3   | 4:e:162:GLY:HA3   | 1.89                     | 0.54              |
| 2:A6:7:ILE:HD11   | 2:A6:137:MET:HE1  | 1.89                     | 0.54              |
| 2:A6:204:LEU:HD13 | 2:A6:231:ILE:HD12 | 1.90                     | 0.54              |
| 2:B6:76:ASP:HA    | 2:B6:79:ARG:HD2   | 1.89                     | 0.54              |
| 2:C6:177:VAL:HG13 | 3:C7:327:ASP:HB3  | 1.89                     | 0.54              |
| 2:D2:180:ALA:HB1  | 3:D3:256:ASN:HD21 | 1.72                     | 0.54              |
| 2:D2:210:TYR:HB3  | 3:D3:324:LYS:HE3  | 1.88                     | 0.54              |
| 2:D4:107:HIS:NE2  | 2:D4:151:CYS:SG   | 2.74                     | 0.54              |
| 3:F1:139:LEU:HA   | 3:F1:145:SER:HB2  | 1.89                     | 0.54              |
| 3:F1:200:GLN:HG3  | 3:F1:268:ILE:HD11 | 1.90                     | 0.54              |
| 4:e:12:VAL:HG12   | 4:e:15:ARG:NH1    | 2.21                     | 0.54              |
| 4:t:181:GLN:HE22  | 4:t:200:ASP:H     | 1.54                     | 0.54              |
| 2:A6:298:PRO:HG3  | 2:A6:308:ARG:HH22 | 1.72                     | 0.54              |
| 2:B2:180:ALA:H    | 3:B3:347:ASN:ND2  | 2.05                     | 0.54              |
| 3:B7:100:ASN:HB3  | 3:B7:103:LYS:HD3  | 1.89                     | 0.54              |
| 3:C9:179:VAL:HG11 | 2:D0:258:ASN:O    | 2.07                     | 0.54              |
| 2:D2:98:ASP:O     | 2:D2:105:ARG:NH2  | 2.31                     | 0.54              |
| 4:c:97:ARG:HG2    | 4:e:161:TYR:OH    | 2.07                     | 0.54              |
| 4:f:107:LYS:HD2   | 4:f:201:TRP:CD1   | 2.43                     | 0.54              |
| 1:11:254:LYS:HD3  | 2:D0:364:PRO:HD2  | 1.89                     | 0.54              |
| 1:23:257:PRO:HG3  | 2:C4:26:LEU:HD12  | 1.89                     | 0.54              |
| 1:8:251:TYR:HE1   | 2:C0:22:GLU:HG2   | 1.72                     | 0.54              |
| 2:A4:291:ILE:HD12 | 2:A4:375:VAL:HG23 | 1.89                     | 0.54              |
| 2:A8:241:SER:HB2  | 2:A8:249:ASN:HB2  | 1.90                     | 0.54              |
| 2:C6:26:LEU:HD21  | 2:C6:363:VAL:HG12 | 1.88                     | 0.54              |
| 3:C7:156:ARG:HG2  | 3:C7:195:ASN:HB2  | 1.90                     | 0.54              |
| 2:D2:207:GLU:HA   | 2:D2:210:TYR:HB2  | 1.89                     | 0.54              |
| 2:D6:222:PRO:CD   | 3:D7:324:LYS:HZ2  | 2.20                     | 0.54              |
| 3:D7:406:MET:HE2  | 3:D7:406:MET:CA   | 2.21                     | 0.54              |
| 2:D8:210:TYR:OH   | 3:D9:323:THR:OG1  | 2.24                     | 0.54              |
| 2:E0:223:THR:CG2  | 2:E0:225:THR:HG22 | 2.38                     | 0.54              |
| 2:E6:107:HIS:NE2  | 2:E6:151:CYS:SG   | 2.75                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:190:HIS:HB2  | 3:E7:414:ASN:HD22 | 1.73                     | 0.54              |
| 4:a:89:LEU:HB3    | 4:a:90:PRO:HD3    | 1.89                     | 0.54              |
| 4:e:71:LYS:HD3    | 4:g:39:PRO:HG3    | 1.89                     | 0.54              |
| 4:i:59:ASN:ND2    | 5:k:100:CYS:SG    | 2.78                     | 0.54              |
| 1:2:251:TYR:OH    | 2:A8:18:ASN:CB    | 2.56                     | 0.54              |
| 3:A3:311:LEU:HD12 | 3:A3:342:VAL:HG11 | 1.89                     | 0.54              |
| 2:B0:283:HIS:O    | 2:B4:56:THR:CB    | 2.55                     | 0.54              |
| 3:B1:292:GLN:NE2  | 3:B1:298:ASN:OD1  | 2.39                     | 0.54              |
| 2:B2:174:SER:HB2  | 2:B2:207:GLU:HG2  | 1.88                     | 0.54              |
| 2:B4:406:HIS:HA   | 2:B4:409:VAL:HG12 | 1.90                     | 0.54              |
| 2:C0:11:GLN:NE2   | 2:C0:15:GLN:OE1   | 2.41                     | 0.54              |
| 2:C0:278:ALA:HA   | 2:C0:369:ALA:HB2  | 1.88                     | 0.54              |
| 2:C6:97:GLU:OE2   | 2:C6:105:ARG:NH2  | 2.31                     | 0.54              |
| 3:C7:183:TYR:HB3  | 3:C7:398:TYR:HE2  | 1.73                     | 0.54              |
| 3:C7:262:ARG:NH1  | 3:C7:421:GLU:OE2  | 2.40                     | 0.54              |
| 2:C8:177:VAL:HG13 | 3:C9:327:ASP:OD2  | 2.07                     | 0.54              |
| 2:D0:119:LEU:HA   | 2:D0:122:ILE:HG22 | 1.90                     | 0.54              |
| 2:D0:179:THR:OG1  | 3:D1:246:LEU:CD2  | 2.55                     | 0.54              |
| 2:D0:288:VAL:HA   | 2:D0:291:ILE:HG12 | 1.90                     | 0.54              |
| 2:D4:210:TYR:CB   | 3:D5:324:LYS:HD3  | 2.37                     | 0.54              |
| 2:D6:181:VAL:H    | 3:D7:256:ASN:ND2  | 2.05                     | 0.54              |
| 2:D6:285:GLN:HB2  | 2:E0:55:GLU:O     | 2.07                     | 0.54              |
| 3:D7:282:ARG:NH1  | 3:D7:288:GLU:OE2  | 2.41                     | 0.54              |
| 2:E8:236:SER:O    | 2:E8:243:ARG:NH2  | 2.38                     | 0.54              |
| 5:l:58:LYS:HD2    | 4:n:161:TYR:CE1   | 2.43                     | 0.54              |
| 4:p:170:VAL:HG22  | 4:p:185:ILE:HD11  | 1.90                     | 0.54              |
| 1:0:248:ARG:NH2   | 4:c:160:GLY:O     | 2.40                     | 0.54              |
| 3:A1:193:VAL:HG12 | 3:A1:265:PHE:CE2  | 2.42                     | 0.54              |
| 3:A3:91:VAL:HG21  | 3:A3:116:VAL:HG12 | 1.89                     | 0.54              |
| 2:B2:234:VAL:HG21 | 2:B2:302:MET:HE1  | 1.88                     | 0.54              |
| 3:B3:152:ILE:HG23 | 3:B3:164:MET:HE1  | 1.90                     | 0.54              |
| 3:B9:311:LEU:HD12 | 3:B9:342:VAL:HG11 | 1.89                     | 0.54              |
| 2:C8:206:ASN:HD22 | 2:C8:227:LEU:HD23 | 1.73                     | 0.54              |
| 3:E1:49:VAL:HG21  | 3:E1:241:ARG:HG2  | 1.90                     | 0.54              |
| 2:E4:369:ALA:HB1  | 5:w:161:PHE:CZ    | 2.43                     | 0.54              |
| 3:E9:220:PRO:HD2  | 2:F0:326:LYS:CE   | 2.38                     | 0.54              |
| 1:5:256:LEU:HD23  | 2:B4:31:GLN:HG2   | 1.88                     | 0.54              |
| 2:A0:168:ASN:ND2  | 2:A0:170:CYS:SG   | 2.81                     | 0.54              |
| 3:A9:345:ILE:O    | 3:A9:348:ASN:ND2  | 2.41                     | 0.54              |
| 2:B8:283:HIS:HB2  | 2:C2:88:HIS:CD2   | 2.43                     | 0.54              |
| 2:C2:306:ASP:OD1  | 2:C2:308:ARG:NH1  | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C8:407:TRP:CZ2  | 3:C9:254:ALA:O    | 2.60                     | 0.54              |
| 3:D1:100:ASN:HB3  | 3:D1:103:LYS:HG2  | 1.90                     | 0.54              |
| 3:D3:392:LYS:O    | 2:D4:262:TYR:OH   | 2.26                     | 0.54              |
| 2:D4:96:LYS:HZ3   | 3:D5:128:ASP:HB2  | 1.70                     | 0.54              |
| 3:D9:412:GLU:O    | 3:D9:416:ASN:ND2  | 2.40                     | 0.54              |
| 3:E1:2:ARG:HB2    | 3:E1:131:GLN:HB2  | 1.90                     | 0.54              |
| 3:E3:64:ILE:HD12  | 3:E3:119:VAL:HG12 | 1.90                     | 0.54              |
| 3:E7:68:LEU:HD12  | 3:E7:143:THR:HG22 | 1.90                     | 0.54              |
| 3:F1:43:GLN:HA    | 3:F1:242:PHE:HE1  | 1.73                     | 0.54              |
| 4:t:175:SER:HA    | 4:t:206:PHE:CE1   | 2.43                     | 0.54              |
| 1:0:241:PHE:CZ    | 3:A5:356:ILE:HG23 | 2.43                     | 0.54              |
| 1:2:244:GLN:CG    | 4:e:162:GLY:HA3   | 2.37                     | 0.54              |
| 2:A0:268:MET:N    | 2:A0:268:MET:SD   | 2.81                     | 0.54              |
| 2:A2:102:ASN:HB2  | 2:A2:105:ARG:HB2  | 1.90                     | 0.54              |
| 2:A8:71:GLU:HB2   | 2:A8:98:ASP:OD1   | 2.08                     | 0.54              |
| 3:A9:208:TYR:HE1  | 3:A9:225:LEU:HD11 | 1.73                     | 0.54              |
| 2:B4:377:MET:HE3  | 2:B4:379:SER:HB3  | 1.90                     | 0.54              |
| 2:C4:121:ARG:HH22 | 2:C4:124:LYS:HE3  | 1.72                     | 0.54              |
| 2:C4:236:SER:O    | 2:C4:243:ARG:NH2  | 2.39                     | 0.54              |
| 2:C6:240:ALA:HB1  | 2:C6:356:ASN:HD22 | 1.72                     | 0.54              |
| 2:C8:282:TYR:CE2  | 2:D2:60:LYS:NZ    | 2.70                     | 0.54              |
| 3:D5:13:GLY:HA2   | 3:D5:16:ILE:HG22  | 1.89                     | 0.54              |
| 2:E0:406:HIS:HA   | 2:E0:409:VAL:HG12 | 1.88                     | 0.54              |
| 2:E6:217:LEU:HD21 | 2:E6:367:ASP:HB3  | 1.89                     | 0.54              |
| 4:o:78:ALA:HB3    | 4:o:112:PHE:HE1   | 1.73                     | 0.54              |
| 4:t:67:HIS:HE1    | 4:v:16:ARG:HG2    | 1.73                     | 0.54              |
| 5:w:130:LEU:HD21  | 5:w:143:ARG:NH1   | 2.22                     | 0.54              |
| 1:21:257:PRO:HD3  | 2:F0:26:LEU:HB2   | 1.89                     | 0.54              |
| 1:5:256:LEU:HD23  | 2:B4:31:GLN:HG3   | 1.90                     | 0.54              |
| 1:7:256:LEU:HD11  | 2:B8:31:GLN:N     | 2.22                     | 0.54              |
| 2:A2:174:SER:HB3  | 2:A2:177:VAL:O    | 2.07                     | 0.54              |
| 2:A6:82:THR:HA    | 4:b:98:THR:HG23   | 1.88                     | 0.54              |
| 2:B0:283:HIS:CD2  | 2:B4:60:LYS:HE2   | 2.43                     | 0.54              |
| 2:C0:241:SER:OG   | 2:C0:250:VAL:O    | 2.25                     | 0.54              |
| 2:D2:173:PRO:HG2  | 2:D2:391:MET:HE1  | 1.89                     | 0.54              |
| 2:D6:100:ALA:HA   | 3:D7:252:LYS:HG3  | 1.89                     | 0.54              |
| 3:D9:39:ASP:HA    | 4:r:90:PRO:HG3    | 1.90                     | 0.54              |
| 2:E6:258:ASN:HB3  | 2:E6:352:LYS:HE3  | 1.89                     | 0.54              |
| 3:F1:180:VAL:O    | 3:F1:184:ASN:ND2  | 2.41                     | 0.54              |
| 4:a:77:PHE:HE2    | 4:a:171:ILE:HD11  | 1.73                     | 0.54              |
| 4:f:198:ARG:HG3   | 4:f:198:ARG:NH1   | 2.23                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:w:153:VAL:HA    | 5:w:156:ARG:HB2   | 1.90                     | 0.54              |
| 1:10:246:CYS:N    | 3:C9:355:ASP:OD2  | 2.41                     | 0.53              |
| 1:13:244:GLN:CD   | 4:r:163:SER:H     | 2.16                     | 0.53              |
| 3:A7:180:VAL:O    | 3:A7:184:ASN:ND2  | 2.40                     | 0.53              |
| 3:B1:260:PHE:HB3  | 3:B1:261:PRO:HD2  | 1.90                     | 0.53              |
| 3:B9:167:PHE:CZ   | 3:B9:233:MET:HG2  | 2.43                     | 0.53              |
| 3:C7:237:THR:HG22 | 3:C7:250:LEU:HD11 | 1.89                     | 0.53              |
| 3:D3:139:LEU:HG   | 3:D3:168:SER:HB2  | 1.90                     | 0.53              |
| 3:D3:311:LEU:HD23 | 3:D3:342:VAL:HG11 | 1.90                     | 0.53              |
| 3:D5:238:CYS:SG   | 3:D5:318:ARG:NE   | 2.81                     | 0.53              |
| 2:D6:172:TRP:HZ2  | 2:D6:391:MET:HE1  | 1.73                     | 0.53              |
| 2:D8:407:TRP:CD2  | 3:D9:255:VAL:HG23 | 2.43                     | 0.53              |
| 2:E4:338:LYS:HZ1  | 2:E4:341:ILE:HG12 | 1.73                     | 0.53              |
| 4:n:97:ARG:HD2    | 4:p:161:TYR:CE2   | 2.43                     | 0.53              |
| 4:s:78:ALA:HB3    | 4:s:112:PHE:HE1   | 1.73                     | 0.53              |
| 5:x:40:LYS:NZ     | 5:x:76:LEU:O      | 2.40                     | 0.53              |
| 1:15:256:LEU:HD12 | 2:D8:31:GLN:CD    | 2.34                     | 0.53              |
| 3:A1:341:PHE:HB3  | 3:A1:348:ASN:HD22 | 1.72                     | 0.53              |
| 3:A5:16:ILE:HG22  | 3:A5:226:ASN:CG   | 2.33                     | 0.53              |
| 2:A8:309:HIS:NE2  | 2:A8:386:GLU:OE1  | 2.39                     | 0.53              |
| 2:B8:306:ASP:OD2  | 2:B8:308:ARG:NH2  | 2.39                     | 0.53              |
| 3:C1:7:VAL:HB     | 3:C1:135:ILE:HD13 | 1.89                     | 0.53              |
| 3:D1:385:PHE:CE2  | 3:D1:412:GLU:HB3  | 2.43                     | 0.53              |
| 2:D2:403:ALA:HB2  | 3:D3:344:TRP:CZ3  | 2.43                     | 0.53              |
| 2:E0:223:THR:OG1  | 3:E1:245:GLN:NE2  | 2.40                     | 0.53              |
| 2:E4:279:GLU:OE2  | 2:E8:89:PRO:HG2   | 2.08                     | 0.53              |
| 2:E6:4:VAL:HG12   | 2:E6:133:GLN:HB3  | 1.91                     | 0.53              |
| 2:E6:277:SER:OG   | 2:E6:278:ALA:N    | 2.38                     | 0.53              |
| 2:F0:407:TRP:HZ2  | 3:F1:258:ILE:CD1  | 2.17                     | 0.53              |
| 4:c:92:LEU:HD21   | 4:c:110:ILE:HD13  | 1.90                     | 0.53              |
| 4:n:172:VAL:HG12  | 4:n:181:GLN:HG2   | 1.91                     | 0.53              |
| 5:w:130:LEU:HD21  | 5:w:143:ARG:HH12  | 1.74                     | 0.53              |
| 1:0:244:GLN:HE22  | 4:c:162:GLY:N     | 2.05                     | 0.53              |
| 2:A0:406:HIS:HE1  | 3:A1:259:PRO:O    | 1.91                     | 0.53              |
| 3:B7:139:LEU:HA   | 3:B7:145:SER:HB3  | 1.91                     | 0.53              |
| 2:B8:123:ARG:NH1  | 2:B8:123:ARG:HB3  | 2.23                     | 0.53              |
| 3:B9:11:GLN:HG3   | 3:B9:12:CYS:N     | 2.22                     | 0.53              |
| 2:C4:274:PRO:HG2  | 2:C4:371:VAL:HG11 | 1.90                     | 0.53              |
| 2:C6:186:ASN:OD1  | 2:C6:408:TYR:OH   | 2.26                     | 0.53              |
| 2:C6:398:MET:HE1  | 3:C7:345:ILE:HG23 | 1.90                     | 0.53              |
| 3:D5:213:ARG:HH12 | 3:D5:297:LYS:HB2  | 1.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D8:238:LEU:HD11 | 2:D8:255:PHE:CE2  | 2.42                     | 0.53              |
| 3:E1:172:SER:HB3  | 3:E1:205:GLU:HG2  | 1.90                     | 0.53              |
| 3:E5:181:GLU:HB2  | 3:E5:182:PRO:HD3  | 1.89                     | 0.53              |
| 2:E6:280:LYS:NZ   | 2:F0:89:PRO:CB    | 2.68                     | 0.53              |
| 3:E7:105:HIS:CD2  | 3:E7:150:LEU:HB2  | 2.43                     | 0.53              |
| 4:j:187:SER:OG    | 4:j:188:GLY:N     | 2.41                     | 0.53              |
| 4:t:78:ALA:HB3    | 4:t:112:PHE:HE1   | 1.73                     | 0.53              |
| 1:17:253:ALA:HB2  | 2:E2:32:PRO:HG2   | 1.91                     | 0.53              |
| 2:A4:221:ARG:HB3  | 3:A5:322:SER:CB   | 2.38                     | 0.53              |
| 2:B4:240:ALA:HB1  | 2:B4:356:ASN:HD22 | 1.73                     | 0.53              |
| 3:C1:263:LEU:HB2  | 3:C1:422:TYR:CZ   | 2.43                     | 0.53              |
| 2:D0:168:ASN:ND2  | 2:D0:170:CYS:SG   | 2.81                     | 0.53              |
| 2:D4:11:GLN:HG3   | 2:D4:74:VAL:HG21  | 1.90                     | 0.53              |
| 3:E1:318:ARG:HG2  | 3:E1:354:CYS:HB3  | 1.91                     | 0.53              |
| 2:E4:11:GLN:HE22  | 3:E5:246:LEU:HA   | 1.74                     | 0.53              |
| 2:E8:12:ALA:HB3   | 2:E8:140:ALA:HB2  | 1.90                     | 0.53              |
| 2:E8:252:VAL:HA   | 2:E8:255:PHE:HD2  | 1.72                     | 0.53              |
| 2:F0:209:ILE:HB   | 2:F0:227:LEU:HD13 | 1.90                     | 0.53              |
| 2:F0:398:MET:HE3  | 3:F1:346:PRO:HD2  | 1.90                     | 0.53              |
| 4:p:23:LEU:HD23   | 4:p:38:LEU:CD2    | 2.39                     | 0.53              |
| 4:r:106:GLN:NE2   | 4:r:109:GLU:OE1   | 2.42                     | 0.53              |
| 1:7:256:LEU:CG    | 2:B8:31:GLN:HB3   | 2.37                     | 0.53              |
| 3:A1:218:THR:O    | 2:A2:326:LYS:CE   | 2.50                     | 0.53              |
| 2:B4:282:TYR:HD2  | 2:B4:283:HIS:CE1  | 2.27                     | 0.53              |
| 3:B5:171:PRO:HB3  | 3:B5:181:GLU:OE1  | 2.09                     | 0.53              |
| 3:B9:293:MET:HE2  | 3:B9:365:VAL:HG11 | 1.89                     | 0.53              |
| 2:C0:286:LEU:O    | 2:C0:373:ARG:NH1  | 2.42                     | 0.53              |
| 2:C4:287:SER:OG   | 2:C4:290:GLU:OE1  | 2.21                     | 0.53              |
| 3:C5:6:HIS:CD2    | 3:C5:134:GLN:HG3  | 2.43                     | 0.53              |
| 2:C6:352:LYS:NZ   | 2:C6:353:CYS:O    | 2.40                     | 0.53              |
| 2:D4:215:ARG:HH12 | 2:D4:299:ALA:CB   | 2.21                     | 0.53              |
| 2:E2:36:MET:HE3   | 2:E2:61:HIS:NE2   | 2.23                     | 0.53              |
| 3:F1:113:ILE:HA   | 3:F1:116:VAL:HG12 | 1.89                     | 0.53              |
| 4:q:181:GLN:NE2   | 4:q:200:ASP:OD1   | 2.40                     | 0.53              |
| 1:1:254:LYS:CB    | 2:A6:364:PRO:HB2  | 2.38                     | 0.53              |
| 1:17:247:TYR:HE2  | 2:E2:82:THR:H     | 1.56                     | 0.53              |
| 1:9:243:ALA:HB1   | 3:C3:356:ILE:HD13 | 1.90                     | 0.53              |
| 2:A0:136:LEU:HD23 | 2:A0:167:LEU:HB3  | 1.89                     | 0.53              |
| 3:A1:32:PRO:O     | 3:A1:83:GLN:NE2   | 2.41                     | 0.53              |
| 2:B2:221:ARG:HG3  | 2:B2:221:ARG:NH1  | 2.24                     | 0.53              |
| 3:B7:15:GLN:O     | 3:B7:226:ASN:ND2  | 2.40                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B7:212:PHE:CD1  | 2:B8:326:LYS:HD3  | 2.43                     | 0.53              |
| 2:B8:278:ALA:HA   | 2:B8:369:ALA:HB2  | 1.89                     | 0.53              |
| 2:C0:306:ASP:N    | 2:C0:386:GLU:OE2  | 2.41                     | 0.53              |
| 3:C9:100:ASN:HB3  | 3:C9:103:LYS:HG2  | 1.91                     | 0.53              |
| 2:D4:203:MET:HE2  | 2:D4:267:PHE:HB3  | 1.90                     | 0.53              |
| 3:D5:100:ASN:ND2  | 3:D5:397:TRP:O    | 2.41                     | 0.53              |
| 3:E7:44:LEU:CD2   | 4:v:91:PHE:HE2    | 2.22                     | 0.53              |
| 4:h:187:SER:OG    | 4:h:188:GLY:N     | 2.41                     | 0.53              |
| 5:k:40:LYS:HB3    | 5:k:76:LEU:HB2    | 1.90                     | 0.53              |
| 5:l:112:PRO:HD2   | 5:l:127:ALA:HB3   | 1.90                     | 0.53              |
| 1:20:245:SER:HB3  | 1:20:248:ARG:HD3  | 1.91                     | 0.53              |
| 1:8:253:ALA:HB2   | 4:i:101:GLU:OE1   | 2.09                     | 0.53              |
| 3:B3:16:ILE:HD11  | 3:B3:229:VAL:CG1  | 2.36                     | 0.53              |
| 3:C3:149:THR:O    | 3:C3:191:GLN:NE2  | 2.42                     | 0.53              |
| 3:C9:174:LYS:NZ   | 2:D0:329:ASN:O    | 2.41                     | 0.53              |
| 2:D2:96:LYS:NZ    | 3:D3:128:ASP:HB2  | 2.23                     | 0.53              |
| 2:D4:230:LEU:HD21 | 2:D4:368:LEU:HD11 | 1.90                     | 0.53              |
| 3:D7:396:HIS:HA   | 3:D7:399:THR:HG22 | 1.90                     | 0.53              |
| 2:E6:64:ARG:HB3   | 2:E6:125:LEU:HD21 | 1.89                     | 0.53              |
| 2:E8:396:ASP:OD1  | 2:E8:422:ARG:NH1  | 2.42                     | 0.53              |
| 2:F0:224:TYR:CD2  | 3:F1:323:THR:HG21 | 2.44                     | 0.53              |
| 4:b:97:ARG:NH1    | 4:d:6:PHE:CG      | 2.73                     | 0.53              |
| 4:c:172:VAL:HG12  | 4:c:204:THR:HG21  | 1.90                     | 0.53              |
| 5:x:57:TYR:HE2    | 5:x:70:GLU:HA     | 1.72                     | 0.53              |
| 2:A0:180:ALA:HB3  | 2:A0:183:GLU:HG2  | 1.90                     | 0.53              |
| 2:A4:208:ALA:HA   | 2:A4:304:LYS:HD3  | 1.91                     | 0.53              |
| 2:A6:174:SER:HB3  | 2:A6:207:GLU:HG2  | 1.91                     | 0.53              |
| 3:B5:44:LEU:HD23  | 4:f:91:PHE:HE1    | 1.72                     | 0.53              |
| 2:D2:75:VAL:HG11  | 2:D2:94:SER:HB3   | 1.90                     | 0.53              |
| 3:D3:101:TRP:CE3  | 3:D3:403:MET:HE1  | 2.44                     | 0.53              |
| 2:D6:69:ASP:OD1   | 2:D6:70:LEU:N     | 2.41                     | 0.53              |
| 2:D8:319:TYR:CD2  | 2:D8:375:VAL:HG22 | 2.43                     | 0.53              |
| 3:E3:46:ARG:HH21  | 3:E3:46:ARG:CG    | 2.22                     | 0.53              |
| 3:E7:234:SER:O    | 3:E7:241:ARG:NH2  | 2.42                     | 0.53              |
| 4:a:97:ARG:HH12   | 4:c:6:PHE:H       | 1.55                     | 0.53              |
| 4:f:73:VAL:HG12   | 4:f:109:GLU:HB3   | 1.91                     | 0.53              |
| 4:g:8:SER:HB2     | 4:g:147:HIS:HA    | 1.91                     | 0.53              |
| 2:A2:176:GLN:HB3  | 3:A3:331:LEU:HD22 | 1.91                     | 0.53              |
| 2:A6:79:ARG:NH1   | 2:A6:94:SER:OG    | 2.42                     | 0.53              |
| 2:C2:265:ILE:HD12 | 2:C2:432:TYR:CE1  | 2.44                     | 0.53              |
| 3:C3:183:TYR:HB3  | 3:C3:398:TYR:HE2  | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C4:2:ARG:CD     | 2:C4:2:ARG:CB     | 2.78                     | 0.53              |
| 3:C7:295:ASP:HB3  | 3:C7:298:ASN:HB2  | 1.90                     | 0.53              |
| 2:C8:141:VAL:HG23 | 2:C8:170:CYS:HB3  | 1.91                     | 0.53              |
| 3:C9:57:GLY:HA3   | 4:m:83:PRO:HB2    | 1.91                     | 0.53              |
| 3:D1:248:SER:HA   | 3:D1:252:LYS:HG3  | 1.91                     | 0.53              |
| 3:D3:100:ASN:HB3  | 3:D3:103:LYS:HB2  | 1.91                     | 0.53              |
| 2:E2:76:ASP:HA    | 2:E2:79:ARG:HD2   | 1.90                     | 0.53              |
| 2:E4:221:ARG:NH2  | 3:E5:322:SER:O    | 2.41                     | 0.53              |
| 3:E9:68:LEU:HG    | 3:E9:147:MET:HE2  | 1.90                     | 0.53              |
| 3:E9:244:GLY:HA2  | 3:E9:355:ASP:HB2  | 1.91                     | 0.53              |
| 4:d:170:VAL:HG23  | 4:d:183:LEU:HB2   | 1.90                     | 0.53              |
| 4:h:75:LEU:O      | 4:h:170:VAL:HA    | 2.09                     | 0.53              |
| 3:A5:317:PHE:CD1  | 3:A5:365:VAL:HG22 | 2.43                     | 0.53              |
| 2:B2:8:HIS:CE1    | 2:B2:17:GLY:HA3   | 2.44                     | 0.53              |
| 2:C2:103:PHE:H    | 2:C2:408:TYR:HE1  | 1.57                     | 0.53              |
| 2:C4:287:SER:HA   | 2:C4:373:ARG:HH21 | 1.73                     | 0.53              |
| 3:D7:135:ILE:HB   | 3:D7:166:THR:HG22 | 1.89                     | 0.53              |
| 2:D8:205:ASP:OD1  | 2:D8:206:ASN:N    | 2.42                     | 0.53              |
| 2:E4:12:ALA:HB3   | 2:E4:140:ALA:HB2  | 1.91                     | 0.53              |
| 2:E6:222:PRO:HD2  | 3:E7:324:LYS:CB   | 2.39                     | 0.53              |
| 3:F1:321:MET:HE3  | 3:F1:363:MET:SD   | 2.49                     | 0.53              |
| 1:10:239:LEU:HG   | 1:10:240:PRO:HD2  | 1.91                     | 0.52              |
| 3:A1:77:ARG:HH22  | 3:A1:92:PHE:HZ    | 1.56                     | 0.52              |
| 2:A4:269:LEU:HB3  | 2:A4:301:MET:CE   | 2.38                     | 0.52              |
| 3:A5:10:GLY:HA2   | 3:A5:143:THR:HG23 | 1.91                     | 0.52              |
| 3:A5:105:HIS:CD2  | 3:A5:150:LEU:HB2  | 2.44                     | 0.52              |
| 2:A6:7:ILE:HD11   | 2:A6:137:MET:CE   | 2.38                     | 0.52              |
| 2:B6:178:SER:HB3  | 3:B7:347:ASN:CG   | 2.34                     | 0.52              |
| 3:B9:283:ALA:HB2  | 3:C3:53:GLU:O     | 2.08                     | 0.52              |
| 3:C3:10:GLY:O     | 3:C3:14:ASN:ND2   | 2.42                     | 0.52              |
| 2:C4:179:THR:O    | 3:C5:350:LYS:HD2  | 2.08                     | 0.52              |
| 2:D0:217:LEU:O    | 4:p:198:ARG:NH2   | 2.42                     | 0.52              |
| 3:D5:228:LEU:HG   | 3:D5:300:MET:HE2  | 1.90                     | 0.52              |
| 3:D9:267:LEU:HB3  | 3:D9:299:MET:HE2  | 1.90                     | 0.52              |
| 2:E8:306:ASP:HB3  | 2:E8:309:HIS:CE1  | 2.45                     | 0.52              |
| 4:c:119:ARG:NH2   | 4:c:137:GLU:HB3   | 2.24                     | 0.52              |
| 2:A8:137:MET:SD   | 2:A8:154:LEU:HD11 | 2.49                     | 0.52              |
| 3:B5:260:PHE:HB3  | 3:B5:261:PRO:CD   | 2.37                     | 0.52              |
| 3:C1:334:GLN:OE1  | 3:C1:348:ASN:N    | 2.41                     | 0.52              |
| 3:C3:35:THR:OG1   | 3:C3:36:TYR:N     | 2.41                     | 0.52              |
| 3:C5:174:LYS:NZ   | 2:C6:336:LYS:HB2  | 2.23                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D2:219:ILE:CG2  | 4:q:198:ARG:HH22  | 2.22                     | 0.52              |
| 2:D8:177:VAL:HG11 | 3:D9:327:ASP:HB3  | 1.91                     | 0.52              |
| 3:E1:164:MET:HB3  | 3:E1:197:ASP:H    | 1.73                     | 0.52              |
| 3:E1:215:LEU:HB3  | 3:E1:217:LEU:HD13 | 1.92                     | 0.52              |
| 2:E4:241:SER:HB2  | 2:E4:249:ASN:HB2  | 1.89                     | 0.52              |
| 3:E5:318:ARG:HG2  | 3:E5:354:CYS:HB3  | 1.90                     | 0.52              |
| 2:E6:84:ARG:NH2   | 4:v:197:LEU:HD11  | 2.23                     | 0.52              |
| 4:c:176:ASP:OD1   | 4:c:176:ASP:N     | 2.42                     | 0.52              |
| 4:p:23:LEU:HD23   | 4:p:38:LEU:HD21   | 1.90                     | 0.52              |
| 2:B0:65:CYS:O     | 2:B0:91:GLN:NE2   | 2.42                     | 0.52              |
| 3:B1:102:ALA:HB2  | 3:B1:403:MET:HE3  | 1.90                     | 0.52              |
| 3:B5:3:GLU:HA     | 3:B5:49:VAL:HA    | 1.91                     | 0.52              |
| 3:B7:287:PRO:HA   | 3:B7:290:THR:HG22 | 1.91                     | 0.52              |
| 3:C1:267:LEU:HD23 | 3:C1:299:MET:HE3  | 1.92                     | 0.52              |
| 2:C4:269:LEU:HD11 | 2:C4:384:ILE:HD11 | 1.90                     | 0.52              |
| 2:C6:277:SER:OG   | 2:C6:278:ALA:N    | 2.41                     | 0.52              |
| 2:D0:175:PRO:HB3  | 2:D0:390:ARG:HD3  | 1.91                     | 0.52              |
| 2:D2:11:GLN:NE2   | 3:D3:245:GLN:O    | 2.42                     | 0.52              |
| 3:D9:7:VAL:HG11   | 3:D9:151:LEU:HD23 | 1.90                     | 0.52              |
| 3:E5:304:ASP:OD2  | 3:E5:306:ARG:NH1  | 2.43                     | 0.52              |
| 2:E6:282:TYR:CG   | 5:x:160:ARG:HD2   | 2.44                     | 0.52              |
| 3:E7:128:ASP:OD1  | 3:E7:129:CYS:N    | 2.41                     | 0.52              |
| 2:F0:65:CYS:SG    | 2:F0:66:VAL:N     | 2.82                     | 0.52              |
| 4:a:139:PRO:O     | 4:a:143:ILE:HD12  | 2.09                     | 0.52              |
| 2:A0:18:ASN:HD21  | 2:A0:78:VAL:HG22  | 1.74                     | 0.52              |
| 2:B2:180:ALA:H    | 3:B3:347:ASN:HD21 | 1.58                     | 0.52              |
| 2:B6:270:SER:HB2  | 2:B6:302:MET:HE2  | 1.90                     | 0.52              |
| 3:B9:290:THR:HA   | 3:B9:293:MET:HE3  | 1.91                     | 0.52              |
| 2:C0:181:VAL:HG22 | 3:C1:256:ASN:CG   | 2.34                     | 0.52              |
| 3:C3:230:SER:HA   | 3:C3:233:MET:HE2  | 1.91                     | 0.52              |
| 2:C4:85:HIS:NE2   | 5:k:60:THR:HA     | 2.25                     | 0.52              |
| 3:C9:66:MET:CE    | 3:C9:151:LEU:HD22 | 2.39                     | 0.52              |
| 2:D8:204:LEU:HD13 | 2:D8:231:ILE:HD12 | 1.90                     | 0.52              |
| 2:F0:103:PHE:CD2  | 2:F0:189:LEU:HB3  | 2.45                     | 0.52              |
| 3:F1:184:ASN:OD1  | 3:F1:398:TYR:OH   | 2.24                     | 0.52              |
| 4:d:18:ASN:HB2    | 4:d:45:MET:HG2    | 1.91                     | 0.52              |
| 4:h:64:PRO:HD2    | 4:h:67:HIS:CE1    | 2.44                     | 0.52              |
| 1:7:251:TYR:CE2   | 2:B8:18:ASN:HB3   | 2.45                     | 0.52              |
| 1:9:241:PHE:CZ    | 3:C3:356:ILE:HG23 | 2.40                     | 0.52              |
| 2:A6:276:ILE:HB   | 2:A6:280:LYS:HB2  | 1.91                     | 0.52              |
| 2:B0:210:TYR:CB   | 3:B1:324:LYS:HD2  | 2.35                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B3:18:ALA:HB2   | 3:B3:76:VAL:HG23  | 1.90                     | 0.52              |
| 2:B6:258:ASN:HB3  | 2:B6:352:LYS:HG3  | 1.91                     | 0.52              |
| 3:C3:100:ASN:HB3  | 3:C3:103:LYS:HG2  | 1.90                     | 0.52              |
| 3:C3:113:ILE:HA   | 3:C3:116:VAL:HG12 | 1.92                     | 0.52              |
| 3:D9:128:ASP:OD1  | 3:D9:128:ASP:N    | 2.42                     | 0.52              |
| 3:D9:173:PRO:HB3  | 3:D9:380:ARG:CZ   | 2.39                     | 0.52              |
| 3:D9:238:CYS:SG   | 3:D9:318:ARG:NE   | 2.82                     | 0.52              |
| 2:E2:79:ARG:NH1   | 2:E2:92:LEU:O     | 2.43                     | 0.52              |
| 4:a:53:GLY:HA2    | 4:a:62:VAL:HG21   | 1.90                     | 0.52              |
| 4:b:78:ALA:HB3    | 4:b:112:PHE:HE1   | 1.74                     | 0.52              |
| 4:b:126:ARG:NH2   | 4:b:131:TRP:O     | 2.42                     | 0.52              |
| 5:k:49:ILE:HG13   | 5:k:129:PRO:HG2   | 1.91                     | 0.52              |
| 5:l:79:ASP:HB3    | 5:l:82:ASP:HB3    | 1.92                     | 0.52              |
| 4:s:151:MET:HE2   | 4:s:163:SER:HB2   | 1.91                     | 0.52              |
| 1:11:246:CYS:SG   | 3:D1:245:GLN:HG2  | 2.50                     | 0.52              |
| 1:18:245:SER:HA   | 3:E5:355:ASP:OD2  | 2.09                     | 0.52              |
| 3:A9:291:GLN:OE1  | 3:B3:122:LYS:NZ   | 2.35                     | 0.52              |
| 3:B3:27:GLU:OE2   | 3:B3:318:ARG:NH2  | 2.29                     | 0.52              |
| 3:B3:283:ALA:HA   | 3:B7:55:THR:HB    | 1.91                     | 0.52              |
| 2:B4:282:TYR:CE2  | 2:B8:85:HIS:HB3   | 2.40                     | 0.52              |
| 2:B6:33:ASP:O     | 2:B6:60:LYS:NZ    | 2.42                     | 0.52              |
| 2:B8:84:ARG:NH2   | 4:h:197:LEU:HD11  | 2.25                     | 0.52              |
| 3:B9:12:CYS:HB3   | 3:B9:138:SER:HB2  | 1.92                     | 0.52              |
| 3:C5:311:LEU:HD23 | 3:C5:342:VAL:HG11 | 1.90                     | 0.52              |
| 3:C9:220:PRO:HG2  | 2:D0:326:LYS:CE   | 2.39                     | 0.52              |
| 3:D1:284:LEU:HB3  | 3:D5:55:THR:CG2   | 2.29                     | 0.52              |
| 2:E0:96:LYS:HE2   | 3:E1:128:ASP:OD2  | 2.09                     | 0.52              |
| 2:F0:208:ALA:HB2  | 2:F0:304:LYS:HB2  | 1.91                     | 0.52              |
| 2:F0:322:ASP:O    | 2:F0:373:ARG:NH2  | 2.42                     | 0.52              |
| 5:l:18:GLN:HG2    | 4:n:146:ARG:NH1   | 2.24                     | 0.52              |
| 4:o:95:TYR:CZ     | 4:o:99:MET:HE3    | 2.45                     | 0.52              |
| 4:t:146:ARG:HD3   | 4:t:156:VAL:HG21  | 1.90                     | 0.52              |
| 2:A0:119:LEU:HD11 | 2:A0:156:ARG:HG2  | 1.92                     | 0.52              |
| 2:A0:339:ARG:O    | 2:A0:342:GLN:NE2  | 2.43                     | 0.52              |
| 2:B4:188:VAL:HG23 | 2:B4:425:LEU:HD22 | 1.92                     | 0.52              |
| 2:B6:282:TYR:CE2  | 2:C0:85:HIS:CG    | 2.97                     | 0.52              |
| 2:B8:50:ASN:O     | 2:B8:64:ARG:NH2   | 2.43                     | 0.52              |
| 3:D5:330:MET:HG2  | 3:D5:349:MET:HE2  | 1.92                     | 0.52              |
| 2:E0:221:ARG:CG   | 3:E1:322:SER:OG   | 2.58                     | 0.52              |
| 3:E3:213:ARG:HH21 | 3:E3:216:LYS:HE3  | 1.74                     | 0.52              |
| 2:E4:10:GLY:HA2   | 2:E4:145:THR:HG23 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E4:85:HIS:NE2   | 4:u:99:MET:HE1    | 2.25                     | 0.52              |
| 3:E7:35:THR:HG22  | 4:v:83:PRO:CG     | 2.37                     | 0.52              |
| 2:E8:214:ARG:HH22 | 2:E8:220:GLU:HG2  | 1.75                     | 0.52              |
| 3:F1:285:SER:N    | 3:F1:288:GLU:OE2  | 2.38                     | 0.52              |
| 4:f:9:PRO:HA      | 4:f:12:VAL:HG22   | 1.91                     | 0.52              |
| 4:m:18:ASN:HB2    | 4:m:45:MET:HG3    | 1.92                     | 0.52              |
| 2:A4:28:HIS:CE1   | 2:A4:243:ARG:HD2  | 2.45                     | 0.52              |
| 2:A6:208:ALA:HB2  | 2:A6:304:LYS:HG2  | 1.92                     | 0.52              |
| 3:B1:282:ARG:O    | 3:B5:55:THR:HG22  | 2.09                     | 0.52              |
| 2:B6:179:THR:HG21 | 3:B7:327:ASP:OD1  | 2.09                     | 0.52              |
| 2:C2:362:VAL:CG1  | 2:C2:370:LYS:HB3  | 2.34                     | 0.52              |
| 3:C3:69:GLU:HG2   | 3:C3:71:GLY:H     | 1.75                     | 0.52              |
| 3:C3:380:ARG:HH11 | 3:C3:381:VAL:HG23 | 1.75                     | 0.52              |
| 2:C6:304:LYS:HD3  | 2:C6:304:LYS:C    | 2.35                     | 0.52              |
| 2:D0:219:ILE:HG23 | 4:p:198:ARG:NH2   | 2.24                     | 0.52              |
| 2:D4:326:LYS:NZ   | 2:D4:327:ASP:OD1  | 2.38                     | 0.52              |
| 2:E8:296:PHE:CE2  | 2:E8:335:ILE:HG21 | 2.45                     | 0.52              |
| 2:F0:176:GLN:HG3  | 3:F1:331:LEU:CD2  | 2.40                     | 0.52              |
| 4:d:71:LYS:NZ     | 4:f:19:GLU:OE2    | 2.43                     | 0.52              |
| 4:s:68:LEU:HA     | 4:s:71:LYS:HZ2    | 1.74                     | 0.52              |
| 4:u:176:ASP:OD1   | 4:u:176:ASP:N     | 2.43                     | 0.52              |
| 1:4:240:PRO:HB2   | 4:g:154:TYR:O     | 2.09                     | 0.52              |
| 2:A0:137:MET:HG3  | 2:A0:154:LEU:HD12 | 1.90                     | 0.52              |
| 2:A2:324:VAL:HG12 | 2:A2:326:LYS:H    | 1.74                     | 0.52              |
| 2:A6:261:PRO:HG3  | 2:A6:313:MET:HE2  | 1.92                     | 0.52              |
| 3:A7:203:ASP:HB2  | 3:A7:301:CYS:HA   | 1.92                     | 0.52              |
| 2:A8:285:GLN:N    | 2:B2:56:THR:CB    | 2.73                     | 0.52              |
| 3:B1:10:GLY:HA2   | 3:B1:143:THR:HG23 | 1.91                     | 0.52              |
| 3:B1:16:ILE:HG22  | 3:B1:226:ASN:CG   | 2.35                     | 0.52              |
| 3:B5:128:ASP:N    | 3:B5:128:ASP:OD1  | 2.42                     | 0.52              |
| 2:B6:88:HIS:HB3   | 2:B6:91:GLN:HG3   | 1.92                     | 0.52              |
| 2:B6:306:ASP:OD2  | 2:B6:308:ARG:NH2  | 2.40                     | 0.52              |
| 2:C4:290:GLU:HA   | 2:C4:293:ASN:HB2  | 1.92                     | 0.52              |
| 3:D3:239:CYS:SG   | 3:D3:248:SER:N    | 2.82                     | 0.52              |
| 3:D5:324:LYS:HA   | 3:D5:327:ASP:HB2  | 1.91                     | 0.52              |
| 2:D8:298:PRO:HB3  | 2:D8:307:PRO:HD2  | 1.91                     | 0.52              |
| 3:D9:6:HIS:CE1    | 3:D9:8:GLN:HG2    | 2.45                     | 0.52              |
| 3:E5:309:ARG:H    | 3:E5:372:THR:HG22 | 1.75                     | 0.52              |
| 3:E7:64:ILE:HD13  | 3:E7:119:VAL:HG13 | 1.91                     | 0.52              |
| 4:e:7:ALA:HB3     | 4:e:161:TYR:HE2   | 1.75                     | 0.52              |
| 4:o:57:ASN:HA     | 4:o:132:LEU:HD23  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4:240:PRO:HG2   | 4:g:154:TYR:CA    | 2.40                     | 0.52              |
| 3:A5:201:VAL:HG13 | 3:A5:301:CYS:SG   | 2.50                     | 0.52              |
| 2:A8:180:ALA:HA   | 3:A9:350:LYS:HB3  | 1.92                     | 0.52              |
| 2:A8:241:SER:OG   | 2:A8:250:VAL:O    | 2.22                     | 0.52              |
| 3:A9:187:LEU:HA   | 3:A9:190:HIS:CE1  | 2.45                     | 0.52              |
| 3:C1:200:GLN:HG3  | 3:C1:268:ILE:HD11 | 1.92                     | 0.52              |
| 2:C2:151:CYS:SG   | 2:C2:193:SER:OG   | 2.49                     | 0.52              |
| 3:C5:68:LEU:HA    | 3:C5:93:GLY:HA3   | 1.91                     | 0.52              |
| 2:C6:101:ASN:HA   | 2:C6:144:GLY:CA   | 2.40                     | 0.52              |
| 2:C8:259:LEU:HD21 | 2:C8:316:CYS:HB2  | 1.92                     | 0.52              |
| 3:D3:7:VAL:HG11   | 3:D3:151:LEU:HD23 | 1.90                     | 0.52              |
| 3:E3:290:THR:HA   | 3:E3:293:MET:HE2  | 1.92                     | 0.52              |
| 2:E6:304:LYS:HG3  | 2:E6:304:LYS:O    | 2.09                     | 0.52              |
| 3:E7:257:LEU:HD21 | 3:E7:314:SER:HB3  | 1.91                     | 0.52              |
| 2:E8:395:PHE:HZ   | 2:E8:418:PHE:HB3  | 1.75                     | 0.52              |
| 3:E9:184:ASN:OD1  | 3:E9:398:TYR:OH   | 2.26                     | 0.52              |
| 4:t:15:ARG:HG2    | 4:t:45:MET:HE1    | 1.92                     | 0.52              |
| 1:11:255:PRO:HG3  | 4:p:178:ARG:NH1   | 2.25                     | 0.51              |
| 3:A1:128:ASP:OD1  | 3:A1:129:CYS:N    | 2.43                     | 0.51              |
| 3:A5:40:SER:HB3   | 3:A5:43:GLN:HG3   | 1.92                     | 0.51              |
| 3:B3:210:ILE:O    | 3:B3:214:THR:OG1  | 2.27                     | 0.51              |
| 3:C5:209:ASP:CG   | 3:C5:213:ARG:HH21 | 2.17                     | 0.51              |
| 2:D2:403:ALA:HB2  | 3:D3:344:TRP:CH2  | 2.44                     | 0.51              |
| 2:E0:76:ASP:HA    | 2:E0:79:ARG:HD2   | 1.92                     | 0.51              |
| 3:E9:267:LEU:HB3  | 3:E9:299:MET:SD   | 2.50                     | 0.51              |
| 5:k:73:TYR:HB2    | 5:k:92:TRP:HE1    | 1.74                     | 0.51              |
| 4:m:14:LYS:HE2    | 4:m:45:MET:HB3    | 1.92                     | 0.51              |
| 4:u:181:GLN:NE2   | 4:u:200:ASP:OD1   | 2.43                     | 0.51              |
| 1:20:240:PRO:O    | 3:E9:359:LYS:HG3  | 2.11                     | 0.51              |
| 1:9:243:ALA:HB3   | 3:C3:356:ILE:CG2  | 2.28                     | 0.51              |
| 3:A3:77:ARG:HH22  | 3:A3:92:PHE:HZ    | 1.58                     | 0.51              |
| 3:A3:398:TYR:HB3  | 3:A3:403:MET:HG3  | 1.92                     | 0.51              |
| 2:A6:210:TYR:C    | 3:A7:324:LYS:HZ1  | 2.18                     | 0.51              |
| 2:A8:212:ILE:HG12 | 2:A8:275:ILE:HD11 | 1.91                     | 0.51              |
| 2:B0:115:VAL:HG21 | 2:B0:152:LEU:HD22 | 1.92                     | 0.51              |
| 3:B5:12:CYS:SG    | 3:B5:138:SER:OG   | 2.63                     | 0.51              |
| 2:C4:313:MET:HE3  | 2:C4:380:ASN:HB3  | 1.92                     | 0.51              |
| 3:D3:112:LEU:HD23 | 3:D3:147:MET:HE1  | 1.92                     | 0.51              |
| 3:D3:128:ASP:N    | 3:D3:128:ASP:OD1  | 2.41                     | 0.51              |
| 3:D3:294:PHE:CD2  | 3:D3:333:VAL:HG21 | 2.45                     | 0.51              |
| 2:D4:309:HIS:NE2  | 2:D4:386:GLU:OE1  | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D8:395:PHE:HD2  | 2:D8:422:ARG:HD3  | 1.75                     | 0.51              |
| 3:D9:283:ALA:HB2  | 3:E3:53:GLU:O     | 2.10                     | 0.51              |
| 3:E5:128:ASP:OD1  | 3:E5:129:CYS:N    | 2.43                     | 0.51              |
| 3:E5:284:LEU:HD23 | 3:E5:362:LYS:HG2  | 1.92                     | 0.51              |
| 2:E6:250:VAL:HG21 | 2:E6:318:MET:SD   | 2.50                     | 0.51              |
| 3:E7:311:LEU:HD12 | 3:E7:342:VAL:HG11 | 1.92                     | 0.51              |
| 3:E9:121:ARG:NH2  | 3:E9:158:GLU:OE2  | 2.43                     | 0.51              |
| 4:r:55:LEU:HD22   | 4:r:111:ILE:HD12  | 1.93                     | 0.51              |
| 4:r:129:MET:SD    | 4:r:131:TRP:NE1   | 2.81                     | 0.51              |
| 4:s:106:GLN:NE2   | 4:s:108:ILE:O     | 2.43                     | 0.51              |
| 1:4:247:TYR:CZ    | 2:B2:81:GLY:HA3   | 2.43                     | 0.51              |
| 2:A0:315:CYS:HB2  | 2:A0:351:PHE:CD1  | 2.46                     | 0.51              |
| 3:A1:139:LEU:HD13 | 3:A1:168:SER:HB2  | 1.92                     | 0.51              |
| 3:A1:205:GLU:HA   | 3:A1:208:TYR:CD2  | 2.45                     | 0.51              |
| 3:B1:281:TYR:HA   | 3:B5:54:ALA:HB1   | 1.91                     | 0.51              |
| 3:B3:181:GLU:HB2  | 3:B3:182:PRO:HD3  | 1.92                     | 0.51              |
| 2:C2:84:ARG:NH1   | 4:j:197:LEU:HD11  | 2.25                     | 0.51              |
| 2:C2:155:GLU:HG2  | 2:C2:197:HIS:CD2  | 2.46                     | 0.51              |
| 2:D0:191:THR:HG21 | 2:D0:425:LEU:HD13 | 1.90                     | 0.51              |
| 2:D4:259:LEU:HD21 | 2:D4:316:CYS:HB2  | 1.92                     | 0.51              |
| 2:D6:298:PRO:HB3  | 2:D6:307:PRO:HD2  | 1.92                     | 0.51              |
| 3:D7:283:ALA:HB2  | 3:E1:54:ALA:HA    | 1.93                     | 0.51              |
| 3:D9:107:THR:OG1  | 3:D9:108:GLU:OE1  | 2.28                     | 0.51              |
| 2:E4:239:THR:OG1  | 2:E4:243:ARG:NH1  | 2.43                     | 0.51              |
| 3:E5:100:ASN:HB3  | 3:E5:103:LYS:HG2  | 1.92                     | 0.51              |
| 3:E5:213:ARG:HH12 | 3:E5:297:LYS:HB3  | 1.75                     | 0.51              |
| 3:F1:375:GLN:HE21 | 3:F1:379:LYS:HD3  | 1.74                     | 0.51              |
| 1:18:248:ARG:NH1  | 3:E5:42:LEU:HD21  | 2.25                     | 0.51              |
| 1:2:240:PRO:HB2   | 4:e:154:TYR:CG    | 2.46                     | 0.51              |
| 3:A1:210:ILE:HD11 | 3:A1:228:LEU:HD21 | 1.91                     | 0.51              |
| 2:A8:336:LYS:O    | 2:A8:339:ARG:NH2  | 2.43                     | 0.51              |
| 3:A9:73:MET:HE1   | 3:A9:90:PHE:CG    | 2.46                     | 0.51              |
| 3:C1:35:THR:OG1   | 3:C1:36:TYR:N     | 2.41                     | 0.51              |
| 2:C2:33:ASP:O     | 2:C2:60:LYS:NZ    | 2.33                     | 0.51              |
| 2:C2:186:ASN:OD1  | 2:C2:408:TYR:OH   | 2.27                     | 0.51              |
| 2:C6:407:TRP:CZ3  | 3:C7:255:VAL:C    | 2.82                     | 0.51              |
| 3:D1:294:PHE:CD2  | 3:D1:333:VAL:HG21 | 2.44                     | 0.51              |
| 2:D2:221:ARG:CZ   | 4:q:190:GLU:HB3   | 2.40                     | 0.51              |
| 3:D3:165:GLU:OE2  | 3:D3:200:GLN:NE2  | 2.43                     | 0.51              |
| 3:D9:139:LEU:HA   | 3:D9:145:SER:HB2  | 1.92                     | 0.51              |
| 3:E3:213:ARG:NH2  | 3:E3:216:LYS:HE3  | 2.25                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:156:ARG:NH1  | 3:E7:162:ARG:O    | 2.42                     | 0.51              |
| 3:F1:44:LEU:HD21  | 5:x:48:GLN:NE2    | 2.24                     | 0.51              |
| 4:r:154:TYR:CE1   | 4:r:158:THR:HG22  | 2.44                     | 0.51              |
| 1:13:251:TYR:HE2  | 2:D4:18:ASN:HB3   | 1.76                     | 0.51              |
| 1:16:246:CYS:N    | 3:E1:320:ARG:HH22 | 2.08                     | 0.51              |
| 1:20:256:LEU:HD21 | 2:E8:30:ILE:O     | 2.10                     | 0.51              |
| 2:A6:155:GLU:OE1  | 2:A6:197:HIS:NE2  | 2.33                     | 0.51              |
| 2:B0:79:ARG:HB3   | 2:B0:92:LEU:HD13  | 1.91                     | 0.51              |
| 3:B7:318:ARG:HD3  | 3:B7:358:PRO:HD3  | 1.92                     | 0.51              |
| 2:C0:106:GLY:HA3  | 2:C0:148:GLY:HA3  | 1.91                     | 0.51              |
| 2:C2:82:THR:HG23  | 4:j:101:GLU:OE2   | 2.10                     | 0.51              |
| 2:C2:217:LEU:HB3  | 2:C2:219:ILE:HG13 | 1.92                     | 0.51              |
| 3:C3:172:SER:OG   | 3:C3:205:GLU:OE2  | 2.29                     | 0.51              |
| 2:C4:222:PRO:HD2  | 3:C5:324:LYS:HB2  | 1.92                     | 0.51              |
| 3:C7:239:CYS:HB3  | 3:C7:248:SER:O    | 2.11                     | 0.51              |
| 3:C9:137:HIS:HE1  | 3:C9:166:THR:HB   | 1.75                     | 0.51              |
| 3:C9:347:ASN:OD1  | 3:C9:349:MET:HB3  | 2.11                     | 0.51              |
| 3:D1:1:MET:N      | 3:D1:128:ASP:OD2  | 2.38                     | 0.51              |
| 3:D1:203:ASP:OD2  | 3:D1:302:ALA:N    | 2.38                     | 0.51              |
| 2:D8:100:ALA:HA   | 3:D9:252:LYS:HG3  | 1.92                     | 0.51              |
| 2:E2:84:ARG:NH2   | 4:t:197:LEU:HD21  | 2.26                     | 0.51              |
| 4:c:100:ASN:ND2   | 4:e:6:PHE:CZ      | 2.79                     | 0.51              |
| 4:h:15:ARG:O      | 4:h:19:GLU:HG3    | 2.11                     | 0.51              |
| 4:s:8:SER:HB2     | 4:s:147:HIS:HA    | 1.91                     | 0.51              |
| 2:A4:210:TYR:CE1  | 2:A4:227:LEU:HD11 | 2.46                     | 0.51              |
| 3:A5:117:LEU:HA   | 3:A5:120:VAL:HG12 | 1.92                     | 0.51              |
| 3:A5:262:ARG:HD3  | 3:A5:421:GLU:OE2  | 2.11                     | 0.51              |
| 3:A9:259:PRO:HG2  | 3:A9:311:LEU:CD2  | 2.39                     | 0.51              |
| 3:C7:100:ASN:HB3  | 3:C7:103:LYS:HG2  | 1.93                     | 0.51              |
| 2:C8:203:MET:HE3  | 2:C8:267:PHE:HD2  | 1.76                     | 0.51              |
| 3:D3:12:CYS:HB3   | 3:D3:138:SER:HB2  | 1.91                     | 0.51              |
| 2:D4:221:ARG:CG   | 3:D5:322:SER:CB   | 2.89                     | 0.51              |
| 2:D6:283:HIS:CD2  | 2:E0:60:LYS:NZ    | 2.79                     | 0.51              |
| 3:D9:7:VAL:HG11   | 3:D9:151:LEU:HD21 | 1.91                     | 0.51              |
| 2:E0:176:GLN:HB3  | 3:E1:331:LEU:CD2  | 2.41                     | 0.51              |
| 2:E8:301:MET:HE1  | 2:E8:307:PRO:HG3  | 1.93                     | 0.51              |
| 4:d:9:PRO:HA      | 4:d:12:VAL:HG22   | 1.92                     | 0.51              |
| 4:v:112:PHE:CD2   | 4:v:129:MET:HE1   | 2.46                     | 0.51              |
| 1:10:254:LYS:HZ1  | 2:C8:22:GLU:HG2   | 1.69                     | 0.51              |
| 2:A0:91:GLN:HA    | 2:A0:121:ARG:HH12 | 1.75                     | 0.51              |
| 3:A7:139:LEU:HA   | 3:A7:145:SER:HB2  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A8:309:HIS:HE2  | 2:A8:386:GLU:CD   | 2.19                     | 0.51              |
| 3:B1:16:ILE:HG22  | 3:B1:226:ASN:OD1  | 2.10                     | 0.51              |
| 3:B9:49:VAL:HG11  | 3:B9:241:ARG:HG2  | 1.92                     | 0.51              |
| 3:C1:20:PHE:CD2   | 3:C1:233:MET:HE3  | 2.46                     | 0.51              |
| 2:C4:204:LEU:CD2  | 2:C4:302:MET:SD   | 2.98                     | 0.51              |
| 2:C6:71:GLU:HB3   | 2:C6:98:ASP:HB3   | 1.93                     | 0.51              |
| 2:D2:12:ALA:CB    | 2:D2:140:ALA:HB2  | 2.37                     | 0.51              |
| 2:D2:285:GLN:HB3  | 2:D6:56:THR:HA    | 1.92                     | 0.51              |
| 3:D7:398:TYR:HB3  | 3:D7:408:PHE:HZ   | 1.76                     | 0.51              |
| 3:E1:64:ILE:HD12  | 3:E1:119:VAL:HG12 | 1.92                     | 0.51              |
| 2:E4:422:ARG:NH1  | 2:E4:426:ALA:HB2  | 2.26                     | 0.51              |
| 2:E6:254:GLU:O    | 2:E6:258:ASN:ND2  | 2.44                     | 0.51              |
| 3:E7:139:LEU:HA   | 3:E7:145:SER:HB2  | 1.93                     | 0.51              |
| 3:E7:176:SER:OG   | 3:E7:181:GLU:OE1  | 2.28                     | 0.51              |
| 3:F1:44:LEU:HD21  | 5:x:48:GLN:CD     | 2.36                     | 0.51              |
| 2:A4:93:ILE:CG2   | 2:A4:117:LEU:HD22 | 2.38                     | 0.51              |
| 3:A5:284:LEU:H    | 3:A9:55:THR:HB    | 1.74                     | 0.51              |
| 2:A8:2:ARG:HG3    | 2:A8:51:THR:HG22  | 1.93                     | 0.51              |
| 3:B1:2:ARG:NH1    | 3:B1:249:ASP:OD2  | 2.43                     | 0.51              |
| 3:B9:170:PHE:HE2  | 3:B9:378:PHE:HE1  | 1.59                     | 0.51              |
| 3:C1:207:LEU:HB3  | 3:C1:225:LEU:HD22 | 1.93                     | 0.51              |
| 3:C7:140:GLY:O    | 3:C7:184:ASN:ND2  | 2.41                     | 0.51              |
| 3:D1:10:GLY:HA2   | 3:D1:143:THR:HG23 | 1.91                     | 0.51              |
| 2:D4:250:VAL:HG22 | 2:D4:352:LYS:NZ   | 2.26                     | 0.51              |
| 3:D7:397:TRP:NE1  | 2:D8:257:THR:HA   | 2.26                     | 0.51              |
| 2:E2:259:LEU:HB3  | 2:E2:268:MET:HE1  | 1.92                     | 0.51              |
| 3:E5:281:TYR:CD2  | 3:E9:86:ARG:HA    | 2.45                     | 0.51              |
| 2:E6:250:VAL:HG12 | 2:E6:254:GLU:HG2  | 1.92                     | 0.51              |
| 2:E8:80:THR:HG22  | 2:E8:84:ARG:HH21  | 1.75                     | 0.51              |
| 3:F1:57:GLY:HA3   | 5:x:44:SER:HB3    | 1.93                     | 0.51              |
| 4:o:18:ASN:ND2    | 4:o:46:ASP:OD1    | 2.44                     | 0.51              |
| 4:o:101:GLU:OE2   | 4:q:6:PHE:N       | 2.44                     | 0.51              |
| 1:17:247:TYR:CE2  | 2:E2:81:GLY:HA3   | 2.46                     | 0.51              |
| 2:B2:291:ILE:HD12 | 2:B2:375:VAL:HG23 | 1.93                     | 0.51              |
| 2:C8:101:ASN:HD22 | 3:C9:256:ASN:HD21 | 1.58                     | 0.51              |
| 2:D2:269:LEU:HD11 | 2:D2:384:ILE:HD11 | 1.92                     | 0.51              |
| 2:D8:53:PHE:O     | 2:D8:64:ARG:NH2   | 2.44                     | 0.51              |
| 2:D8:223:THR:HG23 | 2:D8:225:THR:H    | 1.76                     | 0.51              |
| 3:F1:30:ILE:HD12  | 3:F1:51:TYR:HE2   | 1.76                     | 0.51              |
| 4:j:142:GLU:OE2   | 4:j:146:ARG:NH2   | 2.44                     | 0.51              |
| 4:m:50:PHE:HD2    | 4:m:55:LEU:HD11   | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:p:74:ALA:HB2    | 4:p:172:VAL:HG12  | 1.93                     | 0.51              |
| 4:u:59:ASN:OD1    | 5:w:100:CYS:HB3   | 2.10                     | 0.51              |
| 4:u:149:ARG:HD3   | 4:u:161:TYR:CD1   | 2.46                     | 0.51              |
| 3:A3:383:ASP:HA   | 3:A3:386:THR:HG22 | 1.93                     | 0.51              |
| 2:A6:283:HIS:CD2  | 2:B0:60:LYS:NZ    | 2.79                     | 0.51              |
| 3:A7:281:TYR:C    | 3:B1:54:ALA:HB1   | 2.36                     | 0.51              |
| 3:A9:267:LEU:HD21 | 3:A9:374:ILE:HG22 | 1.93                     | 0.51              |
| 3:B7:313:ALA:HB3  | 3:B7:349:MET:HE2  | 1.92                     | 0.51              |
| 3:C5:7:VAL:HB     | 3:C5:135:ILE:HG22 | 1.92                     | 0.51              |
| 2:D4:298:PRO:HB3  | 2:D4:307:PRO:HD2  | 1.92                     | 0.51              |
| 3:D5:289:LEU:HD13 | 3:D5:365:VAL:HG23 | 1.92                     | 0.51              |
| 2:E4:69:ASP:OD1   | 2:E4:70:LEU:N     | 2.44                     | 0.51              |
| 3:E7:281:TYR:O    | 3:F1:54:ALA:HB1   | 2.11                     | 0.51              |
| 2:F0:28:HIS:NE2   | 2:F0:243:ARG:HD2  | 2.26                     | 0.51              |
| 3:F1:293:MET:HE3  | 3:F1:367:PHE:HB2  | 1.93                     | 0.51              |
| 4:j:175:SER:HA    | 4:j:206:PHE:HE1   | 1.76                     | 0.51              |
| 4:n:78:ALA:HB3    | 4:n:112:PHE:HE1   | 1.76                     | 0.51              |
| 4:q:106:GLN:NE2   | 4:q:109:GLU:OE1   | 2.44                     | 0.51              |
| 4:t:146:ARG:HH11  | 4:t:146:ARG:HG3   | 1.75                     | 0.51              |
| 2:A2:384:ILE:HA   | 2:A2:387:VAL:HG12 | 1.93                     | 0.50              |
| 3:A5:219:THR:HB   | 2:A6:324:VAL:HG21 | 1.93                     | 0.50              |
| 2:B0:172:TRP:HB3  | 2:B0:205:ASP:OD1  | 2.10                     | 0.50              |
| 2:B0:210:TYR:HB3  | 3:B1:324:LYS:NZ   | 2.26                     | 0.50              |
| 2:B4:286:LEU:O    | 2:B4:373:ARG:NH1  | 2.40                     | 0.50              |
| 2:C4:12:ALA:CB    | 2:C4:140:ALA:HB2  | 2.35                     | 0.50              |
| 2:C8:119:LEU:HA   | 2:C8:122:ILE:HG22 | 1.93                     | 0.50              |
| 3:D9:139:LEU:HD12 | 3:D9:170:PHE:CE1  | 2.44                     | 0.50              |
| 2:E2:283:HIS:HB3  | 2:E6:62:VAL:HG11  | 1.93                     | 0.50              |
| 4:f:97:ARG:HH12   | 4:h:161:TYR:HA    | 1.76                     | 0.50              |
| 4:g:9:PRO:HB2     | 4:g:143:ILE:HG23  | 1.93                     | 0.50              |
| 4:h:8:SER:OG      | 4:h:11:ASN:OD1    | 2.29                     | 0.50              |
| 4:h:101:GLU:OE2   | 4:j:161:TYR:OH    | 2.29                     | 0.50              |
| 4:v:5:VAL:O       | 4:v:11:ASN:ND2    | 2.43                     | 0.50              |
| 1:11:244:GLN:O    | 3:D1:355:ASP:CG   | 2.54                     | 0.50              |
| 2:A4:245:ASP:OD1  | 2:A4:245:ASP:N    | 2.40                     | 0.50              |
| 2:C2:261:PRO:HB2  | 2:C2:262:TYR:CD2  | 2.47                     | 0.50              |
| 2:C6:282:TYR:CG   | 4:n:202:ARG:HD2   | 2.46                     | 0.50              |
| 2:C6:407:TRP:CZ2  | 3:C7:258:ILE:HB   | 2.46                     | 0.50              |
| 2:D0:189:LEU:HD11 | 2:D0:418:PHE:CD1  | 2.47                     | 0.50              |
| 2:D0:275:ILE:HG23 | 2:D0:368:LEU:HD11 | 1.93                     | 0.50              |
| 3:D7:103:LYS:HB3  | 3:D7:401:GLU:HG2  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E2:319:TYR:CD1  | 2:E2:375:VAL:HG22 | 2.46                     | 0.50              |
| 3:E5:112:LEU:HD23 | 3:E5:112:LEU:O    | 2.11                     | 0.50              |
| 2:F0:239:THR:OG1  | 2:F0:243:ARG:NH1  | 2.45                     | 0.50              |
| 4:q:111:ILE:HD13  | 4:q:132:LEU:HB2   | 1.93                     | 0.50              |
| 4:t:101:GLU:OE2   | 4:v:6:PHE:HB3     | 2.04                     | 0.50              |
| 1:15:256:LEU:CD1  | 2:D8:31:GLN:N     | 2.70                     | 0.50              |
| 3:A3:205:GLU:HA   | 3:A3:208:TYR:HD2  | 1.76                     | 0.50              |
| 2:A4:221:ARG:C    | 3:A5:322:SER:HB2  | 2.37                     | 0.50              |
| 3:A5:175:VAL:HG21 | 2:A6:329:ASN:O    | 2.11                     | 0.50              |
| 3:A7:278:SER:OG   | 3:B1:87:PRO:HG2   | 2.11                     | 0.50              |
| 2:B4:9:VAL:HG12   | 2:B4:68:LEU:HB2   | 1.93                     | 0.50              |
| 3:B7:107:THR:HG21 | 3:B7:401:GLU:OE2  | 2.10                     | 0.50              |
| 3:C1:68:LEU:HA    | 3:C1:93:GLY:HA3   | 1.93                     | 0.50              |
| 2:C8:217:LEU:HB3  | 2:C8:219:ILE:HG13 | 1.94                     | 0.50              |
| 3:D1:12:CYS:HB3   | 3:D1:138:SER:HB2  | 1.94                     | 0.50              |
| 2:D6:50:ASN:O     | 2:D6:64:ARG:NH2   | 2.44                     | 0.50              |
| 2:D6:265:ILE:HG22 | 2:D6:380:ASN:HD21 | 1.75                     | 0.50              |
| 2:E0:88:HIS:HB3   | 2:E0:91:GLN:HB2   | 1.93                     | 0.50              |
| 2:E0:192:HIS:NE2  | 2:E0:420:GLU:OE2  | 2.44                     | 0.50              |
| 3:E1:259:PRO:HD2  | 3:E1:263:LEU:HD11 | 1.93                     | 0.50              |
| 2:E4:221:ARG:CZ   | 3:E5:322:SER:OG   | 2.60                     | 0.50              |
| 2:E8:268:MET:N    | 2:E8:268:MET:SD   | 2.85                     | 0.50              |
| 4:e:170:VAL:HG23  | 4:e:183:LEU:HB2   | 1.94                     | 0.50              |
| 4:n:10:LEU:HB2    | 4:n:147:HIS:CE1   | 2.46                     | 0.50              |
| 1:23:255:PRO:HG3  | 4:m:178:ARG:HD3   | 1.93                     | 0.50              |
| 1:4:240:PRO:CG    | 4:g:154:TYR:C     | 2.84                     | 0.50              |
| 2:B2:208:ALA:HB2  | 2:B2:304:LYS:HB2  | 1.94                     | 0.50              |
| 2:B8:123:ARG:HB3  | 2:B8:123:ARG:HH11 | 1.77                     | 0.50              |
| 2:C6:79:ARG:NH1   | 2:C6:92:LEU:O     | 2.44                     | 0.50              |
| 2:C8:189:LEU:HD11 | 2:C8:418:PHE:CD1  | 2.46                     | 0.50              |
| 2:D2:134:GLY:HA2  | 2:D2:164:LYS:HE2  | 1.93                     | 0.50              |
| 3:D3:140:GLY:O    | 3:D3:184:ASN:ND2  | 2.42                     | 0.50              |
| 2:D4:12:ALA:CB    | 2:D4:140:ALA:HB2  | 2.42                     | 0.50              |
| 3:D5:93:GLY:HA2   | 3:D5:112:LEU:HD11 | 1.94                     | 0.50              |
| 3:D5:316:MET:HG3  | 3:D5:352:SER:HB2  | 1.92                     | 0.50              |
| 2:E0:178:SER:HB3  | 2:E0:183:GLU:HG2  | 1.93                     | 0.50              |
| 3:E3:153:SER:HB2  | 3:E3:191:GLN:NE2  | 2.27                     | 0.50              |
| 3:E5:68:LEU:HA    | 3:E5:93:GLY:HA3   | 1.93                     | 0.50              |
| 2:E8:274:PRO:HG3  | 2:E8:286:LEU:HD13 | 1.93                     | 0.50              |
| 2:F0:122:ILE:HG21 | 2:F0:157:LEU:HD21 | 1.93                     | 0.50              |
| 4:h:10:LEU:HD21   | 4:h:49:LEU:HD12   | 1.91                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:h:14:LYS:HB2    | 4:h:47:LEU:HD12   | 1.93                     | 0.50              |
| 4:o:170:VAL:HG23  | 4:o:183:LEU:HB2   | 1.93                     | 0.50              |
| 1:14:245:SER:HB2  | 3:D7:42:LEU:HD11  | 1.93                     | 0.50              |
| 2:A0:222:PRO:HD2  | 3:A1:324:LYS:CG   | 2.40                     | 0.50              |
| 2:A0:281:ALA:O    | 4:a:202:ARG:NH2   | 2.45                     | 0.50              |
| 3:A3:230:SER:HA   | 3:A3:233:MET:HB3  | 1.94                     | 0.50              |
| 3:A5:128:ASP:OD1  | 3:A5:129:CYS:N    | 2.40                     | 0.50              |
| 2:A8:238:LEU:HD22 | 2:A8:255:PHE:CE2  | 2.46                     | 0.50              |
| 3:A9:220:PRO:HB2  | 2:B0:326:LYS:HZ3  | 1.77                     | 0.50              |
| 2:B0:135:PHE:HD2  | 2:B0:166:LYS:HG2  | 1.76                     | 0.50              |
| 3:B7:105:HIS:CD2  | 3:B7:150:LEU:HD12 | 2.46                     | 0.50              |
| 3:B7:281:TYR:CD2  | 3:C1:87:PRO:HD2   | 2.44                     | 0.50              |
| 2:B8:5:ILE:HD12   | 2:B8:125:LEU:HD23 | 1.93                     | 0.50              |
| 3:C1:113:ILE:HA   | 3:C1:116:VAL:HG12 | 1.93                     | 0.50              |
| 2:C6:274:PRO:HG2  | 2:C6:371:VAL:HG11 | 1.93                     | 0.50              |
| 3:C9:220:PRO:HB2  | 2:D0:326:LYS:HZ1  | 1.77                     | 0.50              |
| 3:E5:207:LEU:HB3  | 3:E5:225:LEU:HD22 | 1.94                     | 0.50              |
| 2:F0:402:ARG:O    | 3:F1:260:PHE:HE1  | 1.94                     | 0.50              |
| 4:a:96:TYR:CZ     | 4:c:6:PHE:HE2     | 2.29                     | 0.50              |
| 4:e:176:ASP:OD1   | 4:e:176:ASP:N     | 2.44                     | 0.50              |
| 5:l:18:GLN:CG     | 4:n:146:ARG:HH11  | 2.25                     | 0.50              |
| 4:m:55:LEU:HD22   | 4:m:111:ILE:HD12  | 1.93                     | 0.50              |
| 4:r:5:VAL:HG11    | 4:r:149:ARG:HD3   | 1.94                     | 0.50              |
| 4:u:72:SER:HB3    | 4:u:108:ILE:HG22  | 1.94                     | 0.50              |
| 1:10:241:PHE:CZ   | 3:C9:356:ILE:HD12 | 2.44                     | 0.50              |
| 1:19:243:ALA:O    | 3:E7:356:ILE:HD12 | 2.12                     | 0.50              |
| 1:5:240:PRO:HB3   | 4:h:154:TYR:CD2   | 2.45                     | 0.50              |
| 2:A0:172:TRP:N    | 2:A0:204:LEU:O    | 2.45                     | 0.50              |
| 2:A6:191:THR:HA   | 2:A6:194:LEU:HB3  | 1.94                     | 0.50              |
| 2:A8:210:TYR:HB3  | 3:A9:324:LYS:HE2  | 1.94                     | 0.50              |
| 2:B2:151:CYS:SG   | 2:B2:193:SER:OG   | 2.53                     | 0.50              |
| 3:B9:43:GLN:HA    | 3:B9:242:PHE:HE1  | 1.77                     | 0.50              |
| 2:C4:188:VAL:HG13 | 2:C4:425:LEU:HD23 | 1.94                     | 0.50              |
| 3:C5:91:VAL:HB    | 3:C5:112:LEU:HD11 | 1.93                     | 0.50              |
| 3:C5:238:CYS:SG   | 3:C5:239:CYS:N    | 2.84                     | 0.50              |
| 2:C6:288:VAL:HA   | 2:C6:291:ILE:HG12 | 1.94                     | 0.50              |
| 3:D5:334:GLN:HE22 | 3:D5:347:ASN:HA   | 1.76                     | 0.50              |
| 2:D6:116:ASP:OD1  | 2:D6:117:LEU:N    | 2.44                     | 0.50              |
| 3:D9:87:PRO:HA    | 3:D9:90:PHE:CD1   | 2.47                     | 0.50              |
| 3:E3:316:MET:HE1  | 3:E3:368:VAL:HG22 | 1.93                     | 0.50              |
| 2:E8:151:CYS:SG   | 2:E8:193:SER:OG   | 2.55                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:p:18:ASN:ND2    | 4:p:46:ASP:H      | 2.07                     | 0.50              |
| 4:q:151:MET:SD    | 4:q:163:SER:OG    | 2.65                     | 0.50              |
| 3:A3:64:ILE:HD12  | 3:A3:119:VAL:HG12 | 1.93                     | 0.50              |
| 2:A6:85:HIS:NE2   | 4:b:99:MET:CE     | 2.54                     | 0.50              |
| 3:B7:208:TYR:HB3  | 2:B8:326:LYS:CE   | 2.41                     | 0.50              |
| 3:B7:283:ALA:HA   | 3:C1:55:THR:HG23  | 1.94                     | 0.50              |
| 2:C2:105:ARG:HG2  | 2:C2:411:GLU:HG2  | 1.93                     | 0.50              |
| 2:C2:399:TYR:OH   | 2:C2:415:GLU:OE2  | 2.30                     | 0.50              |
| 3:C9:170:PHE:HD1  | 3:C9:171:PRO:HD2  | 1.77                     | 0.50              |
| 3:D1:140:GLY:O    | 3:D1:184:ASN:ND2  | 2.43                     | 0.50              |
| 3:D1:173:PRO:HD3  | 3:D1:380:ARG:CZ   | 2.41                     | 0.50              |
| 2:E4:4:VAL:HG21   | 2:E4:136:LEU:HD13 | 1.94                     | 0.50              |
| 3:E5:94:GLN:HA    | 2:E6:2:ARG:HH22   | 1.76                     | 0.50              |
| 3:E9:105:HIS:HD2  | 3:E9:150:LEU:HD12 | 1.77                     | 0.50              |
| 4:o:115:LEU:HD21  | 4:o:145:LYS:HD3   | 1.93                     | 0.50              |
| 4:t:101:GLU:OE2   | 4:v:6:PHE:N       | 2.44                     | 0.50              |
| 1:2:244:GLN:NE2   | 4:e:163:SER:H     | 2.08                     | 0.50              |
| 1:2:254:LYS:HD3   | 2:A8:364:PRO:O    | 2.12                     | 0.50              |
| 2:A0:242:LEU:HD21 | 2:A0:251:ASP:HB2  | 1.93                     | 0.50              |
| 3:A5:139:LEU:HG   | 3:A5:168:SER:HB3  | 1.94                     | 0.50              |
| 2:A8:280:LYS:O    | 2:A8:284:GLU:HG2  | 2.12                     | 0.50              |
| 2:B4:50:ASN:O     | 2:B4:64:ARG:NH2   | 2.45                     | 0.50              |
| 3:B9:10:GLY:HA2   | 3:B9:143:THR:HG23 | 1.94                     | 0.50              |
| 3:B9:334:GLN:HE21 | 3:B9:349:MET:HG2  | 1.75                     | 0.50              |
| 2:C8:285:GLN:HB3  | 2:D2:56:THR:HA    | 1.94                     | 0.50              |
| 3:C9:167:PHE:HZ   | 3:C9:236:VAL:HG11 | 1.76                     | 0.50              |
| 2:D2:199:ASP:OD2  | 2:D2:256:GLN:NE2  | 2.45                     | 0.50              |
| 2:E0:98:ASP:OD1   | 2:E0:99:ALA:N     | 2.45                     | 0.50              |
| 3:F1:117:LEU:HB3  | 3:F1:121:ARG:HH22 | 1.76                     | 0.50              |
| 4:h:151:MET:HE1   | 4:h:158:THR:HG21  | 1.93                     | 0.50              |
| 4:i:10:LEU:HD22   | 4:i:47:LEU:HD21   | 1.94                     | 0.50              |
| 4:m:78:ALA:HB3    | 4:m:112:PHE:HE1   | 1.76                     | 0.50              |
| 4:v:94:ASN:C      | 4:v:94:ASN:HD22   | 2.20                     | 0.50              |
| 1:12:257:PRO:CD   | 2:D2:26:LEU:HD22  | 2.39                     | 0.50              |
| 1:19:243:ALA:CB   | 3:E7:357:PRO:CD   | 2.55                     | 0.50              |
| 2:A0:103:PHE:HD2  | 2:A0:189:LEU:HD23 | 1.75                     | 0.50              |
| 2:B2:11:GLN:NE2   | 3:B3:246:LEU:CD1  | 2.75                     | 0.50              |
| 3:B9:216:LYS:HE2  | 3:B9:275:SER:HB3  | 1.94                     | 0.50              |
| 3:C9:7:VAL:HG11   | 3:C9:66:MET:HE3   | 1.92                     | 0.50              |
| 3:C9:39:ASP:HA    | 4:m:90:PRO:HG3    | 1.93                     | 0.50              |
| 3:D3:219:THR:HA   | 2:D4:326:LYS:CE   | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:281:TYR:C    | 3:F1:54:ALA:HB1   | 2.35                     | 0.50              |
| 3:F1:128:ASP:OD1  | 3:F1:129:CYS:N    | 2.43                     | 0.50              |
| 4:b:69:LYS:O      | 4:d:39:PRO:HD3    | 2.12                     | 0.50              |
| 4:t:66:SER:HB2    | 4:v:23:LEU:HD13   | 1.93                     | 0.50              |
| 1:7:253:ALA:CB    | 4:h:102:GLY:HA2   | 2.42                     | 0.49              |
| 2:A4:76:ASP:HA    | 2:A4:79:ARG:HG2   | 1.93                     | 0.49              |
| 3:A7:1:MET:N      | 3:A7:128:ASP:OD2  | 2.36                     | 0.49              |
| 3:A7:318:ARG:HD3  | 3:A7:358:PRO:HD3  | 1.93                     | 0.49              |
| 2:A8:30:ILE:HG21  | 2:A8:61:HIS:HD2   | 1.77                     | 0.49              |
| 2:B0:209:ILE:HA   | 2:B0:212:ILE:HG22 | 1.94                     | 0.49              |
| 3:B1:153:SER:HA   | 3:B1:195:ASN:HD22 | 1.75                     | 0.49              |
| 2:B4:274:PRO:HG3  | 2:B4:286:LEU:HD12 | 1.93                     | 0.49              |
| 3:B7:404:ASP:OD1  | 3:B7:405:GLU:N    | 2.43                     | 0.49              |
| 2:C2:398:MET:HE1  | 3:C3:345:ILE:HD13 | 1.93                     | 0.49              |
| 3:C3:57:GLY:HA3   | 4:j:83:PRO:HB2    | 1.92                     | 0.49              |
| 3:D5:114:ASP:OD1  | 3:D5:114:ASP:N    | 2.45                     | 0.49              |
| 2:D8:211:ASP:OD2  | 2:D8:304:LYS:NZ   | 2.38                     | 0.49              |
| 3:D9:320:ARG:HH22 | 4:t:188:GLY:HA3   | 1.77                     | 0.49              |
| 3:E5:163:ILE:HD13 | 3:E5:250:LEU:HB3  | 1.94                     | 0.49              |
| 2:F0:207:GLU:HA   | 2:F0:210:TYR:HB2  | 1.93                     | 0.49              |
| 4:d:106:GLN:HE21  | 4:f:6:PHE:HZ      | 1.59                     | 0.49              |
| 4:e:68:LEU:HB3    | 4:e:206:PHE:HD2   | 1.77                     | 0.49              |
| 1:0:241:PHE:CE1   | 3:A5:356:ILE:HG23 | 2.47                     | 0.49              |
| 2:A6:306:ASP:HB3  | 2:A6:309:HIS:CE1  | 2.46                     | 0.49              |
| 2:A8:27:GLU:OE2   | 2:A8:243:ARG:NH2  | 2.44                     | 0.49              |
| 2:B0:286:LEU:HD13 | 2:B0:371:VAL:HG23 | 1.93                     | 0.49              |
| 3:B5:10:GLY:HA2   | 3:B5:143:THR:HG23 | 1.95                     | 0.49              |
| 2:B6:271:SER:HB2  | 2:B6:301:MET:HE2  | 1.95                     | 0.49              |
| 3:B9:13:GLY:HA2   | 3:B9:136:THR:HG22 | 1.94                     | 0.49              |
| 3:C1:113:ILE:HG21 | 3:C1:154:LYS:CD   | 2.42                     | 0.49              |
| 2:C4:407:TRP:CZ3  | 3:C5:255:VAL:HG22 | 2.47                     | 0.49              |
| 3:D3:313:ALA:HB1  | 3:D3:367:PHE:HE1  | 1.76                     | 0.49              |
| 4:e:75:LEU:O      | 4:e:170:VAL:HA    | 2.12                     | 0.49              |
| 4:f:67:HIS:HA     | 4:h:19:GLU:OE1    | 2.12                     | 0.49              |
| 4:h:72:SER:HG     | 4:h:199:TRP:HE1   | 1.60                     | 0.49              |
| 4:j:78:ALA:HB3    | 4:j:112:PHE:HE1   | 1.75                     | 0.49              |
| 4:v:99:MET:HE1    | 4:v:201:TRP:NE1   | 2.26                     | 0.49              |
| 1:21:256:LEU:CD2  | 2:F0:31:GLN:HA    | 2.43                     | 0.49              |
| 3:A3:52:ASN:ND2   | 3:A3:123:GLU:OE2  | 2.42                     | 0.49              |
| 2:A6:296:PHE:HE2  | 2:A6:335:ILE:HG21 | 1.75                     | 0.49              |
| 2:B2:259:LEU:HB3  | 2:B2:268:MET:HE2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C1:20:PHE:HD2   | 3:C1:233:MET:HE3  | 1.77                     | 0.49              |
| 3:C1:192:LEU:HD11 | 3:C1:199:VAL:HG11 | 1.93                     | 0.49              |
| 2:C6:177:VAL:HB   | 2:C6:207:GLU:HB3  | 1.94                     | 0.49              |
| 2:D2:96:LYS:HZ1   | 3:D3:128:ASP:HB2  | 1.76                     | 0.49              |
| 3:D3:303:SER:HB3  | 3:D3:377:MET:HE3  | 1.95                     | 0.49              |
| 3:D9:87:PRO:HA    | 3:D9:90:PHE:HD1   | 1.77                     | 0.49              |
| 2:E0:96:LYS:CE    | 3:E1:128:ASP:CG   | 2.84                     | 0.49              |
| 2:E8:137:MET:HE3  | 2:E8:154:LEU:HD12 | 1.95                     | 0.49              |
| 4:f:18:ASN:ND2    | 4:f:46:ASP:H      | 2.11                     | 0.49              |
| 4:g:158:THR:HB    | 4:g:161:TYR:HB2   | 1.94                     | 0.49              |
| 5:k:160:ARG:HA    | 5:k:163:LYS:NZ    | 2.28                     | 0.49              |
| 4:p:141:THR:O     | 4:p:145:LYS:HG2   | 2.12                     | 0.49              |
| 5:w:133:VAL:HG11  | 5:w:157:TRP:NE1   | 2.27                     | 0.49              |
| 1:0:244:GLN:CB    | 3:A5:320:ARG:NH2  | 2.69                     | 0.49              |
| 1:6:240:PRO:CG    | 4:i:154:TYR:CD2   | 2.94                     | 0.49              |
| 2:C0:70:LEU:HD21  | 2:C0:149:LEU:HD22 | 1.93                     | 0.49              |
| 2:C4:97:GLU:OE2   | 2:C4:105:ARG:NH2  | 2.30                     | 0.49              |
| 3:C5:262:ARG:O    | 3:C5:264:HIS:ND1  | 2.46                     | 0.49              |
| 2:C6:399:TYR:OH   | 2:C6:415:GLU:OE2  | 2.30                     | 0.49              |
| 2:D4:88:HIS:HB3   | 2:D4:91:GLN:HG2   | 1.94                     | 0.49              |
| 3:D5:107:THR:OG1  | 3:D5:108:GLU:N    | 2.44                     | 0.49              |
| 3:D9:260:PHE:HB3  | 3:D9:261:PRO:CD   | 2.37                     | 0.49              |
| 3:E1:396:HIS:HA   | 3:E1:399:THR:HG22 | 1.93                     | 0.49              |
| 2:E6:22:GLU:OE1   | 2:E6:229:ARG:NH1  | 2.45                     | 0.49              |
| 2:E8:107:HIS:NE2  | 2:E8:151:CYS:SG   | 2.82                     | 0.49              |
| 2:E8:271:SER:HB3  | 2:E8:377:MET:HB3  | 1.93                     | 0.49              |
| 5:k:54:ARG:HG3    | 5:k:91:PRO:HG3    | 1.95                     | 0.49              |
| 1:10:244:GLN:H    | 3:C9:320:ARG:HH11 | 1.60                     | 0.49              |
| 1:15:256:LEU:HD13 | 2:D8:30:ILE:C     | 2.37                     | 0.49              |
| 1:21:252:VAL:HG22 | 1:21:253:ALA:H    | 1.77                     | 0.49              |
| 1:9:241:PHE:CG    | 3:C3:43:GLN:NE2   | 2.81                     | 0.49              |
| 3:A1:341:PHE:HB3  | 3:A1:348:ASN:ND2  | 2.27                     | 0.49              |
| 2:A4:422:ARG:HH12 | 2:A4:426:ALA:HB2  | 1.78                     | 0.49              |
| 2:A8:282:TYR:OH   | 2:B2:33:ASP:CG    | 2.56                     | 0.49              |
| 3:B3:68:LEU:HD23  | 3:B3:112:LEU:HD22 | 1.92                     | 0.49              |
| 3:C7:281:TYR:O    | 3:D1:86:ARG:CD    | 2.60                     | 0.49              |
| 3:D7:117:LEU:HA   | 3:D7:120:VAL:HG12 | 1.94                     | 0.49              |
| 3:E1:57:GLY:HA3   | 4:s:83:PRO:HB2    | 1.94                     | 0.49              |
| 2:E2:242:LEU:HD11 | 2:E2:252:VAL:HG23 | 1.95                     | 0.49              |
| 2:E6:175:PRO:HB3  | 2:E6:390:ARG:HH21 | 1.77                     | 0.49              |
| 2:E8:10:GLY:HA2   | 2:E8:145:THR:HG23 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F0:137:MET:O    | 2:F0:168:ASN:ND2  | 2.42                     | 0.49              |
| 3:F1:262:ARG:NH2  | 3:F1:421:GLU:OE1  | 2.46                     | 0.49              |
| 4:e:63:ILE:HD11   | 4:e:132:LEU:HD13  | 1.95                     | 0.49              |
| 4:h:170:VAL:HG23  | 4:h:183:LEU:HB2   | 1.94                     | 0.49              |
| 1:3:245:SER:HB2   | 3:B1:42:LEU:HD21  | 1.94                     | 0.49              |
| 3:A1:260:PHE:HB3  | 3:A1:261:PRO:HD2  | 1.94                     | 0.49              |
| 2:A6:112:LYS:HA   | 2:A6:115:VAL:HG12 | 1.95                     | 0.49              |
| 3:A9:396:HIS:CE1  | 2:B0:261:PRO:O    | 2.65                     | 0.49              |
| 3:B5:330:MET:HE1  | 3:B5:349:MET:HE3  | 1.94                     | 0.49              |
| 2:B8:208:ALA:HB2  | 2:B8:304:LYS:HB2  | 1.94                     | 0.49              |
| 2:B8:282:TYR:HE2  | 2:C2:85:HIS:ND1   | 2.11                     | 0.49              |
| 3:B9:281:TYR:CD1  | 3:C3:58:ARG:HD3   | 2.47                     | 0.49              |
| 2:C2:261:PRO:HB2  | 2:C2:262:TYR:HD2  | 1.77                     | 0.49              |
| 3:C3:289:LEU:HD12 | 3:C3:365:VAL:HG12 | 1.93                     | 0.49              |
| 2:C6:251:ASP:N    | 2:C6:254:GLU:OE2  | 2.41                     | 0.49              |
| 3:D1:10:GLY:O     | 3:D1:14:ASN:ND2   | 2.41                     | 0.49              |
| 3:D3:293:MET:HG3  | 3:D3:367:PHE:HB2  | 1.95                     | 0.49              |
| 2:D6:209:ILE:HG21 | 2:D6:227:LEU:HG   | 1.94                     | 0.49              |
| 3:F1:19:LYS:NZ    | 3:F1:223:GLY:O    | 2.45                     | 0.49              |
| 4:e:139:PRO:O     | 4:e:143:ILE:HG12  | 2.13                     | 0.49              |
| 4:f:176:ASP:OD1   | 4:f:176:ASP:N     | 2.46                     | 0.49              |
| 4:g:78:ALA:HB3    | 4:g:112:PHE:HE1   | 1.76                     | 0.49              |
| 5:w:36:LEU:HD23   | 5:w:72:ILE:HB     | 1.94                     | 0.49              |
| 1:7:255:PRO:HG3   | 4:j:3:GLN:CD      | 2.37                     | 0.49              |
| 3:A1:105:HIS:CD2  | 3:A1:150:LEU:HB2  | 2.48                     | 0.49              |
| 2:B4:167:LEU:HD22 | 2:B4:200:VAL:HB   | 1.94                     | 0.49              |
| 3:B5:63:ALA:O     | 3:B5:89:ASN:ND2   | 2.45                     | 0.49              |
| 2:C4:82:THR:HA    | 5:k:59:THR:HG23   | 1.93                     | 0.49              |
| 3:C9:334:GLN:HE22 | 3:C9:348:ASN:N    | 2.10                     | 0.49              |
| 2:D2:214:ARG:HG2  | 2:D2:214:ARG:HH11 | 1.77                     | 0.49              |
| 3:D5:232:ALA:HB1  | 3:D5:268:ILE:HG21 | 1.94                     | 0.49              |
| 2:E2:311:LYS:NZ   | 2:E2:342:GLN:OE1  | 2.45                     | 0.49              |
| 4:a:97:ARG:NH1    | 4:c:6:PHE:H       | 2.11                     | 0.49              |
| 4:d:78:ALA:HB3    | 4:d:112:PHE:HE1   | 1.76                     | 0.49              |
| 4:f:14:LYS:HD3    | 4:f:47:LEU:HB2    | 1.94                     | 0.49              |
| 4:f:105:ASN:OD1   | 4:f:106:GLN:N     | 2.46                     | 0.49              |
| 5:k:109:TYR:OH    | 5:k:138:GLY:O     | 2.31                     | 0.49              |
| 4:o:164:ARG:HG2   | 4:o:164:ARG:HH11  | 1.78                     | 0.49              |
| 1:16:247:TYR:HB3  | 2:E0:77:GLU:OE2   | 2.13                     | 0.49              |
| 2:A4:204:LEU:HD13 | 2:A4:231:ILE:HG12 | 1.94                     | 0.49              |
| 2:A8:172:TRP:HB3  | 2:A8:205:ASP:OD1  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B5:156:ARG:HD3  | 3:B5:164:MET:HG2  | 1.94                     | 0.49              |
| 2:B6:234:VAL:HG21 | 2:B6:302:MET:HE1  | 1.95                     | 0.49              |
| 3:C3:270:PHE:O    | 3:C3:298:ASN:ND2  | 2.34                     | 0.49              |
| 3:C7:318:ARG:O    | 3:C7:321:MET:HE1  | 2.13                     | 0.49              |
| 3:D1:180:VAL:O    | 3:D1:184:ASN:ND2  | 2.45                     | 0.49              |
| 3:D1:284:LEU:CB   | 3:D5:55:THR:HG21  | 2.32                     | 0.49              |
| 2:D2:98:ASP:OD1   | 2:D2:99:ALA:N     | 2.45                     | 0.49              |
| 2:D4:316:CYS:SG   | 2:D4:352:LYS:HG2  | 2.52                     | 0.49              |
| 3:D7:128:ASP:OD1  | 3:D7:129:CYS:N    | 2.40                     | 0.49              |
| 2:D8:163:LYS:HD2  | 2:D8:163:LYS:N    | 2.23                     | 0.49              |
| 2:E4:256:GLN:HE21 | 2:E4:256:GLN:H    | 1.59                     | 0.49              |
| 4:b:115:LEU:HD21  | 4:b:145:LYS:HE3   | 1.93                     | 0.49              |
| 4:c:18:ASN:ND2    | 4:c:46:ASP:OD1    | 2.34                     | 0.49              |
| 5:x:133:VAL:HG11  | 5:x:157:TRP:NE1   | 2.28                     | 0.49              |
| 1:12:246:CYS:SG   | 3:D3:245:GLN:HG2  | 2.52                     | 0.49              |
| 3:A5:283:ALA:HB2  | 3:A9:53:GLU:O     | 2.12                     | 0.49              |
| 3:A7:11:GLN:HA    | 3:A7:72:THR:HG21  | 1.95                     | 0.49              |
| 3:A7:293:MET:SD   | 3:A7:365:VAL:HG11 | 2.52                     | 0.49              |
| 3:A9:91:VAL:HG21  | 3:A9:116:VAL:HG22 | 1.95                     | 0.49              |
| 2:B2:163:LYS:H    | 2:B2:163:LYS:HD3  | 1.78                     | 0.49              |
| 3:B7:259:PRO:HD2  | 3:B7:263:LEU:HD11 | 1.94                     | 0.49              |
| 2:B8:305:CYS:HG   | 2:B8:309:HIS:HE2  | 1.60                     | 0.49              |
| 3:B9:354:CYS:SG   | 3:B9:355:ASP:N    | 2.86                     | 0.49              |
| 2:C0:70:LEU:HD12  | 2:C0:99:ALA:HB2   | 1.95                     | 0.49              |
| 3:C1:275:SER:OG   | 3:C1:276:ARG:N    | 2.46                     | 0.49              |
| 3:C5:154:LYS:HB3  | 3:C5:154:LYS:HE2  | 1.59                     | 0.49              |
| 2:C6:198:THR:O    | 2:C6:266:HIS:NE2  | 2.46                     | 0.49              |
| 2:D0:2:ARG:HH21   | 2:D0:133:GLN:NE2  | 2.11                     | 0.49              |
| 2:D4:8:HIS:HD2    | 2:D4:67:PHE:CE1   | 2.31                     | 0.49              |
| 2:D4:23:LEU:HD11  | 2:D4:361:THR:HG23 | 1.94                     | 0.49              |
| 3:D7:323:THR:HA   | 3:D7:326:VAL:HG12 | 1.95                     | 0.49              |
| 2:D8:50:ASN:O     | 2:D8:64:ARG:NH2   | 2.46                     | 0.49              |
| 3:D9:248:SER:HA   | 3:D9:252:LYS:HD2  | 1.94                     | 0.49              |
| 2:E0:96:LYS:NZ    | 3:E1:129:CYS:N    | 2.61                     | 0.49              |
| 3:E1:3:GLU:HA     | 3:E1:49:VAL:HA    | 1.94                     | 0.49              |
| 2:E2:397:LEU:O    | 2:E2:397:LEU:HD23 | 2.12                     | 0.49              |
| 3:E3:321:MET:HG2  | 3:E3:363:MET:SD   | 2.53                     | 0.49              |
| 2:E6:290:GLU:CD   | 2:F0:124:LYS:HE3  | 2.38                     | 0.49              |
| 2:E8:70:LEU:HD12  | 2:E8:99:ALA:HB2   | 1.93                     | 0.49              |
| 4:t:63:ILE:HG22   | 4:v:16:ARG:HD2    | 1.93                     | 0.49              |
| 1:19:243:ALA:HB1  | 3:E7:356:ILE:HA   | 1.89                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:247:TYR:HE2   | 2:B8:81:GLY:HA3   | 1.76                     | 0.49              |
| 3:B3:248:SER:HA   | 3:B3:252:LYS:HE2  | 1.95                     | 0.49              |
| 3:B9:313:ALA:HB3  | 3:B9:349:MET:HE1  | 1.94                     | 0.49              |
| 2:C8:281:ALA:CB   | 4:o:202:ARG:NH2   | 2.76                     | 0.49              |
| 2:D2:189:LEU:HD21 | 2:D2:413:MET:HE1  | 1.95                     | 0.49              |
| 2:D8:5:ILE:HD12   | 2:D8:125:LEU:HG   | 1.94                     | 0.49              |
| 2:E2:204:LEU:CD2  | 2:E2:231:ILE:HD12 | 2.43                     | 0.49              |
| 3:E9:212:PHE:CE1  | 2:F0:326:LYS:NZ   | 2.72                     | 0.49              |
| 4:j:146:ARG:HB2   | 4:j:146:ARG:CZ    | 2.43                     | 0.49              |
| 5:k:27:ASP:HB3    | 4:m:38:LEU:HG     | 1.94                     | 0.49              |
| 4:q:112:PHE:HB2   | 4:q:131:TRP:HE1   | 1.78                     | 0.49              |
| 4:v:129:MET:SD    | 4:v:131:TRP:NE1   | 2.86                     | 0.49              |
| 2:A0:208:ALA:HB2  | 2:A0:304:LYS:HB2  | 1.93                     | 0.48              |
| 3:A7:318:ARG:HH11 | 3:A7:358:PRO:HD3  | 1.77                     | 0.48              |
| 2:B2:183:GLU:OE2  | 2:B2:187:SER:OG   | 2.31                     | 0.48              |
| 3:B5:181:GLU:HB2  | 3:B5:182:PRO:HD3  | 1.95                     | 0.48              |
| 2:C0:1:MET:N      | 2:C0:129:CYS:SG   | 2.73                     | 0.48              |
| 2:C0:356:ASN:OD1  | 2:C0:357:TYR:N    | 2.46                     | 0.48              |
| 2:C0:406:HIS:CD2  | 3:C1:261:PRO:HD3  | 2.48                     | 0.48              |
| 3:C1:73:MET:HB3   | 3:C1:77:ARG:NH2   | 2.29                     | 0.48              |
| 2:C2:7:ILE:HG22   | 2:C2:9:VAL:HG23   | 1.94                     | 0.48              |
| 2:C2:254:GLU:HG2  | 2:C2:352:LYS:HZ3  | 1.78                     | 0.48              |
| 2:C4:2:ARG:HB3    | 2:C4:133:GLN:NE2  | 2.26                     | 0.48              |
| 2:C6:282:TYR:HD2  | 4:n:202:ARG:HD2   | 1.67                     | 0.48              |
| 2:C8:319:TYR:HB3  | 2:C8:323:VAL:HG11 | 1.95                     | 0.48              |
| 3:C9:1:MET:N      | 3:C9:128:ASP:OD2  | 2.38                     | 0.48              |
| 2:D0:279:GLU:CD   | 4:p:197:LEU:O     | 2.51                     | 0.48              |
| 3:D1:189:VAL:HG11 | 3:D1:415:MET:CE   | 2.43                     | 0.48              |
| 3:D7:208:TYR:HB3  | 2:D8:326:LYS:HE3  | 1.95                     | 0.48              |
| 3:D7:281:TYR:CE1  | 3:E1:58:ARG:NH2   | 2.81                     | 0.48              |
| 2:E0:73:THR:CB    | 3:E1:46:ARG:HH22  | 2.25                     | 0.48              |
| 2:F0:9:VAL:HG13   | 2:F0:149:LEU:HD23 | 1.95                     | 0.48              |
| 4:g:15:ARG:O      | 4:g:19:GLU:HB3    | 2.13                     | 0.48              |
| 4:s:15:ARG:O      | 4:s:19:GLU:HG3    | 2.13                     | 0.48              |
| 1:22:241:PHE:HZ   | 3:C7:356:ILE:HG23 | 1.77                     | 0.48              |
| 2:A4:265:ILE:HG23 | 2:A4:432:TYR:CZ   | 2.48                     | 0.48              |
| 2:A4:310:GLY:HA3  | 2:A4:383:ALA:HB2  | 1.95                     | 0.48              |
| 3:B5:44:LEU:HD23  | 4:f:91:PHE:CE1    | 2.48                     | 0.48              |
| 2:B6:195:LEU:HD21 | 2:B6:264:ARG:HE   | 1.78                     | 0.48              |
| 2:C0:103:PHE:H    | 2:C0:408:TYR:HE1  | 1.61                     | 0.48              |
| 2:C4:79:ARG:NH1   | 2:C4:92:LEU:O     | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C7:164:MET:N    | 3:C7:197:ASP:OD2  | 2.41                     | 0.48              |
| 2:E0:66:VAL:HG21  | 2:E0:122:ILE:HD11 | 1.94                     | 0.48              |
| 3:E1:249:ASP:OD1  | 3:E1:252:LYS:HG2  | 2.13                     | 0.48              |
| 3:E3:49:VAL:HG21  | 3:E3:241:ARG:HG2  | 1.95                     | 0.48              |
| 2:E4:236:SER:OG   | 2:E4:243:ARG:NH2  | 2.46                     | 0.48              |
| 2:E8:234:VAL:HG21 | 2:E8:302:MET:HE1  | 1.95                     | 0.48              |
| 3:E9:156:ARG:HH22 | 3:E9:197:ASP:HB2  | 1.78                     | 0.48              |
| 3:E9:169:VAL:HG12 | 3:E9:202:ILE:HB   | 1.94                     | 0.48              |
| 3:E9:183:TYR:OH   | 3:E9:388:MET:O    | 2.21                     | 0.48              |
| 2:F0:274:PRO:HG2  | 2:F0:371:VAL:HG11 | 1.95                     | 0.48              |
| 4:i:74:ALA:HB2    | 4:i:172:VAL:HG12  | 1.95                     | 0.48              |
| 5:l:132:ILE:HA    | 5:l:142:GLY:O     | 2.13                     | 0.48              |
| 4:m:75:LEU:HD23   | 4:m:173:ILE:HG13  | 1.93                     | 0.48              |
| 4:r:142:GLU:O     | 4:r:146:ARG:HG2   | 2.13                     | 0.48              |
| 3:A7:139:LEU:HG   | 3:A7:168:SER:HB3  | 1.95                     | 0.48              |
| 2:B2:80:THR:HA    | 2:B2:84:ARG:HE    | 1.77                     | 0.48              |
| 3:B9:252:LYS:HG3  | 3:B9:350:LYS:HE3  | 1.95                     | 0.48              |
| 3:C1:101:TRP:NE1  | 3:C1:145:SER:O    | 2.39                     | 0.48              |
| 2:E2:107:HIS:NE2  | 2:E2:151:CYS:SG   | 2.83                     | 0.48              |
| 3:E7:274:THR:HG21 | 3:E7:282:ARG:HD2  | 1.95                     | 0.48              |
| 4:p:78:ALA:HB3    | 4:p:112:PHE:HE1   | 1.78                     | 0.48              |
| 4:t:185:ILE:HD13  | 4:t:195:ALA:HB3   | 1.94                     | 0.48              |
| 1:12:241:PHE:CZ   | 3:D3:356:ILE:HG23 | 2.48                     | 0.48              |
| 2:A4:210:TYR:CB   | 3:A5:324:LYS:CE   | 2.83                     | 0.48              |
| 2:B0:76:ASP:HA    | 2:B0:79:ARG:HG2   | 1.96                     | 0.48              |
| 3:B5:73:MET:HA    | 3:B5:76:VAL:HG12  | 1.96                     | 0.48              |
| 2:C2:398:MET:HE1  | 3:C3:345:ILE:CD1  | 2.44                     | 0.48              |
| 3:C7:97:ALA:HA    | 3:C7:103:LYS:HZ2  | 1.79                     | 0.48              |
| 3:C7:407:GLU:HA   | 3:C7:410:GLU:HB3  | 1.96                     | 0.48              |
| 3:D9:174:LYS:HD2  | 3:D9:174:LYS:HA   | 1.79                     | 0.48              |
| 4:f:71:LYS:HG3    | 4:h:39:PRO:HD3    | 1.96                     | 0.48              |
| 5:k:27:ASP:OD2    | 4:m:23:LEU:CD1    | 2.61                     | 0.48              |
| 4:t:79:ASP:OD2    | 4:t:152:LYS:NZ    | 2.37                     | 0.48              |
| 4:v:84:LYS:HB2    | 4:v:168:PRO:HD3   | 1.94                     | 0.48              |
| 1:17:241:PHE:HZ   | 3:E3:356:ILE:HG23 | 1.77                     | 0.48              |
| 2:A2:407:TRP:HH2  | 3:A3:254:ALA:HB1  | 1.78                     | 0.48              |
| 2:A4:174:SER:HB3  | 2:A4:175:PRO:HD2  | 1.95                     | 0.48              |
| 2:A4:221:ARG:HB3  | 3:A5:322:SER:OG   | 2.14                     | 0.48              |
| 3:A5:238:CYS:SG   | 3:A5:318:ARG:NE   | 2.85                     | 0.48              |
| 3:B3:283:ALA:HB2  | 3:B7:53:GLU:O     | 2.14                     | 0.48              |
| 3:B5:97:ALA:HA    | 3:B5:103:LYS:HE2  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C1:73:MET:HB3   | 3:C1:77:ARG:HH22  | 1.77                     | 0.48              |
| 3:C1:102:ALA:HB1  | 3:C1:401:GLU:HB2  | 1.94                     | 0.48              |
| 3:C1:326:VAL:O    | 3:C1:330:MET:HG2  | 2.14                     | 0.48              |
| 2:C6:51:THR:HG23  | 2:C6:52:PHE:HD1   | 1.77                     | 0.48              |
| 2:C6:215:ARG:HB2  | 2:C6:215:ARG:NH1  | 2.28                     | 0.48              |
| 2:D2:282:TYR:O    | 2:D6:60:LYS:HD3   | 2.14                     | 0.48              |
| 2:D8:84:ARG:HH21  | 4:r:197:LEU:CD2   | 2.11                     | 0.48              |
| 2:D8:241:SER:OG   | 2:D8:250:VAL:O    | 2.22                     | 0.48              |
| 3:D9:178:THR:O    | 3:D9:181:GLU:HG2  | 2.13                     | 0.48              |
| 2:E2:392:ASP:OD1  | 2:E2:422:ARG:NH1  | 2.46                     | 0.48              |
| 1:14:256:LEU:CD1  | 2:D6:31:GLN:NE2   | 2.72                     | 0.48              |
| 1:5:240:PRO:CB    | 4:h:154:TYR:HB3   | 2.43                     | 0.48              |
| 1:7:251:TYR:CZ    | 2:B8:18:ASN:HB3   | 2.48                     | 0.48              |
| 3:B7:208:TYR:HB3  | 2:B8:326:LYS:HE2  | 1.96                     | 0.48              |
| 2:B8:286:LEU:O    | 2:B8:373:ARG:NH1  | 2.36                     | 0.48              |
| 2:C6:181:VAL:CB   | 3:C7:256:ASN:OD1  | 2.56                     | 0.48              |
| 2:D8:2:ARG:HD2    | 2:D8:133:GLN:HE21 | 1.78                     | 0.48              |
| 3:D9:3:GLU:HA     | 3:D9:49:VAL:HA    | 1.94                     | 0.48              |
| 3:E5:229:VAL:HA   | 3:E5:300:MET:HE1  | 1.94                     | 0.48              |
| 3:E9:209:ASP:OD1  | 3:E9:213:ARG:NH1  | 2.47                     | 0.48              |
| 4:s:185:ILE:HD13  | 4:s:195:ALA:HB3   | 1.94                     | 0.48              |
| 3:A3:309:ARG:NE   | 3:A3:339:SER:O    | 2.46                     | 0.48              |
| 2:A4:203:MET:HE2  | 2:A4:267:PHE:HB3  | 1.95                     | 0.48              |
| 3:A9:251:ARG:HG2  | 3:A9:251:ARG:O    | 2.13                     | 0.48              |
| 3:A9:391:ARG:CZ   | 3:A9:391:ARG:HB2  | 2.41                     | 0.48              |
| 3:B3:239:CYS:SG   | 3:B3:248:SER:N    | 2.79                     | 0.48              |
| 2:B4:156:ARG:HA   | 2:B4:159:VAL:HG12 | 1.96                     | 0.48              |
| 3:C1:281:TYR:O    | 3:C5:54:ALA:CB    | 2.49                     | 0.48              |
| 2:C6:12:ALA:CB    | 2:C6:140:ALA:HB2  | 2.44                     | 0.48              |
| 3:C7:281:TYR:CE2  | 3:D1:87:PRO:HD3   | 2.43                     | 0.48              |
| 3:C9:334:GLN:HE22 | 3:C9:348:ASN:H    | 1.61                     | 0.48              |
| 2:D0:84:ARG:HH22  | 4:n:94:ASN:HD21   | 1.52                     | 0.48              |
| 3:D1:239:CYS:SG   | 3:D1:248:SER:N    | 2.76                     | 0.48              |
| 3:D1:379:LYS:HE3  | 3:D1:419:VAL:HG11 | 1.96                     | 0.48              |
| 3:D5:299:MET:HE1  | 3:D5:367:PHE:CE2  | 2.49                     | 0.48              |
| 2:D8:214:ARG:NH1  | 3:D9:324:LYS:HE2  | 2.28                     | 0.48              |
| 3:D9:318:ARG:HG2  | 3:D9:354:CYS:HB3  | 1.95                     | 0.48              |
| 2:E0:189:LEU:HD13 | 2:E0:413:MET:HE1  | 1.96                     | 0.48              |
| 2:E2:281:ALA:HB3  | 4:v:202:ARG:HH21  | 1.78                     | 0.48              |
| 2:E4:98:ASP:OD1   | 2:E4:100:ALA:N    | 2.40                     | 0.48              |
| 2:E4:261:PRO:HG3  | 2:E4:313:MET:HE2  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E6:221:ARG:HD2  | 3:E7:325:GLU:HB2  | 1.96                     | 0.48              |
| 3:E7:173:PRO:HB2  | 3:E7:174:LYS:HG3  | 1.95                     | 0.48              |
| 3:E9:66:MET:HG3   | 3:E9:116:VAL:HG21 | 1.94                     | 0.48              |
| 4:c:97:ARG:HG3    | 4:e:161:TYR:OH    | 2.12                     | 0.48              |
| 1:22:246:CYS:HB3  | 3:C7:245:GLN:HE21 | 1.79                     | 0.48              |
| 2:A0:221:ARG:CG   | 3:A1:322:SER:OG   | 2.62                     | 0.48              |
| 2:A0:245:ASP:O    | 2:A0:358:GLN:NE2  | 2.32                     | 0.48              |
| 2:A2:3:GLU:OE1    | 2:A2:64:ARG:NH1   | 2.47                     | 0.48              |
| 3:A3:135:ILE:HD13 | 3:A3:152:ILE:HD11 | 1.95                     | 0.48              |
| 3:A7:139:LEU:HD12 | 3:A7:170:PHE:CE1  | 2.49                     | 0.48              |
| 3:B3:77:ARG:HH22  | 3:B3:92:PHE:HZ    | 1.62                     | 0.48              |
| 3:B5:313:ALA:HB3  | 3:B5:349:MET:SD   | 2.54                     | 0.48              |
| 3:B7:311:LEU:HD12 | 3:B7:342:VAL:HG11 | 1.95                     | 0.48              |
| 2:C0:53:PHE:O     | 2:C0:64:ARG:NH2   | 2.46                     | 0.48              |
| 2:C0:283:HIS:CD2  | 2:C4:60:LYS:HE2   | 2.49                     | 0.48              |
| 2:C4:30:ILE:HD13  | 2:C4:53:PHE:CE2   | 2.49                     | 0.48              |
| 2:C4:277:SER:C    | 2:C4:369:ALA:HB2  | 2.39                     | 0.48              |
| 2:D0:177:VAL:HB   | 3:D1:327:ASP:OD1  | 2.12                     | 0.48              |
| 3:D7:301:CYS:SG   | 3:D7:377:MET:HE1  | 2.54                     | 0.48              |
| 2:D8:79:ARG:HG3   | 2:D8:92:LEU:CD1   | 2.41                     | 0.48              |
| 3:E1:317:PHE:HB3  | 3:E1:321:MET:SD   | 2.54                     | 0.48              |
| 2:E2:224:TYR:HD1  | 2:E2:227:LEU:HD12 | 1.79                     | 0.48              |
| 2:E4:277:SER:OG   | 2:E4:278:ALA:N    | 2.46                     | 0.48              |
| 2:E6:12:ALA:HB3   | 2:E6:140:ALA:HB2  | 1.96                     | 0.48              |
| 3:E7:184:ASN:OD1  | 3:E7:398:TYR:OH   | 2.32                     | 0.48              |
| 3:E7:186:THR:HG22 | 3:E7:415:MET:SD   | 2.53                     | 0.48              |
| 3:E9:69:GLU:OE1   | 2:F0:2:ARG:NH1    | 2.47                     | 0.48              |
| 1:15:257:PRO:CG   | 2:D8:26:LEU:CD2   | 2.91                     | 0.48              |
| 1:6:244:GLN:NE2   | 1:6:248:ARG:HB3   | 2.28                     | 0.48              |
| 3:A1:398:TYR:HB3  | 3:A1:403:MET:HG3  | 1.95                     | 0.48              |
| 3:A5:64:ILE:HD12  | 3:A5:119:VAL:HG12 | 1.96                     | 0.48              |
| 3:B1:40:SER:OG    | 3:B1:43:GLN:OE1   | 2.30                     | 0.48              |
| 2:B4:183:GLU:HG2  | 2:B4:184:PRO:HD3  | 1.95                     | 0.48              |
| 2:B8:27:GLU:OE2   | 2:B8:243:ARG:NH1  | 2.47                     | 0.48              |
| 2:B8:256:GLN:O    | 2:B8:260:VAL:HG22 | 2.14                     | 0.48              |
| 2:C2:191:THR:HG21 | 2:C2:425:LEU:HD21 | 1.94                     | 0.48              |
| 2:C6:28:HIS:HE1   | 2:C6:243:ARG:HD2  | 1.78                     | 0.48              |
| 2:C6:241:SER:HB2  | 2:C6:249:ASN:HB2  | 1.95                     | 0.48              |
| 2:C8:88:HIS:HB3   | 2:C8:91:GLN:HB2   | 1.96                     | 0.48              |
| 2:D6:219:ILE:HG22 | 2:D6:222:PRO:HD3  | 1.94                     | 0.48              |
| 3:D9:239:CYS:SG   | 3:D9:248:SER:N    | 2.83                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E0:5:ILE:CD1    | 2:E0:132:LEU:HD11 | 2.43                     | 0.48              |
| 2:F0:173:PRO:HG2  | 2:F0:391:MET:HE1  | 1.96                     | 0.48              |
| 4:e:107:LYS:HD2   | 4:e:201:TRP:CD1   | 2.48                     | 0.48              |
| 1:9:257:PRO:CG    | 2:C2:26:LEU:HD12  | 2.18                     | 0.48              |
| 2:A0:221:ARG:CG   | 3:A1:325:GLU:HB3  | 2.43                     | 0.48              |
| 3:A1:68:LEU:HD12  | 3:A1:97:ALA:HB2   | 1.96                     | 0.48              |
| 2:A4:328:VAL:O    | 2:A4:332:VAL:HG23 | 2.14                     | 0.48              |
| 3:A5:54:ALA:C     | 3:A5:56:GLY:H     | 2.22                     | 0.48              |
| 3:B1:107:THR:OG1  | 3:B1:108:GLU:OE1  | 2.30                     | 0.48              |
| 3:B1:383:ASP:HA   | 3:B1:386:THR:HG22 | 1.95                     | 0.48              |
| 3:C5:6:HIS:HE2    | 3:C5:136:THR:HG23 | 1.79                     | 0.48              |
| 2:C8:217:LEU:HD13 | 2:C8:277:SER:HB3  | 1.96                     | 0.48              |
| 2:D4:306:ASP:HB3  | 2:D4:309:HIS:CE1  | 2.49                     | 0.48              |
| 4:f:99:MET:HE2    | 4:f:99:MET:HB3    | 1.54                     | 0.48              |
| 5:k:78:LYS:HE3    | 5:k:78:LYS:HB2    | 1.53                     | 0.48              |
| 4:q:95:TYR:HA     | 4:q:98:THR:HG22   | 1.96                     | 0.48              |
| 1:13:240:PRO:HB2  | 4:r:154:TYR:HD2   | 1.78                     | 0.47              |
| 3:A1:141:GLY:O    | 3:A1:184:ASN:ND2  | 2.39                     | 0.47              |
| 2:A6:30:ILE:HG22  | 2:A6:36:MET:HB3   | 1.95                     | 0.47              |
| 2:A6:174:SER:HB2  | 2:A6:177:VAL:O    | 2.13                     | 0.47              |
| 3:B1:100:ASN:HB3  | 3:B1:103:LYS:HG2  | 1.95                     | 0.47              |
| 2:C4:174:SER:HB3  | 2:C4:177:VAL:O    | 2.13                     | 0.47              |
| 3:C9:53:GLU:OE2   | 3:C9:54:ALA:N     | 2.47                     | 0.47              |
| 3:D5:307:HIS:ND1  | 3:D5:376:GLU:OE2  | 2.45                     | 0.47              |
| 3:D5:310:TYR:HD1  | 3:D5:371:SER:HB2  | 1.78                     | 0.47              |
| 2:D8:75:VAL:CG2   | 2:D8:92:LEU:HB3   | 2.44                     | 0.47              |
| 2:D8:262:TYR:HB2  | 2:D8:265:ILE:HD12 | 1.96                     | 0.47              |
| 2:E8:9:VAL:HG22   | 2:E8:68:LEU:HB3   | 1.96                     | 0.47              |
| 2:E8:319:TYR:HB3  | 2:E8:323:VAL:HG11 | 1.95                     | 0.47              |
| 2:F0:33:ASP:HB2   | 5:x:63:SER:O      | 2.14                     | 0.47              |
| 4:h:75:LEU:HD23   | 4:h:111:ILE:HB    | 1.96                     | 0.47              |
| 4:t:9:PRO:HA      | 4:t:12:VAL:HG22   | 1.94                     | 0.47              |
| 4:v:40:PRO:HG2    | 4:v:45:MET:HE2    | 1.96                     | 0.47              |
| 1:15:240:PRO:HB2  | 4:t:154:TYR:CD2   | 2.49                     | 0.47              |
| 1:17:253:ALA:HB1  | 2:E2:32:PRO:HG2   | 1.95                     | 0.47              |
| 1:8:248:ARG:HH12  | 4:i:94:ASN:HD21   | 1.63                     | 0.47              |
| 3:B3:257:LEU:HD21 | 3:B3:314:SER:HB2  | 1.96                     | 0.47              |
| 3:B5:66:MET:HG3   | 3:B5:116:VAL:HG21 | 1.96                     | 0.47              |
| 2:B6:406:HIS:HA   | 2:B6:409:VAL:HG12 | 1.95                     | 0.47              |
| 2:B8:73:THR:HA    | 3:B9:46:ARG:HH22  | 1.79                     | 0.47              |
| 3:C1:1:MET:N      | 3:C1:128:ASP:OD2  | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C5:133:PHE:HB2  | 3:C5:164:MET:CB   | 2.44                     | 0.47              |
| 3:C7:192:LEU:HG   | 3:C7:199:VAL:HG21 | 1.95                     | 0.47              |
| 2:C8:175:PRO:HB3  | 2:C8:390:ARG:HD3  | 1.96                     | 0.47              |
| 3:D1:14:ASN:ND2   | 3:D1:67:ASP:OD1   | 2.47                     | 0.47              |
| 3:D7:383:ASP:HA   | 3:D7:386:THR:HG22 | 1.96                     | 0.47              |
| 3:E1:13:GLY:HA2   | 3:E1:136:THR:HG22 | 1.95                     | 0.47              |
| 3:E5:303:SER:HB3  | 3:E5:377:MET:HE3  | 1.96                     | 0.47              |
| 3:F1:87:PRO:HA    | 3:F1:90:PHE:HD1   | 1.79                     | 0.47              |
| 4:d:53:GLY:HA2    | 4:d:62:VAL:HG21   | 1.97                     | 0.47              |
| 4:v:12:VAL:HG22   | 4:v:15:ARG:HH12   | 1.79                     | 0.47              |
| 5:x:61:ASN:OD1    | 5:x:67:ALA:HA     | 2.13                     | 0.47              |
| 1:16:256:LEU:CD2  | 2:E0:31:GLN:CG    | 2.90                     | 0.47              |
| 1:23:240:PRO:CG   | 4:m:154:TYR:HB3   | 2.42                     | 0.47              |
| 3:A1:208:TYR:CE2  | 2:A2:329:ASN:ND2  | 2.82                     | 0.47              |
| 2:A2:320:ARG:NH1  | 2:A2:360:PRO:HA   | 2.30                     | 0.47              |
| 2:A4:306:ASP:HB3  | 2:A4:309:HIS:CE1  | 2.50                     | 0.47              |
| 2:A6:212:ILE:HG12 | 2:A6:275:ILE:HD11 | 1.96                     | 0.47              |
| 2:B2:277:SER:OG   | 2:B2:278:ALA:N    | 2.47                     | 0.47              |
| 3:B3:18:ALA:HB2   | 3:B3:76:VAL:CG2   | 2.44                     | 0.47              |
| 3:B9:383:ASP:HA   | 3:B9:386:THR:HG22 | 1.95                     | 0.47              |
| 2:C0:279:GLU:OE2  | 5:k:155:GLN:O     | 2.32                     | 0.47              |
| 2:C2:168:ASN:OD1  | 2:C2:169:PHE:N    | 2.48                     | 0.47              |
| 2:C2:219:ILE:HG22 | 2:C2:222:PRO:HD3  | 1.96                     | 0.47              |
| 3:C3:141:GLY:O    | 3:C3:184:ASN:ND2  | 2.44                     | 0.47              |
| 3:C7:385:PHE:HZ   | 3:C7:408:PHE:HD2  | 1.61                     | 0.47              |
| 2:D0:189:LEU:HD11 | 2:D0:418:PHE:HD1  | 1.79                     | 0.47              |
| 2:D0:306:ASP:HB3  | 2:D0:309:HIS:CE1  | 2.49                     | 0.47              |
| 2:D6:309:HIS:NE2  | 2:D6:386:GLU:OE1  | 2.47                     | 0.47              |
| 3:D9:289:LEU:HD11 | 3:D9:363:MET:HG2  | 1.95                     | 0.47              |
| 3:F1:207:LEU:HD21 | 3:F1:225:LEU:HB3  | 1.95                     | 0.47              |
| 4:d:96:TYR:OH     | 4:f:6:PHE:CE2     | 2.66                     | 0.47              |
| 4:e:100:ASN:HB3   | 4:g:6:PHE:CZ      | 2.49                     | 0.47              |
| 5:k:91:PRO:HB3    | 4:m:159:TYR:CD2   | 2.48                     | 0.47              |
| 5:l:132:ILE:HD11  | 5:l:143:ARG:HD2   | 1.95                     | 0.47              |
| 4:n:201:TRP:H     | 4:n:201:TRP:CD1   | 2.31                     | 0.47              |
| 4:t:85:CYS:SG     | 4:t:167:VAL:HG22  | 2.54                     | 0.47              |
| 1:11:244:GLN:HB2  | 3:D1:320:ARG:HH22 | 1.79                     | 0.47              |
| 1:13:252:VAL:HA   | 2:D4:82:THR:HG21  | 1.97                     | 0.47              |
| 1:2:247:TYR:CB    | 2:A8:77:GLU:OE2   | 2.58                     | 0.47              |
| 2:A0:73:THR:CA    | 3:A1:46:ARG:HH11  | 2.26                     | 0.47              |
| 2:A4:220:GLU:HG2  | 2:A4:221:ARG:HG3  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A5:73:MET:HE3   | 3:A5:92:PHE:HD1   | 1.79                     | 0.47              |
| 2:A6:33:ASP:OD2   | 4:b:103:GLY:CA    | 2.52                     | 0.47              |
| 2:A6:430:LYS:HB2  | 2:A6:430:LYS:HE2  | 1.50                     | 0.47              |
| 2:C0:2:ARG:NH2    | 2:C0:133:GLN:OE1  | 2.38                     | 0.47              |
| 3:C3:54:ALA:HB3   | 3:C3:58:ARG:HG2   | 1.95                     | 0.47              |
| 3:C5:228:LEU:HD12 | 3:C5:300:MET:HE1  | 1.97                     | 0.47              |
| 2:C8:282:TYR:CD2  | 2:D2:60:LYS:NZ    | 2.72                     | 0.47              |
| 3:D5:239:CYS:SG   | 3:D5:248:SER:N    | 2.87                     | 0.47              |
| 2:D6:283:HIS:CD2  | 2:E0:60:LYS:HZ1   | 2.31                     | 0.47              |
| 3:D7:292:GLN:O    | 3:D7:298:ASN:ND2  | 2.46                     | 0.47              |
| 2:E0:181:VAL:HG23 | 3:E1:347:ASN:O    | 2.14                     | 0.47              |
| 3:E1:19:LYS:HD2   | 3:E1:227:HIS:ND1  | 2.28                     | 0.47              |
| 2:E6:8:HIS:ND1    | 2:E6:65:CYS:SG    | 2.87                     | 0.47              |
| 2:E6:111:GLY:O    | 2:E6:115:VAL:HG23 | 2.14                     | 0.47              |
| 3:E7:389:PHE:CE1  | 3:E7:395:LEU:HD11 | 2.48                     | 0.47              |
| 3:E9:299:MET:HE2  | 3:E9:299:MET:HA   | 1.95                     | 0.47              |
| 4:a:57:ASN:HA     | 4:a:132:LEU:HD23  | 1.97                     | 0.47              |
| 4:b:80:GLY:N      | 4:b:116:ASP:OD1   | 2.40                     | 0.47              |
| 4:t:96:TYR:CE2    | 4:v:6:PHE:CE2     | 2.98                     | 0.47              |
| 1:12:254:LYS:HD3  | 2:D2:364:PRO:O    | 2.15                     | 0.47              |
| 1:21:239:LEU:HB3  | 1:21:240:PRO:HD2  | 1.97                     | 0.47              |
| 1:21:256:LEU:CD1  | 2:F0:37:PRO:HG3   | 2.44                     | 0.47              |
| 3:A1:12:CYS:CB    | 3:A1:138:SER:HB2  | 2.44                     | 0.47              |
| 3:A3:8:GLN:HE22   | 3:A3:17:GLY:HA3   | 1.79                     | 0.47              |
| 2:A4:119:LEU:HD13 | 2:A4:122:ILE:HD11 | 1.96                     | 0.47              |
| 2:A6:32:PRO:HG2   | 4:b:102:GLY:HA2   | 1.97                     | 0.47              |
| 3:A7:200:GLN:HG2  | 3:A7:268:ILE:HD11 | 1.96                     | 0.47              |
| 2:B2:252:VAL:HA   | 2:B2:255:PHE:HD2  | 1.78                     | 0.47              |
| 2:B6:265:ILE:HG23 | 2:B6:432:TYR:CZ   | 2.49                     | 0.47              |
| 3:C1:105:HIS:CE1  | 3:C1:150:LEU:HD13 | 2.50                     | 0.47              |
| 3:C1:274:THR:OG1  | 3:C1:282:ARG:NE   | 2.44                     | 0.47              |
| 3:C5:196:ALA:O    | 3:C5:264:HIS:NE2  | 2.46                     | 0.47              |
| 3:C7:321:MET:N    | 3:C7:321:MET:SD   | 2.88                     | 0.47              |
| 3:C9:64:ILE:HG12  | 3:C9:119:VAL:HG12 | 1.96                     | 0.47              |
| 2:D2:298:PRO:HB3  | 2:D2:307:PRO:HD2  | 1.97                     | 0.47              |
| 3:D3:101:TRP:HE3  | 3:D3:403:MET:HE1  | 1.80                     | 0.47              |
| 3:D5:127:CYS:SG   | 3:D5:128:ASP:N    | 2.82                     | 0.47              |
| 3:D5:323:THR:O    | 3:D5:327:ASP:N    | 2.46                     | 0.47              |
| 3:D7:179:VAL:HG11 | 2:D8:258:ASN:O    | 2.15                     | 0.47              |
| 3:D9:27:GLU:OE2   | 3:D9:241:ARG:NH1  | 2.44                     | 0.47              |
| 2:E2:11:GLN:HE22  | 3:E3:246:LEU:CD1  | 2.27                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E4:221:ARG:NH2  | 3:E5:322:SER:OG   | 2.47                     | 0.47              |
| 2:E6:290:GLU:OE1  | 2:F0:124:LYS:HE3  | 2.14                     | 0.47              |
| 3:E7:382:SER:OG   | 3:E7:412:GLU:OE1  | 2.32                     | 0.47              |
| 2:E8:329:ASN:HA   | 2:E8:332:VAL:HG12 | 1.95                     | 0.47              |
| 4:h:41:ASN:O      | 4:h:45:MET:HG3    | 2.14                     | 0.47              |
| 4:o:165:THR:OG1   | 4:o:166:GLY:N     | 2.48                     | 0.47              |
| 4:u:59:ASN:ND2    | 5:w:100:CYS:HB3   | 2.24                     | 0.47              |
| 1:10:247:TYR:CG   | 2:C8:77:GLU:OE2   | 2.67                     | 0.47              |
| 3:A3:192:LEU:HG   | 3:A3:199:VAL:HG21 | 1.97                     | 0.47              |
| 3:A5:183:TYR:HB3  | 3:A5:398:TYR:HE2  | 1.80                     | 0.47              |
| 3:B5:65:LEU:HB3   | 3:B5:73:MET:HE2   | 1.96                     | 0.47              |
| 3:C1:135:ILE:HG22 | 3:C1:137:HIS:HD2  | 1.79                     | 0.47              |
| 3:C1:219:THR:HB   | 2:C2:324:VAL:HG11 | 1.96                     | 0.47              |
| 2:C2:251:ASP:OD1  | 2:C2:254:GLU:N    | 2.47                     | 0.47              |
| 3:C7:66:MET:HB3   | 3:C7:91:VAL:HG23  | 1.96                     | 0.47              |
| 3:C9:283:ALA:HB2  | 3:D3:53:GLU:O     | 2.14                     | 0.47              |
| 2:D0:298:PRO:HB3  | 2:D0:307:PRO:HD2  | 1.96                     | 0.47              |
| 3:D1:238:CYS:SG   | 3:D1:318:ARG:NE   | 2.86                     | 0.47              |
| 2:D4:221:ARG:HG2  | 2:D4:221:ARG:O    | 2.13                     | 0.47              |
| 2:E0:36:MET:HE3   | 2:E0:61:HIS:NE2   | 2.30                     | 0.47              |
| 2:E2:251:ASP:OD1  | 2:E2:254:GLU:HG2  | 2.14                     | 0.47              |
| 3:E3:213:ARG:NE   | 3:E3:213:ARG:HA   | 2.29                     | 0.47              |
| 2:E8:265:ILE:HD12 | 2:E8:432:TYR:CE1  | 2.50                     | 0.47              |
| 4:b:67:HIS:O      | 4:b:71:LYS:NZ     | 2.47                     | 0.47              |
| 4:d:126:ARG:HD3   | 4:d:133:SER:HB3   | 1.96                     | 0.47              |
| 5:l:46:CYS:HA     | 5:l:49:ILE:HG22   | 1.95                     | 0.47              |
| 4:p:172:VAL:HG23  | 4:p:180:ALA:HB3   | 1.96                     | 0.47              |
| 4:t:63:ILE:HG22   | 4:v:16:ARG:CD     | 2.43                     | 0.47              |
| 5:w:38:PHE:HE1    | 5:w:106:ILE:HD13  | 1.78                     | 0.47              |
| 1:14:240:PRO:CB   | 4:s:154:TYR:CD2   | 2.98                     | 0.47              |
| 1:6:240:PRO:HG3   | 4:i:154:TYR:HD2   | 1.79                     | 0.47              |
| 2:A0:315:CYS:HB2  | 2:A0:351:PHE:HD1  | 1.78                     | 0.47              |
| 2:A2:284:GLU:HG2  | 2:A2:286:LEU:HD22 | 1.95                     | 0.47              |
| 2:A4:135:PHE:CE2  | 2:A4:157:LEU:HD12 | 2.50                     | 0.47              |
| 3:A5:267:LEU:HD11 | 3:A5:371:SER:HB3  | 1.96                     | 0.47              |
| 2:A6:281:ALA:O    | 4:d:202:ARG:NH2   | 2.47                     | 0.47              |
| 2:A8:277:SER:OG   | 2:A8:278:ALA:N    | 2.47                     | 0.47              |
| 2:B0:138:PHE:HZ   | 2:B0:235:ILE:HD12 | 1.80                     | 0.47              |
| 2:B0:223:THR:OG1  | 2:B0:225:THR:HG22 | 2.15                     | 0.47              |
| 2:B0:282:TYR:CZ   | 4:f:201:TRP:HZ2   | 2.32                     | 0.47              |
| 3:B3:176:SER:HB2  | 2:B4:349:THR:CG2  | 2.41                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B6:52:PHE:HD2   | 2:B6:243:ARG:HD3  | 1.78                     | 0.47              |
| 2:B6:72:PRO:HG2   | 3:B7:46:ARG:NH1   | 2.29                     | 0.47              |
| 3:B7:28:HIS:ND1   | 3:B7:43:GLN:O     | 2.45                     | 0.47              |
| 2:B8:26:LEU:HD21  | 2:B8:364:PRO:HD3  | 1.96                     | 0.47              |
| 2:B8:88:HIS:HB3   | 2:B8:91:GLN:HG3   | 1.96                     | 0.47              |
| 3:C1:215:LEU:HD21 | 3:C1:273:LEU:HD22 | 1.95                     | 0.47              |
| 3:C1:382:SER:O    | 3:C1:386:THR:N    | 2.43                     | 0.47              |
| 2:C4:18:ASN:O     | 2:C4:22:GLU:HG2   | 2.15                     | 0.47              |
| 2:C8:1:MET:N      | 2:C8:129:CYS:SG   | 2.80                     | 0.47              |
| 2:C8:7:ILE:HG23   | 2:C8:66:VAL:HG23  | 1.97                     | 0.47              |
| 2:C8:70:LEU:HD12  | 2:C8:145:THR:HG22 | 1.96                     | 0.47              |
| 2:C8:370:LYS:HG3  | 2:C8:370:LYS:O    | 2.14                     | 0.47              |
| 2:D0:245:ASP:OD1  | 2:D0:245:ASP:N    | 2.48                     | 0.47              |
| 2:D2:33:ASP:OD1   | 2:D2:34:GLY:N     | 2.48                     | 0.47              |
| 2:D2:210:TYR:HB3  | 3:D3:324:LYS:CE   | 2.45                     | 0.47              |
| 3:D7:2:ARG:HH11   | 3:D7:240:LEU:HD22 | 1.79                     | 0.47              |
| 2:D8:174:SER:HB2  | 2:D8:177:VAL:O    | 2.13                     | 0.47              |
| 3:E1:7:VAL:HB     | 3:E1:135:ILE:HG13 | 1.97                     | 0.47              |
| 3:E1:33:THR:HG23  | 3:E1:35:THR:HG23  | 1.97                     | 0.47              |
| 2:E2:274:PRO:HB2  | 2:E2:276:ILE:HG12 | 1.96                     | 0.47              |
| 2:E2:277:SER:OG   | 2:E2:278:ALA:N    | 2.48                     | 0.47              |
| 3:E3:247:ASN:C    | 3:E3:247:ASN:HD22 | 2.22                     | 0.47              |
| 2:E4:210:TYR:CE1  | 2:E4:227:LEU:HD21 | 2.49                     | 0.47              |
| 3:E5:344:TRP:CE3  | 3:E5:345:ILE:HG13 | 2.50                     | 0.47              |
| 2:E6:286:LEU:O    | 2:E6:373:ARG:NH1  | 2.44                     | 0.47              |
| 3:E9:66:MET:HE3   | 3:E9:66:MET:HB3   | 1.84                     | 0.47              |
| 2:F0:329:ASN:HA   | 2:F0:332:VAL:HG12 | 1.97                     | 0.47              |
| 2:F0:367:ASP:OD1  | 2:F0:367:ASP:N    | 2.48                     | 0.47              |
| 3:F1:20:PHE:HA    | 3:F1:230:SER:HB2  | 1.96                     | 0.47              |
| 4:c:96:TYR:HA     | 4:c:108:ILE:HD11  | 1.97                     | 0.47              |
| 4:d:70:GLY:HA3    | 4:f:38:LEU:O      | 2.14                     | 0.47              |
| 4:i:111:ILE:CG2   | 4:i:134:ILE:HG13  | 2.44                     | 0.47              |
| 5:k:54:ARG:NH2    | 5:k:89:LEU:O      | 2.47                     | 0.47              |
| 4:m:111:ILE:HD13  | 4:m:132:LEU:HB2   | 1.95                     | 0.47              |
| 4:n:80:GLY:N      | 4:n:116:ASP:OD1   | 2.38                     | 0.47              |
| 4:p:37:GLN:NE2    | 4:p:41:ASN:OD1    | 2.48                     | 0.47              |
| 4:q:63:ILE:HG22   | 4:s:16:ARG:HD3    | 1.96                     | 0.47              |
| 4:s:25:GLN:HE22   | 4:s:36:ILE:HG21   | 1.79                     | 0.47              |
| 4:v:118:ASP:N     | 4:v:118:ASP:OD1   | 2.47                     | 0.47              |
| 4:v:140:LEU:HA    | 4:v:143:ILE:HG22  | 1.96                     | 0.47              |
| 1:11:251:TYR:CE2  | 2:D0:18:ASN:ND2   | 2.82                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:244:GLN:NE2   | 4:e:162:GLY:HA3   | 2.27                     | 0.47              |
| 1:22:243:ALA:HB1  | 3:C7:357:PRO:HD2  | 1.94                     | 0.47              |
| 2:A0:133:GLN:O    | 2:A0:165:SER:OG   | 2.33                     | 0.47              |
| 2:A0:323:VAL:HG11 | 2:A0:328:VAL:HG23 | 1.96                     | 0.47              |
| 2:A2:6:SER:OG     | 2:A2:8:HIS:NE2    | 2.48                     | 0.47              |
| 2:A8:53:PHE:HB3   | 2:A8:61:HIS:HB3   | 1.97                     | 0.47              |
| 2:B0:241:SER:OG   | 2:B0:250:VAL:O    | 2.26                     | 0.47              |
| 2:B4:392:ASP:OD1  | 2:B4:422:ARG:NE   | 2.47                     | 0.47              |
| 2:C4:405:VAL:HG13 | 2:C4:418:PHE:HE2  | 1.79                     | 0.47              |
| 3:C7:91:VAL:HG21  | 3:C7:116:VAL:HG12 | 1.96                     | 0.47              |
| 3:D1:211:CYS:HA   | 3:D1:215:LEU:HB2  | 1.96                     | 0.47              |
| 2:D6:269:LEU:HD23 | 2:D6:301:MET:HG2  | 1.96                     | 0.47              |
| 2:E4:27:GLU:HB3   | 2:E4:361:THR:HG21 | 1.97                     | 0.47              |
| 3:E5:211:CYS:SG   | 3:E5:220:PRO:HB3  | 2.55                     | 0.47              |
| 4:d:71:LYS:CD     | 4:f:39:PRO:HG3    | 2.26                     | 0.47              |
| 4:e:10:LEU:HG     | 4:e:143:ILE:HG22  | 1.97                     | 0.47              |
| 4:j:98:THR:HA     | 4:j:101:GLU:HG3   | 1.97                     | 0.47              |
| 4:t:96:TYR:CZ     | 4:v:6:PHE:HE2     | 2.33                     | 0.47              |
| 1:12:256:LEU:HA   | 2:D2:26:LEU:HD22  | 1.97                     | 0.47              |
| 1:8:257:PRO:CB    | 2:C0:29:GLY:HA2   | 2.45                     | 0.47              |
| 1:9:243:ALA:CB    | 3:C3:357:PRO:CD   | 2.75                     | 0.47              |
| 3:A1:13:GLY:HA2   | 3:A1:16:ILE:HG22  | 1.96                     | 0.47              |
| 2:A6:210:TYR:O    | 3:A7:324:LYS:NZ   | 2.47                     | 0.47              |
| 2:B8:282:TYR:CE2  | 2:C2:85:HIS:HB3   | 2.50                     | 0.47              |
| 2:C0:279:GLU:CD   | 5:k:155:GLN:O     | 2.58                     | 0.47              |
| 3:C1:139:LEU:HA   | 3:C1:145:SER:HB2  | 1.96                     | 0.47              |
| 2:C6:101:ASN:HA   | 2:C6:144:GLY:HA3  | 1.95                     | 0.47              |
| 3:C7:403:MET:HB3  | 3:C7:408:PHE:HE1  | 1.79                     | 0.47              |
| 3:D3:155:VAL:HG13 | 3:D3:164:MET:CE   | 2.44                     | 0.47              |
| 2:D6:269:LEU:CD1  | 2:D6:384:ILE:HD11 | 2.44                     | 0.47              |
| 2:E8:210:TYR:CG   | 3:E9:324:LYS:HD3  | 2.49                     | 0.47              |
| 4:b:97:ARG:HH12   | 4:d:6:PHE:CB      | 2.10                     | 0.47              |
| 4:g:55:LEU:HD23   | 4:g:55:LEU:HA     | 1.79                     | 0.47              |
| 4:j:115:LEU:HD12  | 4:j:167:VAL:HB    | 1.97                     | 0.47              |
| 4:r:146:ARG:HG3   | 4:r:146:ARG:HH11  | 1.80                     | 0.47              |
| 1:7:244:GLN:HE22  | 1:7:249:SER:N     | 2.13                     | 0.47              |
| 2:A0:26:LEU:HD22  | 2:A0:364:PRO:HD3  | 1.97                     | 0.47              |
| 2:A2:103:PHE:H    | 2:A2:408:TYR:HE1  | 1.63                     | 0.47              |
| 2:A6:367:ASP:OD1  | 2:A6:367:ASP:N    | 2.48                     | 0.47              |
| 3:A9:163:ILE:HD13 | 3:A9:250:LEU:HB3  | 1.97                     | 0.47              |
| 3:B3:6:HIS:CE1    | 3:B3:20:PHE:CD2   | 3.03                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B5:57:GLY:O     | 4:f:83:PRO:HB3    | 2.15                     | 0.47              |
| 2:B6:339:ARG:NH1  | 2:B6:342:GLN:OE1  | 2.47                     | 0.47              |
| 3:B7:280:GLN:O    | 3:C1:58:ARG:HD3   | 2.14                     | 0.47              |
| 3:B7:326:VAL:O    | 3:B7:330:MET:HG2  | 2.15                     | 0.47              |
| 2:B8:1:MET:N      | 2:B8:129:CYS:SG   | 2.86                     | 0.47              |
| 2:C0:286:LEU:HD12 | 2:C0:371:VAL:HG12 | 1.97                     | 0.47              |
| 3:C1:279:GLN:HG3  | 3:C1:282:ARG:NH1  | 2.30                     | 0.47              |
| 2:C2:9:VAL:HG22   | 2:C2:68:LEU:HB2   | 1.96                     | 0.47              |
| 2:C4:84:ARG:HE    | 5:k:59:THR:HG21   | 1.80                     | 0.47              |
| 3:C5:220:PRO:HD2  | 2:C6:326:LYS:HB2  | 1.97                     | 0.47              |
| 2:C8:98:ASP:O     | 2:C8:105:ARG:NH2  | 2.48                     | 0.47              |
| 3:C9:336:LYS:HB3  | 3:C9:336:LYS:HE3  | 1.60                     | 0.47              |
| 2:D0:156:ARG:HG2  | 2:D0:156:ARG:HH21 | 1.79                     | 0.47              |
| 2:D2:36:MET:HE3   | 2:D2:61:HIS:NE2   | 2.30                     | 0.47              |
| 3:D5:152:ILE:HA   | 3:D5:155:VAL:HG12 | 1.97                     | 0.47              |
| 3:D5:156:ARG:HH22 | 3:D5:197:ASP:HB2  | 1.80                     | 0.47              |
| 2:D6:276:ILE:HD12 | 2:D6:281:ALA:HA   | 1.97                     | 0.47              |
| 3:D7:178:THR:HG22 | 2:D8:352:LYS:HZ3  | 1.79                     | 0.47              |
| 2:E0:97:GLU:OE2   | 3:E1:251:ARG:NH1  | 2.43                     | 0.47              |
| 2:E6:192:HIS:ND1  | 2:E6:424:ASP:OD2  | 2.48                     | 0.47              |
| 2:E6:236:SER:OG   | 2:E6:243:ARG:NH2  | 2.48                     | 0.47              |
| 3:E7:67:ASP:OD1   | 3:E7:68:LEU:N     | 2.48                     | 0.47              |
| 2:F0:265:ILE:HG23 | 2:F0:432:TYR:HE1  | 1.80                     | 0.47              |
| 4:i:78:ALA:HB3    | 4:i:112:PHE:HE1   | 1.79                     | 0.47              |
| 4:o:166:GLY:O     | 4:o:169:SER:OG    | 2.33                     | 0.47              |
| 1:0:244:GLN:N     | 3:A5:320:ARG:CZ   | 2.78                     | 0.46              |
| 2:A0:139:ASN:OD1  | 2:A0:139:ASN:N    | 2.46                     | 0.46              |
| 2:A8:88:HIS:NE2   | 2:A8:90:GLU:OE1   | 2.48                     | 0.46              |
| 2:B0:90:GLU:HB2   | 2:B0:121:ARG:NH2  | 2.30                     | 0.46              |
| 3:B3:220:PRO:HD2  | 2:B4:326:LYS:HB2  | 1.97                     | 0.46              |
| 3:C5:259:PRO:HB2  | 3:C5:260:PHE:CD1  | 2.49                     | 0.46              |
| 3:C7:281:TYR:HE1  | 3:D1:58:ARG:CZ    | 2.28                     | 0.46              |
| 2:D2:277:SER:OG   | 2:D2:278:ALA:N    | 2.47                     | 0.46              |
| 3:D5:21:TRP:HA    | 3:D5:24:ILE:HG22  | 1.97                     | 0.46              |
| 3:D5:310:TYR:CD1  | 3:D5:371:SER:HB2  | 2.49                     | 0.46              |
| 2:D8:262:TYR:HB3  | 2:D8:263:PRO:CD   | 2.44                     | 0.46              |
| 4:a:97:ARG:NH2    | 4:c:7:ALA:CB      | 2.67                     | 0.46              |
| 4:h:198:ARG:HA    | 4:h:198:ARG:HD2   | 1.79                     | 0.46              |
| 4:i:115:LEU:HD21  | 4:i:145:LYS:HD3   | 1.97                     | 0.46              |
| 1:16:253:ALA:HB1  | 2:E0:32:PRO:HG2   | 1.97                     | 0.46              |
| 1:6:240:PRO:HG2   | 4:i:154:TYR:CD2   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:256:LEU:HG    | 2:B8:31:GLN:HB3   | 1.96                     | 0.46              |
| 2:A4:265:ILE:HG23 | 2:A4:432:TYR:OH   | 2.14                     | 0.46              |
| 3:A5:203:ASP:OD2  | 3:A5:302:ALA:N    | 2.37                     | 0.46              |
| 2:B0:102:ASN:HB3  | 2:B0:105:ARG:H    | 1.80                     | 0.46              |
| 3:B3:282:ARG:O    | 3:B7:55:THR:HG21  | 2.14                     | 0.46              |
| 3:B5:105:HIS:CE1  | 3:B5:150:LEU:HD12 | 2.49                     | 0.46              |
| 3:B7:209:ASP:O    | 3:B7:213:ARG:HG2  | 2.14                     | 0.46              |
| 3:B7:267:LEU:HD13 | 3:B7:371:SER:HB3  | 1.97                     | 0.46              |
| 2:C0:172:TRP:HB2  | 2:C0:203:MET:HB3  | 1.96                     | 0.46              |
| 2:C0:223:THR:OG1  | 3:C1:245:GLN:CD   | 2.58                     | 0.46              |
| 3:D1:282:ARG:NH1  | 3:D1:288:GLU:OE2  | 2.47                     | 0.46              |
| 3:D5:155:VAL:HG13 | 3:D5:164:MET:HE2  | 1.98                     | 0.46              |
| 2:D6:370:LYS:HZ3  | 4:s:202:ARG:HH12  | 1.63                     | 0.46              |
| 2:E2:181:VAL:HG12 | 3:E3:256:ASN:ND2  | 2.30                     | 0.46              |
| 2:E2:220:GLU:HG3  | 2:E2:220:GLU:O    | 2.14                     | 0.46              |
| 2:E4:217:LEU:HD21 | 2:E4:367:ASP:OD2  | 2.16                     | 0.46              |
| 2:F0:25:CYS:SG    | 2:F0:86:LEU:HD11  | 2.55                     | 0.46              |
| 3:F1:171:PRO:HG3  | 3:F1:181:GLU:HG3  | 1.97                     | 0.46              |
| 4:c:22:ALA:HB1    | 4:c:38:LEU:HD22   | 1.97                     | 0.46              |
| 4:d:84:LYS:HE3    | 4:d:168:PRO:HD2   | 1.96                     | 0.46              |
| 4:e:63:ILE:HG22   | 4:g:16:ARG:HD2    | 1.88                     | 0.46              |
| 4:n:191:GLU:OE1   | 4:n:198:ARG:NH2   | 2.47                     | 0.46              |
| 4:p:70:GLY:HA3    | 4:r:38:LEU:O      | 2.15                     | 0.46              |
| 2:A0:132:LEU:HD23 | 2:A0:132:LEU:H    | 1.80                     | 0.46              |
| 2:A0:244:PHE:CD2  | 2:A0:358:GLN:HG2  | 2.50                     | 0.46              |
| 2:A2:326:LYS:HB2  | 2:A2:326:LYS:HE2  | 1.54                     | 0.46              |
| 2:A2:345:ASP:OD1  | 2:A2:346:TRP:N    | 2.48                     | 0.46              |
| 3:A9:135:ILE:HG13 | 3:A9:152:ILE:HG12 | 1.97                     | 0.46              |
| 3:C1:105:HIS:O    | 3:C1:105:HIS:ND1  | 2.48                     | 0.46              |
| 2:C4:167:LEU:HA   | 2:C4:200:VAL:HG13 | 1.98                     | 0.46              |
| 2:C4:417:GLU:HA   | 2:C4:420:GLU:HG3  | 1.97                     | 0.46              |
| 2:C8:97:GLU:HB3   | 2:C8:110:ILE:CD1  | 2.45                     | 0.46              |
| 2:C8:101:ASN:ND2  | 3:C9:252:LYS:HD3  | 2.30                     | 0.46              |
| 3:C9:309:ARG:NH1  | 3:C9:341:PHE:O    | 2.48                     | 0.46              |
| 3:D5:372:THR:HA   | 3:D5:422:TYR:CD2  | 2.50                     | 0.46              |
| 2:E0:100:ALA:HA   | 3:E1:252:LYS:HD2  | 1.96                     | 0.46              |
| 2:E2:176:GLN:HB3  | 3:E3:331:LEU:HD13 | 1.97                     | 0.46              |
| 2:E4:215:ARG:NH1  | 2:E4:216:ASN:OD1  | 2.49                     | 0.46              |
| 2:E4:309:HIS:NE2  | 2:E4:386:GLU:OE1  | 2.40                     | 0.46              |
| 2:E6:176:GLN:HB3  | 3:E7:331:LEU:CD1  | 2.45                     | 0.46              |
| 3:E9:5:VAL:HB     | 3:E9:133:PHE:HD1  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E9:149:THR:HA   | 3:E9:152:ILE:HD12 | 1.97                     | 0.46              |
| 2:F0:50:ASN:O     | 2:F0:64:ARG:NH2   | 2.42                     | 0.46              |
| 4:b:96:TYR:HA     | 4:b:108:ILE:HD11  | 1.97                     | 0.46              |
| 1:20:256:LEU:HD13 | 2:E8:29:GLY:O     | 2.16                     | 0.46              |
| 1:4:247:TYR:HE1   | 2:B2:81:GLY:CA    | 2.20                     | 0.46              |
| 1:6:240:PRO:CG    | 4:i:154:TYR:HD2   | 2.29                     | 0.46              |
| 3:A1:229:VAL:O    | 3:A1:233:MET:HB2  | 2.16                     | 0.46              |
| 3:A3:274:THR:HG21 | 3:A3:282:ARG:HD2  | 1.97                     | 0.46              |
| 3:A5:57:GLY:HA3   | 4:a:83:PRO:HB2    | 1.97                     | 0.46              |
| 3:A5:135:ILE:CD1  | 3:A5:152:ILE:HG12 | 2.45                     | 0.46              |
| 2:A6:331:ALA:O    | 2:A6:334:THR:OG1  | 2.31                     | 0.46              |
| 2:B0:286:LEU:CD1  | 2:B0:371:VAL:HG23 | 2.45                     | 0.46              |
| 2:B4:240:ALA:O    | 2:B4:356:ASN:ND2  | 2.47                     | 0.46              |
| 3:B9:396:HIS:HA   | 3:B9:399:THR:HG22 | 1.97                     | 0.46              |
| 2:C4:210:TYR:CE1  | 2:C4:227:LEU:HD11 | 2.50                     | 0.46              |
| 3:C5:329:GLN:HA   | 3:C5:332:ASN:HB3  | 1.97                     | 0.46              |
| 2:C6:231:ILE:HD13 | 2:C6:302:MET:CE   | 2.45                     | 0.46              |
| 3:C7:291:GLN:NE2  | 3:D1:125:GLU:CD   | 2.70                     | 0.46              |
| 3:C9:101:TRP:HB3  | 3:C9:398:TYR:HE1  | 1.80                     | 0.46              |
| 2:D0:222:PRO:HD2  | 3:D1:324:LYS:HB3  | 1.97                     | 0.46              |
| 3:D3:65:LEU:HB3   | 3:D3:73:MET:HE2   | 1.98                     | 0.46              |
| 3:D5:141:GLY:O    | 3:D5:145:SER:OG   | 2.29                     | 0.46              |
| 3:D5:253:LEU:HD11 | 3:D5:316:MET:HE1  | 1.94                     | 0.46              |
| 2:D6:119:LEU:HA   | 2:D6:122:ILE:HG22 | 1.97                     | 0.46              |
| 2:D8:265:ILE:HG22 | 2:D8:380:ASN:HD21 | 1.79                     | 0.46              |
| 2:D8:324:VAL:HG23 | 2:D8:327:ASP:H    | 1.79                     | 0.46              |
| 3:E1:309:ARG:H    | 3:E1:372:THR:HG22 | 1.80                     | 0.46              |
| 2:E2:185:TYR:HE2  | 2:E2:404:PHE:HB2  | 1.81                     | 0.46              |
| 2:E4:221:ARG:HA   | 2:E4:221:ARG:HD2  | 1.56                     | 0.46              |
| 2:E6:223:THR:CG2  | 2:E6:225:THR:HG22 | 2.43                     | 0.46              |
| 3:E7:323:THR:HA   | 3:E7:326:VAL:HG12 | 1.97                     | 0.46              |
| 3:E9:1:MET:N      | 3:E9:128:ASP:OD2  | 2.34                     | 0.46              |
| 4:c:171:ILE:HD11  | 4:c:182:PHE:HD1   | 1.79                     | 0.46              |
| 4:g:72:SER:HB3    | 4:g:108:ILE:HG22  | 1.97                     | 0.46              |
| 4:n:182:PHE:HE2   | 4:n:187:SER:HB3   | 1.81                     | 0.46              |
| 4:q:53:GLY:HA2    | 4:q:62:VAL:HG21   | 1.98                     | 0.46              |
| 3:A1:415:MET:HE2  | 3:A1:415:MET:HB3  | 1.86                     | 0.46              |
| 3:A3:130:LEU:H    | 3:A3:162:ARG:HH21 | 1.64                     | 0.46              |
| 2:A8:285:GLN:HG3  | 2:A8:286:LEU:N    | 2.31                     | 0.46              |
| 3:A9:213:ARG:HE   | 3:A9:297:LYS:HG3  | 1.81                     | 0.46              |
| 3:B1:114:ASP:N    | 3:B1:114:ASP:OD1  | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:145:THR:O    | 2:B2:149:LEU:HB2  | 2.16                     | 0.46              |
| 3:B3:281:TYR:O    | 3:B7:54:ALA:HB1   | 2.16                     | 0.46              |
| 3:C1:200:GLN:HB3  | 3:C1:266:PHE:HB2  | 1.96                     | 0.46              |
| 2:C6:336:LYS:HB3  | 2:C6:336:LYS:HE3  | 1.68                     | 0.46              |
| 3:D1:151:LEU:HD12 | 3:D1:151:LEU:HA   | 1.79                     | 0.46              |
| 2:E0:183:GLU:HG3  | 2:E0:184:PRO:HD3  | 1.98                     | 0.46              |
| 2:E2:406:HIS:HA   | 2:E2:409:VAL:HG12 | 1.97                     | 0.46              |
| 3:E9:42:LEU:HD21  | 3:E9:356:ILE:HD11 | 1.97                     | 0.46              |
| 4:b:141:THR:O     | 4:b:145:LYS:HG2   | 2.16                     | 0.46              |
| 5:k:73:TYR:HB2    | 5:k:92:TRP:NE1    | 2.31                     | 0.46              |
| 5:l:73:TYR:HB2    | 5:l:92:TRP:HE1    | 1.81                     | 0.46              |
| 4:u:181:GLN:HE22  | 4:u:200:ASP:H     | 1.62                     | 0.46              |
| 3:A1:117:LEU:HD13 | 3:A1:154:LYS:HZ1  | 1.81                     | 0.46              |
| 2:B4:298:PRO:HB3  | 2:B4:307:PRO:HD2  | 1.96                     | 0.46              |
| 2:C0:403:ALA:HA   | 3:C1:260:PHE:CE1  | 2.50                     | 0.46              |
| 2:C2:306:ASP:N    | 2:C2:386:GLU:OE2  | 2.48                     | 0.46              |
| 2:C4:178:SER:HB3  | 3:C5:347:ASN:ND2  | 2.31                     | 0.46              |
| 2:C6:406:HIS:CE1  | 3:C7:260:PHE:HA   | 2.51                     | 0.46              |
| 3:C7:2:ARG:HG3    | 3:C7:131:GLN:HB2  | 1.98                     | 0.46              |
| 3:C7:257:LEU:HD21 | 3:C7:314:SER:HB2  | 1.98                     | 0.46              |
| 3:C9:286:VAL:N    | 3:C9:287:PRO:CD   | 2.78                     | 0.46              |
| 2:D0:229:ARG:HG3  | 2:D0:229:ARG:NH1  | 2.29                     | 0.46              |
| 3:D3:181:GLU:HB2  | 3:D3:182:PRO:HD3  | 1.97                     | 0.46              |
| 2:D4:79:ARG:HH21  | 2:D4:79:ARG:HD3   | 1.43                     | 0.46              |
| 3:D7:238:CYS:SG   | 3:D7:318:ARG:NE   | 2.88                     | 0.46              |
| 2:D8:372:MET:HE2  | 2:D8:372:MET:HB3  | 1.73                     | 0.46              |
| 2:E0:5:ILE:HD12   | 2:E0:132:LEU:HD11 | 1.97                     | 0.46              |
| 3:E1:63:ALA:O     | 3:E1:89:ASN:ND2   | 2.48                     | 0.46              |
| 2:E4:132:LEU:HG   | 2:E4:164:LYS:NZ   | 2.31                     | 0.46              |
| 2:E6:8:HIS:HE1    | 2:E6:21:TRP:HE1   | 1.62                     | 0.46              |
| 3:E7:8:GLN:HE21   | 3:E7:65:LEU:CD2   | 2.29                     | 0.46              |
| 3:E9:207:LEU:HB3  | 3:E9:225:LEU:HD22 | 1.98                     | 0.46              |
| 2:F0:406:HIS:NE2  | 3:F1:261:PRO:HD3  | 2.29                     | 0.46              |
| 3:F1:309:ARG:H    | 3:F1:372:THR:HG22 | 1.81                     | 0.46              |
| 4:f:146:ARG:NH2   | 4:f:156:VAL:HB    | 2.30                     | 0.46              |
| 5:k:91:PRO:HD2    | 5:k:92:TRP:CZ3    | 2.51                     | 0.46              |
| 5:l:144:MET:CE    | 5:l:156:ARG:HB3   | 2.46                     | 0.46              |
| 4:q:78:ALA:HB3    | 4:q:112:PHE:HE1   | 1.81                     | 0.46              |
| 4:r:23:LEU:HD12   | 4:r:38:LEU:HD22   | 1.97                     | 0.46              |
| 4:r:97:ARG:HH22   | 4:t:161:TYR:HA    | 1.81                     | 0.46              |
| 4:r:113:VAL:HG13  | 4:r:141:THR:HG23  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:s:159:TYR:HB2   | 4:s:161:TYR:CE2   | 2.51                     | 0.46              |
| 1:19:241:PHE:CE1  | 3:E7:356:ILE:HG22 | 2.43                     | 0.46              |
| 3:A1:215:LEU:HD11 | 3:A1:273:LEU:HD22 | 1.98                     | 0.46              |
| 3:A3:8:GLN:HG3    | 3:A3:65:LEU:HD13  | 1.98                     | 0.46              |
| 2:A8:288:VAL:HG13 | 2:A8:319:TYR:HE2  | 1.81                     | 0.46              |
| 2:B4:96:LYS:HE3   | 3:B5:1:MET:C      | 2.40                     | 0.46              |
| 2:B8:141:VAL:HA   | 2:B8:147:SER:HB2  | 1.98                     | 0.46              |
| 2:C2:250:VAL:HG23 | 2:C2:352:LYS:NZ   | 2.29                     | 0.46              |
| 2:C4:137:MET:HB3  | 2:C4:168:ASN:HA   | 1.96                     | 0.46              |
| 2:C8:98:ASP:OD1   | 2:C8:99:ALA:N     | 2.49                     | 0.46              |
| 3:C9:54:ALA:C     | 3:C9:56:GLY:H     | 2.24                     | 0.46              |
| 2:D0:107:HIS:CE1  | 2:D0:151:CYS:HG   | 2.31                     | 0.46              |
| 2:D2:241:SER:HB2  | 2:D2:249:ASN:HB2  | 1.98                     | 0.46              |
| 2:D4:285:GLN:CG   | 2:D8:55:GLU:O     | 2.53                     | 0.46              |
| 3:D7:2:ARG:HH11   | 3:D7:240:LEU:CD2  | 2.29                     | 0.46              |
| 3:D9:320:ARG:NH2  | 4:t:188:GLY:HA3   | 2.31                     | 0.46              |
| 2:E0:282:TYR:HB2  | 2:E0:283:HIS:CD2  | 2.50                     | 0.46              |
| 2:E2:185:TYR:CZ   | 2:E2:398:MET:HE3  | 2.51                     | 0.46              |
| 3:E7:289:LEU:HD12 | 3:E7:365:VAL:HG12 | 1.98                     | 0.46              |
| 2:E8:79:ARG:NH1   | 2:E8:92:LEU:O     | 2.48                     | 0.46              |
| 2:E8:313:MET:HE3  | 2:E8:346:TRP:HZ2  | 1.81                     | 0.46              |
| 4:e:71:LYS:CG     | 4:g:39:PRO:HG3    | 2.46                     | 0.46              |
| 4:n:138:ASN:O     | 4:n:141:THR:HG22  | 2.16                     | 0.46              |
| 1:21:256:LEU:HD21 | 2:F0:31:GLN:HA    | 1.98                     | 0.46              |
| 1:21:256:LEU:HD11 | 2:F0:31:GLN:HE21  | 1.81                     | 0.46              |
| 2:A2:336:LYS:HA   | 2:A2:336:LYS:HD2  | 1.77                     | 0.46              |
| 2:A4:222:PRO:HD2  | 3:A5:324:LYS:CB   | 2.42                     | 0.46              |
| 3:A9:181:GLU:HB2  | 3:A9:182:PRO:HD3  | 1.98                     | 0.46              |
| 2:B0:210:TYR:HB3  | 3:B1:324:LYS:CD   | 2.39                     | 0.46              |
| 3:B1:27:GLU:OE1   | 3:B1:318:ARG:NH2  | 2.49                     | 0.46              |
| 3:B1:27:GLU:OE2   | 3:B1:241:ARG:NH1  | 2.38                     | 0.46              |
| 3:B1:281:TYR:HB3  | 3:B5:60:VAL:HG11  | 1.97                     | 0.46              |
| 3:B3:207:LEU:HB3  | 3:B3:225:LEU:HD22 | 1.98                     | 0.46              |
| 2:B6:27:GLU:OE2   | 2:B6:320:ARG:NH2  | 2.49                     | 0.46              |
| 3:B7:281:TYR:CE2  | 3:C1:87:PRO:CD    | 2.88                     | 0.46              |
| 2:C0:188:VAL:HG12 | 2:C0:425:LEU:HD13 | 1.98                     | 0.46              |
| 3:C1:156:ARG:HD3  | 3:C1:160:PRO:HA   | 1.97                     | 0.46              |
| 3:C7:149:THR:HG23 | 3:C7:152:ILE:HD12 | 1.96                     | 0.46              |
| 2:D0:36:MET:SD    | 2:D0:61:HIS:NE2   | 2.76                     | 0.46              |
| 3:D1:274:THR:OG1  | 3:D1:279:GLN:OE1  | 2.34                     | 0.46              |
| 3:D3:64:ILE:HD12  | 3:D3:119:VAL:HG22 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D9:132:GLY:HA3  | 3:D9:163:ILE:HG22 | 1.96                     | 0.46              |
| 3:D9:374:ILE:HD11 | 3:D9:422:TYR:CZ   | 2.51                     | 0.46              |
| 3:E1:19:LYS:NZ    | 3:E1:223:GLY:O    | 2.49                     | 0.46              |
| 3:E1:128:ASP:OD1  | 3:E1:129:CYS:N    | 2.46                     | 0.46              |
| 3:E5:174:LYS:HA   | 3:E5:174:LYS:HD2  | 1.78                     | 0.46              |
| 3:E7:256:ASN:HB3  | 3:E7:350:LYS:HE2  | 1.98                     | 0.46              |
| 2:F0:51:THR:HG23  | 2:F0:52:PHE:CD2   | 2.50                     | 0.46              |
| 2:F0:101:ASN:HB3  | 2:F0:182:VAL:HG21 | 1.98                     | 0.46              |
| 2:F0:390:ARG:NH2  | 2:F0:390:ARG:HB3  | 2.30                     | 0.46              |
| 3:F1:216:LYS:HD3  | 3:F1:216:LYS:HA   | 1.78                     | 0.46              |
| 4:i:185:ILE:HD12  | 4:i:193:ASP:H     | 1.81                     | 0.46              |
| 5:l:54:ARG:HG3    | 5:l:55:GLN:N      | 2.31                     | 0.46              |
| 4:q:10:LEU:HG     | 4:q:143:ILE:HG22  | 1.97                     | 0.46              |
| 1:21:244:GLN:O    | 3:F1:320:ARG:NH2  | 2.49                     | 0.46              |
| 1:8:255:PRO:CG    | 2:C0:364:PRO:HG2  | 2.46                     | 0.46              |
| 2:A0:279:GLU:OE2  | 4:a:198:ARG:CD    | 2.64                     | 0.46              |
| 2:A0:312:TYR:CE1  | 2:A0:379:SER:HB3  | 2.42                     | 0.46              |
| 2:A2:221:ARG:HD3  | 3:A3:322:SER:OG   | 2.16                     | 0.46              |
| 2:A4:2:ARG:HG3    | 2:A4:2:ARG:O      | 2.15                     | 0.46              |
| 2:B0:204:LEU:HD12 | 2:B0:209:ILE:HD11 | 1.97                     | 0.46              |
| 3:B7:66:MET:HE3   | 3:B7:116:VAL:HG21 | 1.98                     | 0.46              |
| 3:B7:112:LEU:O    | 3:B7:112:LEU:HD23 | 2.16                     | 0.46              |
| 3:C1:324:LYS:HA   | 3:C1:324:LYS:HD2  | 1.52                     | 0.46              |
| 3:C3:184:ASN:OD1  | 3:C3:398:TYR:OH   | 2.31                     | 0.46              |
| 3:D3:247:ASN:O    | 3:D3:252:LYS:HE2  | 2.15                     | 0.46              |
| 2:D4:172:TRP:HB3  | 2:D4:205:ASP:OD1  | 2.16                     | 0.46              |
| 3:D9:64:ILE:HD12  | 3:D9:119:VAL:HG12 | 1.98                     | 0.46              |
| 2:E2:244:PHE:HB2  | 2:E2:356:ASN:HD21 | 1.80                     | 0.46              |
| 2:E4:72:PRO:HD2   | 3:E5:2:ARG:HH22   | 1.79                     | 0.46              |
| 4:e:9:PRO:HA      | 4:e:12:VAL:HG22   | 1.98                     | 0.46              |
| 4:i:15:ARG:O      | 4:i:19:GLU:HG3    | 2.15                     | 0.46              |
| 4:r:110:ILE:O     | 4:r:131:TRP:HB2   | 2.16                     | 0.46              |
| 4:v:75:LEU:HD23   | 4:v:111:ILE:HB    | 1.98                     | 0.46              |
| 4:v:96:TYR:HA     | 4:v:108:ILE:HD11  | 1.98                     | 0.46              |
| 5:w:87:ARG:HD2    | 5:w:94:SER:HB3    | 1.97                     | 0.46              |
| 1:9:257:PRO:HG2   | 2:C2:26:LEU:CA    | 2.45                     | 0.46              |
| 2:A0:241:SER:HB3  | 2:A0:249:ASN:HB3  | 1.98                     | 0.46              |
| 3:A1:22:GLU:OE2   | 3:A1:81:PHE:HB2   | 2.15                     | 0.46              |
| 3:A1:260:PHE:CE2  | 3:A1:425:TYR:HE2  | 2.34                     | 0.46              |
| 2:A4:163:LYS:HZ3  | 2:A4:163:LYS:HG3  | 1.49                     | 0.46              |
| 2:A4:340:THR:HG23 | 2:A4:341:ILE:HG13 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A5:206:ALA:HB2  | 3:A5:302:ALA:HB2  | 1.98                     | 0.46              |
| 2:A8:174:SER:HB2  | 2:A8:177:VAL:O    | 2.15                     | 0.46              |
| 3:A9:213:ARG:HH11 | 3:A9:213:ARG:HD2  | 1.58                     | 0.46              |
| 2:B0:27:GLU:OE1   | 2:B0:243:ARG:NH2  | 2.49                     | 0.46              |
| 3:B5:147:MET:HE3  | 3:B5:147:MET:HB3  | 1.75                     | 0.46              |
| 3:C9:164:MET:HE3  | 3:C9:164:MET:HB2  | 1.76                     | 0.46              |
| 2:D2:156:ARG:HD2  | 2:D2:156:ARG:HA   | 1.69                     | 0.46              |
| 2:D2:404:PHE:HZ   | 3:D3:312:THR:HG21 | 1.81                     | 0.46              |
| 2:D4:189:LEU:HD11 | 2:D4:418:PHE:CD1  | 2.51                     | 0.46              |
| 3:D5:164:MET:HE3  | 3:D5:164:MET:HB2  | 1.77                     | 0.46              |
| 2:E6:221:ARG:CG   | 3:E7:325:GLU:HB2  | 2.45                     | 0.46              |
| 2:E8:91:GLN:HB3   | 2:E8:121:ARG:HG2  | 1.97                     | 0.46              |
| 3:E9:220:PRO:HD2  | 2:F0:326:LYS:HE2  | 1.98                     | 0.46              |
| 4:a:181:GLN:HG3   | 4:a:183:LEU:HD22  | 1.98                     | 0.46              |
| 4:e:73:VAL:HA     | 4:e:109:GLU:O     | 2.16                     | 0.46              |
| 4:e:96:TYR:HA     | 4:e:108:ILE:HD11  | 1.98                     | 0.46              |
| 4:m:53:GLY:HA2    | 4:m:62:VAL:HG21   | 1.98                     | 0.46              |
| 4:p:170:VAL:HG23  | 4:p:183:LEU:HB2   | 1.98                     | 0.46              |
| 1:13:244:GLN:CD   | 4:r:162:GLY:HA3   | 2.39                     | 0.45              |
| 3:A5:105:HIS:CE1  | 3:A5:150:LEU:HD12 | 2.51                     | 0.45              |
| 3:B3:324:LYS:O    | 3:B3:328:GLU:N    | 2.49                     | 0.45              |
| 2:B6:339:ARG:HA   | 2:B6:339:ARG:HD2  | 1.65                     | 0.45              |
| 3:B7:190:HIS:HA   | 3:B7:193:VAL:HG12 | 1.98                     | 0.45              |
| 2:B8:188:VAL:HG23 | 2:B8:189:LEU:HD12 | 1.98                     | 0.45              |
| 3:B9:68:LEU:HD23  | 3:B9:112:LEU:HD13 | 1.98                     | 0.45              |
| 2:C0:181:VAL:H    | 3:C1:256:ASN:ND2  | 2.13                     | 0.45              |
| 2:C8:28:HIS:CE1   | 2:C8:243:ARG:HH11 | 2.35                     | 0.45              |
| 2:D2:137:MET:HE3  | 2:D2:137:MET:HB2  | 1.93                     | 0.45              |
| 3:D5:61:PRO:HD3   | 3:D5:84:LEU:HG    | 1.99                     | 0.45              |
| 3:E1:212:PHE:HE1  | 2:E2:326:LYS:HE3  | 1.82                     | 0.45              |
| 3:E1:388:MET:HG2  | 2:E2:346:TRP:O    | 2.15                     | 0.45              |
| 3:E3:2:ARG:HB2    | 3:E3:131:GLN:HB2  | 1.98                     | 0.45              |
| 2:E6:401:LYS:HD2  | 3:E7:344:TRP:CG   | 2.51                     | 0.45              |
| 2:E8:325:PRO:HA   | 2:E8:328:VAL:HG12 | 1.97                     | 0.45              |
| 4:m:90:PRO:HA     | 4:m:93:LEU:HD12   | 1.98                     | 0.45              |
| 4:p:8:SER:HG      | 4:p:11:ASN:HD22   | 1.60                     | 0.45              |
| 1:0:247:TYR:CE2   | 2:A4:81:GLY:HA3   | 2.51                     | 0.45              |
| 2:A4:28:HIS:NE2   | 2:A4:243:ARG:HD2  | 2.32                     | 0.45              |
| 3:B1:239:CYS:SG   | 3:B1:248:SER:N    | 2.87                     | 0.45              |
| 2:C0:313:MET:HE3  | 2:C0:382:THR:HG23 | 1.97                     | 0.45              |
| 3:C3:253:LEU:HD11 | 3:C3:368:VAL:HG21 | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C4:296:PHE:CD1  | 2:C4:377:MET:HE2  | 2.51                     | 0.45              |
| 3:C5:140:GLY:O    | 3:C5:184:ASN:ND2  | 2.41                     | 0.45              |
| 2:C6:191:THR:OG1  | 2:C6:425:LEU:HD21 | 2.15                     | 0.45              |
| 2:C6:279:GLU:OE1  | 4:n:197:LEU:HB3   | 2.15                     | 0.45              |
| 3:C9:139:LEU:CD1  | 3:C9:168:SER:HB2  | 2.43                     | 0.45              |
| 2:D0:221:ARG:N    | 2:D0:222:PRO:HD3  | 2.31                     | 0.45              |
| 2:D0:377:MET:HE2  | 2:D0:379:SER:HB3  | 1.98                     | 0.45              |
| 3:D5:309:ARG:H    | 3:D5:372:THR:HG22 | 1.81                     | 0.45              |
| 3:D5:318:ARG:HD3  | 3:D5:358:PRO:HD3  | 1.98                     | 0.45              |
| 3:D9:135:ILE:HG22 | 3:D9:137:HIS:CD2  | 2.52                     | 0.45              |
| 3:D9:281:TYR:CE1  | 3:E3:58:ARG:CZ    | 3.00                     | 0.45              |
| 2:E4:306:ASP:HB3  | 2:E4:309:HIS:CE1  | 2.51                     | 0.45              |
| 3:E9:330:MET:SD   | 3:E9:349:MET:HG3  | 2.56                     | 0.45              |
| 3:F1:292:GLN:O    | 3:F1:298:ASN:ND2  | 2.39                     | 0.45              |
| 4:t:51:PRO:HD2    | 4:t:54:SER:OG     | 2.16                     | 0.45              |
| 1:20:243:ALA:CB   | 3:E9:357:PRO:HD2  | 2.42                     | 0.45              |
| 2:A0:282:TYR:N    | 4:a:202:ARG:HH22  | 1.98                     | 0.45              |
| 2:A8:238:LEU:HD22 | 2:A8:255:PHE:HE2  | 1.81                     | 0.45              |
| 2:B2:177:VAL:HG12 | 3:B3:331:LEU:HD22 | 1.97                     | 0.45              |
| 3:B5:57:GLY:C     | 4:f:83:PRO:HB3    | 2.41                     | 0.45              |
| 2:C0:133:GLN:HG3  | 2:C0:252:VAL:HG22 | 1.97                     | 0.45              |
| 3:C1:317:PHE:CB   | 3:C1:321:MET:HE1  | 2.45                     | 0.45              |
| 3:C9:181:GLU:HB2  | 3:C9:182:PRO:HD3  | 1.96                     | 0.45              |
| 2:D0:121:ARG:HA   | 2:D0:121:ARG:HD2  | 1.68                     | 0.45              |
| 3:D5:105:HIS:CE1  | 3:D5:150:LEU:HB2  | 2.50                     | 0.45              |
| 2:D6:301:MET:HE1  | 2:D6:312:TYR:OH   | 2.16                     | 0.45              |
| 3:D7:374:ILE:HD11 | 3:D7:422:TYR:CZ   | 2.52                     | 0.45              |
| 3:D9:63:ALA:O     | 3:D9:89:ASN:ND2   | 2.50                     | 0.45              |
| 3:E1:238:CYS:SG   | 3:E1:239:CYS:N    | 2.90                     | 0.45              |
| 2:E8:296:PHE:CZ   | 2:E8:317:LEU:HD21 | 2.51                     | 0.45              |
| 3:E9:238:CYS:SG   | 3:E9:239:CYS:N    | 2.89                     | 0.45              |
| 2:F0:174:SER:HB3  | 2:F0:177:VAL:O    | 2.15                     | 0.45              |
| 2:F0:177:VAL:HG22 | 3:F1:331:LEU:HD22 | 1.99                     | 0.45              |
| 2:F0:306:ASP:HB3  | 2:F0:309:HIS:CE1  | 2.50                     | 0.45              |
| 4:c:75:LEU:O      | 4:c:170:VAL:HA    | 2.16                     | 0.45              |
| 4:h:63:ILE:HG23   | 4:h:67:HIS:ND1    | 2.31                     | 0.45              |
| 5:l:27:ASP:OD2    | 4:n:23:LEU:HD22   | 2.16                     | 0.45              |
| 4:n:148:PHE:O     | 4:n:149:ARG:HG2   | 2.15                     | 0.45              |
| 4:p:154:TYR:HE1   | 4:p:158:THR:HG22  | 1.82                     | 0.45              |
| 1:11:244:GLN:CA   | 3:D1:320:ARG:NH2  | 2.79                     | 0.45              |
| 1:13:256:LEU:HD13 | 2:D4:29:GLY:C     | 2.41                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A2:210:TYR:HB3  | 3:A3:324:LYS:HG3  | 1.98                     | 0.45              |
| 3:A3:187:LEU:HD11 | 3:A3:408:PHE:CE1  | 2.51                     | 0.45              |
| 2:A6:313:MET:HE3  | 2:A6:435:VAL:HG11 | 1.98                     | 0.45              |
| 2:A8:338:LYS:HG2  | 2:A8:340:THR:HG22 | 1.98                     | 0.45              |
| 3:A9:67:ASP:OD1   | 3:A9:68:LEU:N     | 2.48                     | 0.45              |
| 2:B2:12:ALA:HB3   | 2:B2:140:ALA:HB2  | 1.99                     | 0.45              |
| 2:B2:404:PHE:HZ   | 3:B3:345:ILE:HD13 | 1.82                     | 0.45              |
| 3:B3:6:HIS:HE1    | 3:B3:20:PHE:CD2   | 2.34                     | 0.45              |
| 2:B6:132:LEU:HB3  | 2:B6:164:LYS:HE2  | 1.98                     | 0.45              |
| 2:C2:209:ILE:HG22 | 2:C2:227:LEU:HG   | 1.98                     | 0.45              |
| 3:C3:173:PRO:HG3  | 3:C3:302:ALA:HB1  | 1.99                     | 0.45              |
| 2:C4:88:HIS:O     | 2:C4:90:GLU:N     | 2.49                     | 0.45              |
| 2:C4:396:ASP:OD1  | 2:C4:396:ASP:N    | 2.49                     | 0.45              |
| 2:C6:310:GLY:HA3  | 2:C6:383:ALA:HB2  | 1.99                     | 0.45              |
| 3:C7:183:TYR:HB3  | 3:C7:398:TYR:CE2  | 2.51                     | 0.45              |
| 2:C8:147:SER:HB2  | 2:C8:190:SER:HB3  | 1.97                     | 0.45              |
| 2:C8:279:GLU:HG3  | 4:o:197:LEU:O     | 2.16                     | 0.45              |
| 3:C9:282:ARG:NH1  | 3:C9:292:GLN:OE1  | 2.49                     | 0.45              |
| 3:D3:68:LEU:HA    | 3:D3:93:GLY:HA3   | 1.99                     | 0.45              |
| 3:D3:294:PHE:CE2  | 3:D3:333:VAL:HG21 | 2.51                     | 0.45              |
| 3:D3:313:ALA:HB1  | 3:D3:367:PHE:CE1  | 2.51                     | 0.45              |
| 2:D6:64:ARG:HG2   | 2:D6:125:LEU:HD11 | 1.97                     | 0.45              |
| 2:D6:209:ILE:CG2  | 2:D6:227:LEU:HG   | 2.46                     | 0.45              |
| 2:D8:178:SER:HB2  | 3:D9:347:ASN:HD22 | 1.82                     | 0.45              |
| 2:F0:328:VAL:HG21 | 2:F0:355:ILE:HD11 | 1.98                     | 0.45              |
| 2:F0:390:ARG:HB3  | 2:F0:390:ARG:HH21 | 1.81                     | 0.45              |
| 4:d:74:ALA:HB2    | 4:d:172:VAL:HG12  | 1.98                     | 0.45              |
| 4:e:181:GLN:NE2   | 4:e:198:ARG:O     | 2.42                     | 0.45              |
| 4:f:69:LYS:HE3    | 4:f:69:LYS:HB2    | 1.57                     | 0.45              |
| 4:i:176:ASP:OD2   | 4:i:178:ARG:NH1   | 2.49                     | 0.45              |
| 4:r:78:ALA:HB3    | 4:r:112:PHE:HE1   | 1.81                     | 0.45              |
| 1:11:254:LYS:HB3  | 2:D0:364:PRO:HG2  | 1.99                     | 0.45              |
| 1:20:241:PHE:CE1  | 3:E9:356:ILE:CG2  | 3.00                     | 0.45              |
| 2:A0:195:LEU:HD21 | 2:A0:264:ARG:HE   | 1.82                     | 0.45              |
| 2:A4:422:ARG:NH1  | 2:A4:426:ALA:HB2  | 2.31                     | 0.45              |
| 2:A6:11:GLN:HG3   | 2:A6:74:VAL:HG21  | 1.97                     | 0.45              |
| 2:A8:356:ASN:OD1  | 2:A8:357:TYR:N    | 2.49                     | 0.45              |
| 2:B6:70:LEU:HD12  | 2:B6:99:ALA:HB2   | 1.98                     | 0.45              |
| 2:B8:238:LEU:HD12 | 2:B8:238:LEU:HA   | 1.85                     | 0.45              |
| 2:B8:288:VAL:HA   | 2:B8:291:ILE:HG12 | 1.97                     | 0.45              |
| 2:C2:313:MET:HE1  | 2:C2:346:TRP:CZ2  | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C5:209:ASP:OD1  | 3:C5:213:ARG:NH2  | 2.46                     | 0.45              |
| 2:C6:180:ALA:O    | 3:C7:347:ASN:ND2  | 2.50                     | 0.45              |
| 2:C8:60:LYS:NZ    | 2:C8:61:HIS:O     | 2.48                     | 0.45              |
| 2:D2:11:GLN:HE22  | 3:D3:246:LEU:HA   | 1.81                     | 0.45              |
| 2:D2:272:TYR:HD2  | 2:D2:275:ILE:HG12 | 1.81                     | 0.45              |
| 3:D7:213:ARG:CB   | 3:D7:297:LYS:HD2  | 2.46                     | 0.45              |
| 2:E0:306:ASP:OD1  | 2:E0:308:ARG:NH1  | 2.49                     | 0.45              |
| 3:E3:239:CYS:SG   | 3:E3:248:SER:N    | 2.83                     | 0.45              |
| 3:E3:291:GLN:OE1  | 3:E7:122:LYS:HD3  | 2.15                     | 0.45              |
| 2:E4:195:LEU:HD11 | 2:E4:428:LEU:HD22 | 1.98                     | 0.45              |
| 2:E8:69:ASP:OD1   | 2:E8:70:LEU:N     | 2.49                     | 0.45              |
| 2:E8:172:TRP:N    | 2:E8:204:LEU:O    | 2.41                     | 0.45              |
| 3:E9:289:LEU:HD23 | 3:E9:365:VAL:HG12 | 1.98                     | 0.45              |
| 4:e:175:SER:HA    | 4:e:206:PHE:CE1   | 2.51                     | 0.45              |
| 4:n:74:ALA:HB3    | 4:n:110:ILE:HD13  | 1.99                     | 0.45              |
| 4:p:101:GLU:HG3   | 4:r:2:SER:OG      | 2.17                     | 0.45              |
| 4:t:10:LEU:HG     | 4:t:143:ILE:HG22  | 1.97                     | 0.45              |
| 4:v:112:PHE:CG    | 4:v:129:MET:HE1   | 2.52                     | 0.45              |
| 5:x:66:LYS:HG3    | 5:x:67:ALA:H      | 1.81                     | 0.45              |
| 1:6:240:PRO:HG3   | 4:i:154:TYR:CD2   | 2.52                     | 0.45              |
| 2:A4:157:LEU:HB3  | 2:A4:166:LYS:HE2  | 1.99                     | 0.45              |
| 3:A5:73:MET:HE3   | 3:A5:92:PHE:CD1   | 2.52                     | 0.45              |
| 3:B1:362:LYS:HE2  | 3:B1:362:LYS:HB2  | 1.50                     | 0.45              |
| 2:C4:14:ILE:O     | 2:C4:18:ASN:N     | 2.48                     | 0.45              |
| 3:C5:291:GLN:HE22 | 3:C9:122:LYS:HE2  | 1.81                     | 0.45              |
| 3:D1:7:VAL:HB     | 3:D1:135:ILE:HG12 | 1.98                     | 0.45              |
| 3:D3:67:ASP:OD1   | 3:D3:68:LEU:N     | 2.50                     | 0.45              |
| 2:D4:222:PRO:HD2  | 3:D5:324:LYS:HB3  | 1.99                     | 0.45              |
| 3:D5:404:ASP:OD1  | 3:D5:405:GLU:N    | 2.49                     | 0.45              |
| 3:D7:212:PHE:CE1  | 2:D8:326:LYS:HD3  | 2.40                     | 0.45              |
| 2:D8:179:THR:HG21 | 3:D9:327:ASP:OD1  | 2.16                     | 0.45              |
| 3:D9:129:CYS:O    | 3:D9:129:CYS:SG   | 2.74                     | 0.45              |
| 3:E3:218:THR:HG23 | 3:E3:219:THR:HG23 | 1.99                     | 0.45              |
| 2:E4:221:ARG:HH12 | 3:E5:324:LYS:H    | 1.65                     | 0.45              |
| 2:E6:223:THR:OG1  | 3:E7:245:GLN:NE2  | 2.48                     | 0.45              |
| 2:E6:280:LYS:HZ3  | 2:F0:89:PRO:CB    | 2.10                     | 0.45              |
| 2:E6:423:GLU:O    | 2:E6:427:ALA:N    | 2.44                     | 0.45              |
| 2:E8:137:MET:HB3  | 2:E8:168:ASN:HA   | 1.99                     | 0.45              |
| 3:E9:49:VAL:HG21  | 3:E9:241:ARG:HG2  | 1.98                     | 0.45              |
| 4:b:53:GLY:HA2    | 4:b:62:VAL:HG21   | 1.98                     | 0.45              |
| 4:f:15:ARG:HA     | 4:f:45:MET:HE1    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A0:290:GLU:CB   | 2:A4:124:LYS:NZ   | 2.79                     | 0.45              |
| 3:A1:326:VAL:O    | 3:A1:330:MET:HG2  | 2.16                     | 0.45              |
| 2:A2:199:ASP:OD1  | 2:A2:200:VAL:N    | 2.49                     | 0.45              |
| 3:A3:414:ASN:HD22 | 3:A3:414:ASN:C    | 2.25                     | 0.45              |
| 3:A7:54:ALA:C     | 3:A7:56:GLY:H     | 2.25                     | 0.45              |
| 2:B2:28:HIS:CE1   | 2:B2:243:ARG:HD2  | 2.51                     | 0.45              |
| 2:B6:1:MET:N      | 2:B6:129:CYS:SG   | 2.90                     | 0.45              |
| 2:C6:207:GLU:HA   | 2:C6:210:TYR:HB2  | 1.99                     | 0.45              |
| 2:C6:281:ALA:HB3  | 4:n:202:ARG:HH12  | 1.81                     | 0.45              |
| 2:C8:282:TYR:CE1  | 4:o:201:TRP:CZ2   | 2.87                     | 0.45              |
| 2:C8:420:GLU:O    | 2:C8:420:GLU:HG3  | 2.16                     | 0.45              |
| 3:C9:99:ASN:ND2   | 3:C9:178:THR:HG22 | 2.32                     | 0.45              |
| 3:D1:206:ALA:HB2  | 3:D1:302:ALA:HB2  | 1.99                     | 0.45              |
| 2:D2:219:ILE:HG22 | 4:q:198:ARG:HH22  | 1.82                     | 0.45              |
| 3:D5:96:GLY:N     | 3:D5:108:GLU:OE2  | 2.50                     | 0.45              |
| 3:E1:198:GLU:HB2  | 3:E1:266:PHE:CE2  | 2.47                     | 0.45              |
| 2:E4:271:SER:HB2  | 2:E4:377:MET:HB3  | 1.98                     | 0.45              |
| 3:E5:256:ASN:HD21 | 3:E5:350:LYS:CG   | 2.29                     | 0.45              |
| 3:E9:28:HIS:CE1   | 3:E9:241:ARG:HE   | 2.34                     | 0.45              |
| 2:F0:395:PHE:CD2  | 2:F0:422:ARG:HD2  | 2.51                     | 0.45              |
| 3:F1:170:PHE:HB3  | 3:F1:171:PRO:HD2  | 1.99                     | 0.45              |
| 4:h:111:ILE:HD13  | 4:h:132:LEU:HB2   | 1.98                     | 0.45              |
| 4:q:64:PRO:HD2    | 4:q:67:HIS:CE1    | 2.52                     | 0.45              |
| 1:19:256:LEU:H    | 1:19:256:LEU:HG   | 1.64                     | 0.45              |
| 1:4:240:PRO:HG2   | 4:g:154:TYR:CB    | 2.44                     | 0.45              |
| 3:A1:100:ASN:HB3  | 3:A1:103:LYS:HB2  | 1.98                     | 0.45              |
| 3:B1:91:VAL:HG21  | 3:B1:116:VAL:HG12 | 1.97                     | 0.45              |
| 2:B8:5:ILE:HG12   | 2:B8:132:LEU:HD11 | 1.98                     | 0.45              |
| 2:C0:276:ILE:HG23 | 2:C0:281:ALA:HB2  | 1.99                     | 0.45              |
| 3:C7:289:LEU:HD23 | 3:C7:289:LEU:HA   | 1.87                     | 0.45              |
| 3:C9:190:HIS:HB2  | 3:C9:414:ASN:HD21 | 1.82                     | 0.45              |
| 3:D3:164:MET:HE3  | 3:D3:164:MET:HB2  | 1.75                     | 0.45              |
| 2:D4:116:ASP:OD1  | 2:D4:116:ASP:N    | 2.49                     | 0.45              |
| 3:D5:113:ILE:HD12 | 3:D5:116:VAL:CG1  | 2.47                     | 0.45              |
| 2:D6:3:GLU:HA     | 2:D6:51:THR:HA    | 1.98                     | 0.45              |
| 2:D8:73:THR:HA    | 3:D9:46:ARG:HH12  | 1.82                     | 0.45              |
| 2:D8:388:PHE:HD1  | 2:D8:391:MET:HE2  | 1.82                     | 0.45              |
| 2:E0:195:LEU:HD13 | 2:E0:264:ARG:HH21 | 1.81                     | 0.45              |
| 3:E1:122:LYS:HD3  | 3:E1:122:LYS:HA   | 1.57                     | 0.45              |
| 3:E1:268:ILE:HD12 | 3:E1:368:VAL:HG22 | 1.98                     | 0.45              |
| 2:E4:23:LEU:HD11  | 2:E4:361:THR:HG23 | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E4:241:SER:OG   | 2:E4:250:VAL:O    | 2.33                     | 0.45              |
| 3:F1:198:GLU:OE2  | 3:F1:200:GLN:NE2  | 2.45                     | 0.45              |
| 4:e:5:VAL:HG23    | 4:e:8:SER:HB3     | 1.99                     | 0.45              |
| 4:f:56:LYS:HE2    | 4:f:56:LYS:HB2    | 1.71                     | 0.45              |
| 4:j:95:TYR:O      | 4:j:99:MET:HB2    | 2.17                     | 0.45              |
| 4:s:59:ASN:HD21   | 4:u:9:PRO:HA      | 1.82                     | 0.45              |
| 5:x:73:TYR:HB2    | 5:x:92:TRP:HE1    | 1.80                     | 0.45              |
| 2:A0:338:LYS:HE3  | 2:A0:338:LYS:HB3  | 1.73                     | 0.45              |
| 3:A5:135:ILE:HD12 | 3:A5:152:ILE:HG12 | 1.98                     | 0.45              |
| 2:A8:269:LEU:HD22 | 2:A8:303:ALA:HB3  | 1.99                     | 0.45              |
| 2:A8:304:LYS:HD2  | 2:A8:304:LYS:HA   | 1.75                     | 0.45              |
| 3:A9:202:ILE:HD13 | 3:A9:229:VAL:HG22 | 1.99                     | 0.45              |
| 3:A9:259:PRO:HB2  | 3:A9:260:PHE:CD1  | 2.52                     | 0.45              |
| 3:A9:313:ALA:HB3  | 3:A9:349:MET:HG2  | 1.99                     | 0.45              |
| 2:B0:2:ARG:HB2    | 2:B0:133:GLN:NE2  | 2.29                     | 0.45              |
| 2:B2:1:MET:N      | 2:B2:129:CYS:SG   | 2.76                     | 0.45              |
| 2:B4:158:SER:OG   | 2:B4:166:LYS:NZ   | 2.49                     | 0.45              |
| 2:B4:178:SER:OG   | 2:B4:179:THR:N    | 2.49                     | 0.45              |
| 2:B4:311:LYS:H    | 2:B4:382:THR:HG22 | 1.82                     | 0.45              |
| 2:B8:168:ASN:HD22 | 2:B8:198:THR:HG21 | 1.81                     | 0.45              |
| 3:C1:103:LYS:HA   | 3:C1:107:THR:HB   | 1.98                     | 0.45              |
| 2:C4:181:VAL:HG12 | 3:C5:256:ASN:CB   | 2.40                     | 0.45              |
| 2:C6:189:LEU:HD11 | 2:C6:413:MET:HE2  | 1.97                     | 0.45              |
| 2:C8:399:TYR:OH   | 2:C8:415:GLU:OE1  | 2.30                     | 0.45              |
| 3:C9:77:ARG:HH21  | 3:C9:92:PHE:HZ    | 1.63                     | 0.45              |
| 3:C9:174:LYS:HZ2  | 2:D0:329:ASN:CG   | 2.23                     | 0.45              |
| 3:D3:397:TRP:CH2  | 2:D4:260:VAL:O    | 2.69                     | 0.45              |
| 3:D5:4:ILE:HD11   | 3:D5:240:LEU:HD13 | 1.98                     | 0.45              |
| 3:D7:214:THR:OG1  | 3:D7:215:LEU:N    | 2.48                     | 0.45              |
| 2:D8:292:THR:HG21 | 2:D8:331:ALA:HB1  | 1.99                     | 0.45              |
| 2:E6:209:ILE:HG22 | 2:E6:227:LEU:HD22 | 1.98                     | 0.45              |
| 3:E7:49:VAL:HG11  | 3:E7:241:ARG:HG2  | 1.98                     | 0.45              |
| 4:h:19:GLU:HB3    | 4:h:40:PRO:CD     | 2.47                     | 0.45              |
| 5:l:162:ASN:HB3   | 5:l:164:TRP:HE1   | 1.82                     | 0.45              |
| 4:q:185:ILE:HD13  | 4:q:195:ALA:HB3   | 1.99                     | 0.45              |
| 1:0:247:TYR:CZ    | 2:A4:81:GLY:HA3   | 2.52                     | 0.45              |
| 1:3:257:PRO:HD3   | 2:B0:26:LEU:HD12  | 1.97                     | 0.45              |
| 2:A2:244:PHE:HD2  | 2:A2:358:GLN:HG2  | 1.82                     | 0.45              |
| 3:A5:200:GLN:HG3  | 3:A5:268:ILE:HD11 | 1.98                     | 0.45              |
| 2:A8:116:ASP:N    | 2:A8:116:ASP:OD1  | 2.47                     | 0.45              |
| 2:B0:82:THR:CG2   | 4:d:101:GLU:OE2   | 2.65                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B0:262:TYR:HB3  | 2:B0:263:PRO:HD2  | 1.98                     | 0.45              |
| 3:B5:336:LYS:HA   | 3:B5:336:LYS:CE   | 2.47                     | 0.45              |
| 2:B6:52:PHE:CD2   | 2:B6:243:ARG:HD3  | 2.52                     | 0.45              |
| 3:C1:137:HIS:ND1  | 3:C1:138:SER:O    | 2.38                     | 0.45              |
| 2:C2:346:TRP:HZ2  | 2:C2:435:VAL:HG13 | 1.82                     | 0.45              |
| 3:C9:299:MET:HE3  | 3:C9:305:PRO:HG3  | 1.98                     | 0.45              |
| 3:D3:267:LEU:HB3  | 3:D3:299:MET:HE2  | 1.99                     | 0.45              |
| 3:D5:138:SER:HA   | 3:D5:169:VAL:HG22 | 1.99                     | 0.45              |
| 3:E5:105:HIS:CD2  | 3:E5:150:LEU:HB2  | 2.51                     | 0.45              |
| 3:E9:167:PHE:CE1  | 3:E9:233:MET:HG2  | 2.52                     | 0.45              |
| 3:E9:349:MET:C    | 3:E9:350:LYS:HD2  | 2.42                     | 0.45              |
| 2:F0:195:LEU:HD21 | 2:F0:428:LEU:HD22 | 1.98                     | 0.45              |
| 5:l:128:ILE:HD12  | 5:l:129:PRO:HA    | 1.99                     | 0.45              |
| 4:n:171:ILE:HG22  | 4:n:182:PHE:HA    | 2.00                     | 0.45              |
| 4:p:28:LYS:HA     | 4:p:28:LYS:HD3    | 1.78                     | 0.45              |
| 4:v:119:ARG:NH1   | 4:v:137:GLU:OE1   | 2.50                     | 0.45              |
| 5:w:33:SER:OG     | 5:w:162:ASN:O     | 2.28                     | 0.45              |
| 5:x:17:GLN:NE2    | 5:x:20:ASN:OD1    | 2.50                     | 0.45              |
| 1:11:247:TYR:CG   | 2:D0:77:GLU:OE2   | 2.70                     | 0.44              |
| 1:18:255:PRO:HG2  | 2:E4:364:PRO:CG   | 2.47                     | 0.44              |
| 3:A9:173:PRO:HG2  | 3:A9:205:GLU:OE2  | 2.17                     | 0.44              |
| 3:B3:11:GLN:HE22  | 2:B4:248:LEU:HD12 | 1.82                     | 0.44              |
| 3:B3:171:PRO:HB3  | 3:B3:181:GLU:OE1  | 2.17                     | 0.44              |
| 2:C0:66:VAL:HG21  | 2:C0:122:ILE:HD11 | 1.99                     | 0.44              |
| 2:C0:320:ARG:NH2  | 2:C0:358:GLN:OE1  | 2.51                     | 0.44              |
| 2:C2:2:ARG:O      | 2:C2:2:ARG:HG2    | 2.16                     | 0.44              |
| 2:C2:432:TYR:O    | 2:C2:436:GLY:N    | 2.50                     | 0.44              |
| 3:C3:215:LEU:HD21 | 3:C3:273:LEU:HD22 | 1.98                     | 0.44              |
| 2:C4:390:ARG:O    | 2:C4:394:LYS:N    | 2.50                     | 0.44              |
| 3:C5:174:LYS:HZ1  | 2:C6:336:LYS:HB2  | 1.82                     | 0.44              |
| 2:C6:135:PHE:HB2  | 2:C6:166:LYS:HA   | 1.99                     | 0.44              |
| 2:C8:28:HIS:HE1   | 2:C8:243:ARG:HH11 | 1.63                     | 0.44              |
| 3:C9:226:ASN:HA   | 3:C9:229:VAL:HG22 | 1.98                     | 0.44              |
| 3:D1:173:PRO:HD2  | 3:D1:205:GLU:OE2  | 2.16                     | 0.44              |
| 3:D1:311:LEU:HD12 | 3:D1:311:LEU:HA   | 1.89                     | 0.44              |
| 2:D4:405:VAL:HG12 | 2:D4:409:VAL:HG23 | 2.00                     | 0.44              |
| 2:E0:96:LYS:NZ    | 3:E1:128:ASP:CG   | 2.75                     | 0.44              |
| 3:E3:7:VAL:HB     | 3:E3:135:ILE:HG13 | 1.99                     | 0.44              |
| 3:E5:246:LEU:HA   | 3:E5:246:LEU:HD12 | 1.88                     | 0.44              |
| 2:E8:210:TYR:HE2  | 3:E9:327:ASP:OD2  | 2.00                     | 0.44              |
| 4:e:71:LYS:HG3    | 4:g:39:PRO:HD3    | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:m:97:ARG:NH1    | 4:m:101:GLU:OE1   | 2.51                     | 0.44              |
| 4:r:77:PHE:HE2    | 4:r:171:ILE:HD12  | 1.82                     | 0.44              |
| 4:t:66:SER:HB3    | 4:v:23:LEU:HD13   | 1.99                     | 0.44              |
| 4:v:71:LYS:HZ1    | 4:v:106:GLN:HG3   | 1.83                     | 0.44              |
| 1:1:246:CYS:SG    | 1:1:247:TYR:N     | 2.91                     | 0.44              |
| 1:21:251:TYR:HE1  | 2:F0:225:THR:HG1  | 1.63                     | 0.44              |
| 2:A6:250:VAL:HB   | 2:A6:318:MET:HE1  | 1.99                     | 0.44              |
| 2:A8:11:GLN:HE22  | 3:A9:246:LEU:HA   | 1.82                     | 0.44              |
| 3:A9:225:LEU:HD21 | 2:B0:326:LYS:NZ   | 2.32                     | 0.44              |
| 3:B1:149:THR:OG1  | 3:B1:191:GLN:OE1  | 2.22                     | 0.44              |
| 3:B1:230:SER:HA   | 3:B1:233:MET:HG2  | 1.99                     | 0.44              |
| 2:B8:70:LEU:HD12  | 2:B8:99:ALA:HB2   | 1.99                     | 0.44              |
| 3:C1:262:ARG:HA   | 3:C1:262:ARG:HD2  | 1.74                     | 0.44              |
| 2:C6:172:TRP:HB3  | 2:C6:205:ASP:OD1  | 2.17                     | 0.44              |
| 2:C6:188:VAL:HG13 | 2:C6:425:LEU:HD23 | 1.98                     | 0.44              |
| 3:D1:53:GLU:OE2   | 3:D1:54:ALA:N     | 2.50                     | 0.44              |
| 2:D8:319:TYR:CE2  | 2:D8:375:VAL:HG22 | 2.52                     | 0.44              |
| 2:E0:210:TYR:CD2  | 3:E1:324:LYS:HG3  | 2.52                     | 0.44              |
| 2:E4:84:ARG:NH1   | 4:u:197:LEU:HD11  | 2.32                     | 0.44              |
| 3:E7:246:LEU:HD12 | 3:E7:246:LEU:HA   | 1.89                     | 0.44              |
| 3:E9:293:MET:HE3  | 3:E9:365:VAL:HG13 | 1.99                     | 0.44              |
| 2:F0:107:HIS:NE2  | 2:F0:151:CYS:SG   | 2.84                     | 0.44              |
| 4:d:67:HIS:O      | 4:d:71:LYS:NZ     | 2.48                     | 0.44              |
| 5:l:51:PRO:HA     | 5:l:54:ARG:HG2    | 1.99                     | 0.44              |
| 4:v:78:ALA:HB3    | 4:v:112:PHE:HE1   | 1.81                     | 0.44              |
| 1:1:256:LEU:HA    | 1:1:257:PRO:HD3   | 1.87                     | 0.44              |
| 1:3:254:LYS:HB3   | 1:3:255:PRO:HD2   | 1.98                     | 0.44              |
| 3:A7:44:LEU:HD12  | 3:A7:47:ILE:HD12  | 2.00                     | 0.44              |
| 2:B4:6:SER:OG     | 2:B4:8:HIS:NE2    | 2.48                     | 0.44              |
| 2:B4:141:VAL:O    | 2:B4:147:SER:OG   | 2.36                     | 0.44              |
| 3:C1:295:ASP:HB3  | 3:C1:297:LYS:HG2  | 2.00                     | 0.44              |
| 2:C2:282:TYR:CE2  | 5:l:160:ARG:CZ    | 3.01                     | 0.44              |
| 2:C6:1:MET:HA     | 2:C6:129:CYS:HB3  | 2.00                     | 0.44              |
| 2:C8:34:GLY:O     | 2:C8:61:HIS:N     | 2.45                     | 0.44              |
| 2:D6:183:GLU:HA   | 2:D6:186:ASN:HD22 | 1.82                     | 0.44              |
| 3:E5:209:ASP:CG   | 3:E5:213:ARG:HH21 | 2.26                     | 0.44              |
| 3:E5:281:TYR:CD2  | 3:E9:87:PRO:CD    | 2.97                     | 0.44              |
| 3:F1:237:THR:O    | 3:F1:241:ARG:NH1  | 2.50                     | 0.44              |
| 1:11:240:PRO:HB2  | 4:p:154:TYR:HB3   | 1.95                     | 0.44              |
| 1:21:241:PHE:CZ   | 3:F1:356:ILE:HG23 | 2.35                     | 0.44              |
| 2:A0:228:ASN:HA   | 2:A0:231:ILE:HG22 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A0:332:VAL:HG13 | 2:A0:351:PHE:HD2  | 1.82                     | 0.44              |
| 2:A2:292:THR:HG21 | 2:A2:331:ALA:HB1  | 1.99                     | 0.44              |
| 3:B3:63:ALA:O     | 3:B3:89:ASN:ND2   | 2.51                     | 0.44              |
| 3:B5:150:LEU:HD23 | 3:B5:154:LYS:HD2  | 1.99                     | 0.44              |
| 3:C1:149:THR:O    | 3:C1:191:GLN:NE2  | 2.50                     | 0.44              |
| 2:C2:277:SER:OG   | 2:C2:278:ALA:N    | 2.51                     | 0.44              |
| 2:C2:288:VAL:HA   | 2:C2:291:ILE:HG12 | 2.00                     | 0.44              |
| 2:C4:319:TYR:HB3  | 2:C4:323:VAL:HG21 | 1.99                     | 0.44              |
| 3:C5:100:ASN:HB3  | 3:C5:103:LYS:HG2  | 1.99                     | 0.44              |
| 3:C5:293:MET:HE2  | 3:C5:293:MET:HB2  | 1.65                     | 0.44              |
| 2:D4:69:ASP:OD1   | 2:D4:70:LEU:N     | 2.51                     | 0.44              |
| 2:D6:98:ASP:OD1   | 2:D6:99:ALA:N     | 2.50                     | 0.44              |
| 3:D9:8:GLN:NE2    | 3:D9:17:GLY:HA3   | 2.32                     | 0.44              |
| 3:E1:163:ILE:HD12 | 3:E1:250:LEU:HB2  | 1.98                     | 0.44              |
| 3:E5:173:PRO:HB3  | 3:E5:380:ARG:CZ   | 2.47                     | 0.44              |
| 3:E7:66:MET:HB3   | 3:E7:147:MET:HE1  | 1.99                     | 0.44              |
| 4:e:48:ILE:HG13   | 4:e:48:ILE:O      | 2.16                     | 0.44              |
| 3:A1:73:MET:HA    | 3:A1:76:VAL:HG12  | 1.99                     | 0.44              |
| 3:A7:404:ASP:OD1  | 3:A7:405:GLU:N    | 2.51                     | 0.44              |
| 3:B5:67:ASP:OD1   | 3:B5:68:LEU:N     | 2.49                     | 0.44              |
| 3:B9:67:ASP:OD1   | 3:B9:68:LEU:N     | 2.51                     | 0.44              |
| 3:C5:167:PHE:CE2  | 3:C5:233:MET:HG2  | 2.53                     | 0.44              |
| 3:C5:187:LEU:HD11 | 3:C5:408:PHE:CZ   | 2.52                     | 0.44              |
| 3:C5:295:ASP:HB3  | 3:C5:298:ASN:HB2  | 2.00                     | 0.44              |
| 3:D1:281:TYR:OH   | 3:D5:83:GLN:HB3   | 2.18                     | 0.44              |
| 3:D7:112:LEU:HD12 | 3:D7:112:LEU:HA   | 1.79                     | 0.44              |
| 2:D8:231:ILE:O    | 2:D8:235:ILE:HG12 | 2.17                     | 0.44              |
| 3:D9:263:LEU:HD12 | 3:D9:370:ASN:HD21 | 1.82                     | 0.44              |
| 3:E3:336:LYS:HE2  | 3:E3:336:LYS:HA   | 1.99                     | 0.44              |
| 3:E5:257:LEU:HD21 | 3:E5:314:SER:HB2  | 1.99                     | 0.44              |
| 2:E6:369:ALA:CB   | 5:x:158:ASP:OD2   | 2.66                     | 0.44              |
| 2:E6:417:GLU:HA   | 2:E6:420:GLU:HG3  | 2.00                     | 0.44              |
| 3:E9:198:GLU:HG3  | 3:E9:266:PHE:CE2  | 2.53                     | 0.44              |
| 2:F0:339:ARG:O    | 2:F0:342:GLN:NE2  | 2.50                     | 0.44              |
| 5:l:34:VAL:HG23   | 5:l:70:GLU:HB3    | 1.98                     | 0.44              |
| 4:q:170:VAL:HG23  | 4:q:183:LEU:HB2   | 1.99                     | 0.44              |
| 5:w:68:VAL:HB     | 5:w:159:TYR:CE2   | 2.53                     | 0.44              |
| 5:w:73:TYR:CG     | 5:w:90:MET:HE1    | 2.53                     | 0.44              |
| 2:A0:240:ALA:HA   | 2:A0:243:ARG:HE   | 1.82                     | 0.44              |
| 2:A0:290:GLU:HB3  | 2:A4:124:LYS:HZ1  | 1.82                     | 0.44              |
| 2:A0:343:PHE:HZ   | 2:A0:351:PHE:CE1  | 2.35                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A2:103:PHE:CD2  | 2:A2:413:MET:HE1  | 2.53                     | 0.44              |
| 2:A2:133:GLN:NE2  | 2:A2:251:ASP:HB3  | 2.33                     | 0.44              |
| 3:A9:208:TYR:CD1  | 2:B0:326:LYS:HE3  | 2.53                     | 0.44              |
| 2:B4:10:GLY:HA2   | 2:B4:145:THR:HG23 | 1.99                     | 0.44              |
| 3:B5:279:GLN:O    | 3:B5:279:GLN:HG2  | 2.17                     | 0.44              |
| 3:B5:383:ASP:HA   | 3:B5:386:THR:HG22 | 1.99                     | 0.44              |
| 2:C2:296:PHE:HD1  | 2:C2:377:MET:HE2  | 1.82                     | 0.44              |
| 2:C2:404:PHE:CE1  | 3:C3:259:PRO:HG3  | 2.52                     | 0.44              |
| 3:C3:42:LEU:HD21  | 3:C3:356:ILE:HG13 | 2.00                     | 0.44              |
| 2:C4:135:PHE:HB2  | 2:C4:166:LYS:HA   | 2.00                     | 0.44              |
| 3:C7:318:ARG:C    | 3:C7:321:MET:HE1  | 2.42                     | 0.44              |
| 2:C8:191:THR:HG21 | 2:C8:425:LEU:HD13 | 2.00                     | 0.44              |
| 2:D0:285:GLN:HB3  | 2:D4:56:THR:CB    | 2.47                     | 0.44              |
| 2:D0:319:TYR:N    | 2:D0:354:GLY:O    | 2.47                     | 0.44              |
| 2:D4:425:LEU:HD12 | 2:D4:425:LEU:HA   | 1.85                     | 0.44              |
| 3:D5:54:ALA:C     | 3:D5:56:GLY:H     | 2.26                     | 0.44              |
| 3:D5:276:ARG:HH21 | 3:D5:279:GLN:HG3  | 1.82                     | 0.44              |
| 2:E0:166:LYS:N    | 2:E0:199:ASP:OD2  | 2.51                     | 0.44              |
| 3:E1:272:PRO:HG3  | 3:E1:284:LEU:HD11 | 2.00                     | 0.44              |
| 2:E6:195:LEU:HD21 | 2:E6:428:LEU:HD22 | 1.99                     | 0.44              |
| 2:E8:269:LEU:CD2  | 2:E8:384:ILE:HD11 | 2.47                     | 0.44              |
| 2:F0:8:HIS:CD2    | 2:F0:17:GLY:HA3   | 2.52                     | 0.44              |
| 2:F0:213:CYS:HA   | 2:F0:217:LEU:HB2  | 1.99                     | 0.44              |
| 4:c:194:ARG:NE    | 4:c:194:ARG:HA    | 2.31                     | 0.44              |
| 4:f:75:LEU:O      | 4:f:170:VAL:HA    | 2.17                     | 0.44              |
| 4:i:175:SER:HA    | 4:i:206:PHE:HE1   | 1.81                     | 0.44              |
| 4:n:142:GLU:HA    | 4:n:145:LYS:HE3   | 2.00                     | 0.44              |
| 4:q:88:LEU:HD22   | 4:q:185:ILE:HG21  | 1.99                     | 0.44              |
| 4:t:101:GLU:OE2   | 4:v:6:PHE:CA      | 2.65                     | 0.44              |
| 3:A1:291:GLN:CB   | 3:A5:122:LYS:HE3  | 2.48                     | 0.44              |
| 2:A4:11:GLN:HG3   | 2:A4:74:VAL:HG21  | 1.99                     | 0.44              |
| 2:B0:173:PRO:HG3  | 2:B0:187:SER:OG   | 2.18                     | 0.44              |
| 3:B5:8:GLN:OE1    | 3:B5:17:GLY:HA3   | 2.18                     | 0.44              |
| 3:B5:68:LEU:HG    | 3:B5:147:MET:HE2  | 1.99                     | 0.44              |
| 2:C2:23:LEU:HD13  | 2:C2:363:VAL:HG13 | 1.99                     | 0.44              |
| 3:C3:49:VAL:HG11  | 3:C3:241:ARG:HG2  | 2.00                     | 0.44              |
| 2:C4:204:LEU:HD13 | 2:C4:231:ILE:HD12 | 2.00                     | 0.44              |
| 2:C6:7:ILE:HG21   | 2:C6:153:LEU:CD2  | 2.47                     | 0.44              |
| 3:C9:397:TRP:NE1  | 2:D0:257:THR:HA   | 2.32                     | 0.44              |
| 2:D0:132:LEU:HB3  | 2:D0:164:LYS:NZ   | 2.32                     | 0.44              |
| 3:D1:189:VAL:HG11 | 3:D1:415:MET:HE2  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D1:334:GLN:HE22 | 3:D1:347:ASN:HA   | 1.82                     | 0.44              |
| 2:D4:172:TRP:HE1  | 2:D4:391:MET:CE   | 2.31                     | 0.44              |
| 3:D5:117:LEU:O    | 3:D5:121:ARG:HG2  | 2.18                     | 0.44              |
| 2:D6:20:CYS:SG    | 2:D6:235:ILE:HG21 | 2.57                     | 0.44              |
| 3:D7:167:PHE:CE1  | 3:D7:233:MET:HG2  | 2.53                     | 0.44              |
| 3:E3:147:MET:HE3  | 3:E3:147:MET:HB3  | 1.89                     | 0.44              |
| 2:E4:223:THR:CG2  | 2:E4:225:THR:HG22 | 2.43                     | 0.44              |
| 3:E5:3:GLU:HA     | 3:E5:49:VAL:HA    | 2.00                     | 0.44              |
| 3:E5:49:VAL:HG11  | 3:E5:241:ARG:HG2  | 1.99                     | 0.44              |
| 3:E5:136:THR:HG22 | 3:E5:167:PHE:HB2  | 1.99                     | 0.44              |
| 3:E5:156:ARG:HA   | 3:E5:156:ARG:HD2  | 1.82                     | 0.44              |
| 2:E6:27:GLU:OE2   | 2:E6:320:ARG:NH2  | 2.51                     | 0.44              |
| 4:d:158:THR:OG1   | 4:d:161:TYR:HB2   | 2.18                     | 0.44              |
| 4:g:42:TYR:HA     | 4:g:45:MET:HG3    | 1.99                     | 0.44              |
| 4:i:113:VAL:HG12  | 4:i:145:LYS:HZ3   | 1.82                     | 0.44              |
| 3:A1:219:THR:CG2  | 2:A2:326:LYS:HZ1  | 2.31                     | 0.44              |
| 3:A1:289:LEU:HD21 | 3:A1:365:VAL:CG1  | 2.47                     | 0.44              |
| 3:A3:316:MET:HE2  | 3:A3:366:THR:HG23 | 2.00                     | 0.44              |
| 2:A4:107:HIS:HB3  | 2:A4:108:TYR:HD1  | 1.82                     | 0.44              |
| 3:A5:77:ARG:HG3   | 3:A5:90:PHE:HE2   | 1.81                     | 0.44              |
| 3:A7:178:THR:O    | 3:A7:181:GLU:HG2  | 2.18                     | 0.44              |
| 2:B0:306:ASP:HB3  | 2:B0:309:HIS:CE1  | 2.53                     | 0.44              |
| 3:B1:63:ALA:O     | 3:B1:89:ASN:ND2   | 2.51                     | 0.44              |
| 2:C0:71:GLU:HB3   | 2:C0:98:ASP:HB3   | 2.00                     | 0.44              |
| 2:C0:224:TYR:HA   | 2:C0:227:LEU:HD12 | 2.00                     | 0.44              |
| 3:C3:73:MET:HB3   | 3:C3:77:ARG:NH2   | 2.33                     | 0.44              |
| 3:C5:327:ASP:OD1  | 3:C5:327:ASP:N    | 2.47                     | 0.44              |
| 3:D1:152:ILE:CD1  | 3:D1:166:THR:HG21 | 2.47                     | 0.44              |
| 3:D3:7:VAL:HG11   | 3:D3:151:LEU:CD2  | 2.47                     | 0.44              |
| 3:D3:257:LEU:O    | 3:D3:312:THR:OG1  | 2.36                     | 0.44              |
| 2:D4:33:ASP:OD2   | 4:p:107:LYS:NZ    | 2.48                     | 0.44              |
| 2:D4:96:LYS:HZ3   | 3:D5:129:CYS:HB2  | 1.83                     | 0.44              |
| 3:D7:289:LEU:HD23 | 3:D7:289:LEU:HA   | 1.91                     | 0.44              |
| 3:D7:324:LYS:HE2  | 3:D7:324:LYS:HB2  | 1.60                     | 0.44              |
| 2:E0:311:LYS:NZ   | 2:E0:342:GLN:OE1  | 2.45                     | 0.44              |
| 2:E0:352:LYS:HD3  | 2:E0:352:LYS:HA   | 1.74                     | 0.44              |
| 3:E1:273:LEU:H    | 3:E1:292:GLN:HE22 | 1.65                     | 0.44              |
| 3:E1:398:TYR:HB3  | 3:E1:408:PHE:HZ   | 1.82                     | 0.44              |
| 2:E2:269:LEU:HD13 | 2:E2:301:MET:HE2  | 1.99                     | 0.44              |
| 2:E4:132:LEU:O    | 2:E4:164:LYS:NZ   | 2.51                     | 0.44              |
| 3:E5:379:LYS:O    | 3:E5:383:ASP:N    | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E8:53:PHE:HB3   | 2:E8:61:HIS:HB3   | 1.99                     | 0.44              |
| 2:E8:296:PHE:HZ   | 2:E8:317:LEU:HD21 | 1.83                     | 0.44              |
| 3:E9:382:SER:HA   | 3:E9:415:MET:HE1  | 1.99                     | 0.44              |
| 4:f:196:LEU:HD23  | 4:f:196:LEU:HA    | 1.74                     | 0.44              |
| 4:g:184:PRO:HB2   | 4:g:189:LEU:HB2   | 1.99                     | 0.44              |
| 4:o:9:PRO:HA      | 4:o:12:VAL:HG12   | 2.00                     | 0.44              |
| 4:u:142:GLU:OE2   | 4:u:146:ARG:NH2   | 2.48                     | 0.44              |
| 5:x:109:TYR:O     | 5:x:110:ARG:CB    | 2.66                     | 0.44              |
| 1:2:256:LEU:CD1   | 2:A8:31:GLN:HG3   | 2.48                     | 0.44              |
| 1:6:256:LEU:CD2   | 2:B6:31:GLN:HA    | 2.28                     | 0.44              |
| 1:6:257:PRO:HG2   | 2:B6:26:LEU:O     | 2.18                     | 0.44              |
| 2:A2:241:SER:HB3  | 2:A2:249:ASN:HB3  | 2.00                     | 0.44              |
| 2:A4:98:ASP:O     | 2:A4:105:ARG:NH1  | 2.49                     | 0.44              |
| 2:A4:124:LYS:HA   | 2:A4:124:LYS:HD2  | 1.80                     | 0.44              |
| 3:A5:167:PHE:CE2  | 3:A5:233:MET:HG2  | 2.53                     | 0.44              |
| 3:A5:217:LEU:HD23 | 3:A5:220:PRO:HG3  | 2.00                     | 0.44              |
| 2:B0:10:GLY:O     | 2:B0:14:ILE:HG12  | 2.18                     | 0.44              |
| 2:C0:403:ALA:HA   | 3:C1:260:PHE:HE1  | 1.83                     | 0.44              |
| 3:C1:318:ARG:HD3  | 3:C1:358:PRO:HD3  | 2.00                     | 0.44              |
| 2:C2:70:LEU:HD12  | 2:C2:99:ALA:HB2   | 1.99                     | 0.44              |
| 3:C7:200:GLN:HB3  | 3:C7:266:PHE:HB2  | 1.99                     | 0.44              |
| 2:C8:304:LYS:O    | 2:C8:304:LYS:HD3  | 2.18                     | 0.44              |
| 3:D1:117:LEU:HA   | 3:D1:120:VAL:HG12 | 2.00                     | 0.44              |
| 3:D5:208:TYR:O    | 3:D5:212:PHE:HB3  | 2.17                     | 0.44              |
| 2:E0:132:LEU:HB3  | 2:E0:164:LYS:NZ   | 2.33                     | 0.44              |
| 2:E2:204:LEU:HD21 | 2:E2:231:ILE:HD12 | 1.99                     | 0.44              |
| 3:E5:293:MET:HE3  | 3:E5:293:MET:HB3  | 1.73                     | 0.44              |
| 3:E7:208:TYR:CE1  | 3:E7:225:LEU:HD11 | 2.52                     | 0.44              |
| 3:E9:175:VAL:HG23 | 2:F0:332:VAL:CG1  | 2.47                     | 0.44              |
| 4:f:110:ILE:HB    | 4:f:131:TRP:CG    | 2.53                     | 0.44              |
| 4:u:7:ALA:N       | 4:u:161:TYR:OH    | 2.50                     | 0.44              |
| 4:u:187:SER:OG    | 4:u:188:GLY:N     | 2.51                     | 0.44              |
| 5:w:35:ALA:HB2    | 5:w:133:VAL:HG12  | 2.00                     | 0.44              |
| 3:A1:107:THR:HG21 | 3:A1:401:GLU:HG2  | 1.99                     | 0.43              |
| 3:A3:297:LYS:NZ   | 3:A3:306:ARG:HH22 | 2.16                     | 0.43              |
| 3:A3:349:MET:HE3  | 3:A3:349:MET:HB2  | 1.65                     | 0.43              |
| 2:A8:262:TYR:CB   | 2:A8:263:PRO:HD2  | 2.44                     | 0.43              |
| 2:A8:282:TYR:HD2  | 2:A8:283:HIS:CE1  | 2.36                     | 0.43              |
| 3:B5:13:GLY:HA2   | 3:B5:16:ILE:HG22  | 2.00                     | 0.43              |
| 3:B5:287:PRO:HA   | 3:B5:290:THR:HG22 | 2.00                     | 0.43              |
| 3:C1:295:ASP:CB   | 3:C1:297:LYS:HG2  | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C1:330:MET:HB3  | 3:C1:349:MET:HG2  | 2.00                     | 0.43              |
| 3:C3:12:CYS:HB3   | 3:C3:138:SER:HB2  | 2.00                     | 0.43              |
| 3:C3:136:THR:HG23 | 3:C3:167:PHE:HB2  | 1.99                     | 0.43              |
| 2:C4:178:SER:HB3  | 3:C5:347:ASN:CG   | 2.43                     | 0.43              |
| 2:C6:119:LEU:HD21 | 2:C6:156:ARG:HB3  | 2.00                     | 0.43              |
| 2:C8:241:SER:HB2  | 2:C8:249:ASN:HB2  | 1.99                     | 0.43              |
| 2:D2:276:ILE:HD11 | 2:D2:286:LEU:HD11 | 1.99                     | 0.43              |
| 3:D5:200:GLN:HB3  | 3:D5:268:ILE:HD11 | 2.00                     | 0.43              |
| 2:D6:126:ALA:HB1  | 2:D6:132:LEU:HD22 | 1.99                     | 0.43              |
| 3:D9:6:HIS:HD2    | 3:D9:134:GLN:NE2  | 2.16                     | 0.43              |
| 3:D9:107:THR:HG1  | 3:D9:108:GLU:CD   | 2.26                     | 0.43              |
| 2:E2:262:TYR:HD2  | 2:E2:265:ILE:HD12 | 1.83                     | 0.43              |
| 2:E2:268:MET:HE2  | 2:E2:268:MET:HB3  | 1.80                     | 0.43              |
| 3:E7:113:ILE:HA   | 3:E7:116:VAL:HG12 | 2.00                     | 0.43              |
| 3:E7:282:ARG:O    | 3:F1:55:THR:HG23  | 2.18                     | 0.43              |
| 3:F1:30:ILE:HD12  | 3:F1:51:TYR:CE2   | 2.53                     | 0.43              |
| 3:F1:33:THR:O     | 3:F1:58:ARG:NH2   | 2.51                     | 0.43              |
| 4:c:129:MET:HE3   | 4:c:131:TRP:HE1   | 1.83                     | 0.43              |
| 4:d:23:LEU:HD11   | 4:d:38:LEU:HD12   | 1.99                     | 0.43              |
| 5:k:74:VAL:HG21   | 5:k:105:LEU:HD22  | 1.99                     | 0.43              |
| 4:r:94:ASN:O      | 4:r:97:ARG:HB3    | 2.17                     | 0.43              |
| 4:r:97:ARG:NH2    | 4:t:161:TYR:CD1   | 2.86                     | 0.43              |
| 5:w:45:LYS:HE2    | 5:w:45:LYS:HA     | 2.00                     | 0.43              |
| 1:21:245:SER:OG   | 3:F1:355:ASP:OD2  | 2.24                     | 0.43              |
| 2:A0:306:ASP:HB3  | 2:A0:309:HIS:CE1  | 2.53                     | 0.43              |
| 2:A0:334:THR:O    | 2:A0:337:THR:OG1  | 2.34                     | 0.43              |
| 2:A8:298:PRO:HB3  | 2:A8:307:PRO:HD2  | 2.00                     | 0.43              |
| 3:B1:190:HIS:HB2  | 3:B1:414:ASN:HD22 | 1.83                     | 0.43              |
| 3:B3:93:GLY:CA    | 3:B3:112:LEU:HD21 | 2.45                     | 0.43              |
| 2:B4:208:ALA:HB2  | 2:B4:304:LYS:HB2  | 1.99                     | 0.43              |
| 3:B5:57:GLY:HA3   | 4:f:83:PRO:CG     | 2.46                     | 0.43              |
| 2:B8:262:TYR:HB2  | 2:B8:265:ILE:HD12 | 1.99                     | 0.43              |
| 2:C0:256:GLN:O    | 2:C0:260:VAL:HG22 | 2.18                     | 0.43              |
| 2:C0:336:LYS:HG3  | 2:C0:351:PHE:HE1  | 1.83                     | 0.43              |
| 3:C7:68:LEU:HA    | 3:C7:93:GLY:HA3   | 1.99                     | 0.43              |
| 2:D0:137:MET:HE1  | 2:D0:154:LEU:CD1  | 2.47                     | 0.43              |
| 2:E0:329:ASN:HA   | 2:E0:332:VAL:HG12 | 1.99                     | 0.43              |
| 2:E4:277:SER:HB3  | 2:E4:280:LYS:HB2  | 2.00                     | 0.43              |
| 2:F0:65:CYS:O     | 2:F0:91:GLN:HG3   | 2.18                     | 0.43              |
| 4:m:80:GLY:N      | 4:m:116:ASP:OD1   | 2.39                     | 0.43              |
| 4:t:146:ARG:HG3   | 4:t:146:ARG:NH1   | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:21:241:PHE:CZ   | 3:F1:356:ILE:CG2  | 2.97                     | 0.43              |
| 1:8:241:PHE:HZ    | 3:C1:356:ILE:CD1  | 2.09                     | 0.43              |
| 3:A1:311:LEU:HD12 | 3:A1:311:LEU:HA   | 1.93                     | 0.43              |
| 3:A1:379:LYS:HB2  | 3:A1:379:LYS:HZ3  | 1.76                     | 0.43              |
| 2:A2:205:ASP:OD1  | 2:A2:206:ASN:N    | 2.51                     | 0.43              |
| 3:A3:152:ILE:HD12 | 3:A3:164:MET:HE1  | 2.00                     | 0.43              |
| 3:A3:252:LYS:O    | 3:A3:256:ASN:ND2  | 2.52                     | 0.43              |
| 3:B1:156:ARG:HH21 | 3:B1:164:MET:HB2  | 1.84                     | 0.43              |
| 2:B6:326:LYS:HD2  | 2:B6:326:LYS:HA   | 1.56                     | 0.43              |
| 3:B7:10:GLY:HA2   | 3:B7:143:THR:HG23 | 2.00                     | 0.43              |
| 2:B8:391:MET:O    | 2:B8:395:PHE:N    | 2.50                     | 0.43              |
| 2:C0:121:ARG:HD2  | 2:C0:121:ARG:HA   | 1.67                     | 0.43              |
| 3:C1:172:SER:HB3  | 3:C1:176:SER:HB3  | 1.98                     | 0.43              |
| 3:C1:392:LYS:HA   | 3:C1:395:LEU:HD23 | 2.00                     | 0.43              |
| 3:C5:220:PRO:HB2  | 3:C5:225:LEU:CD2  | 2.49                     | 0.43              |
| 2:C8:28:HIS:NE2   | 2:C8:243:ARG:HD2  | 2.33                     | 0.43              |
| 3:C9:263:LEU:O    | 3:C9:263:LEU:HD12 | 2.17                     | 0.43              |
| 3:D1:57:GLY:CA    | 4:n:83:PRO:HB2    | 2.34                     | 0.43              |
| 2:D2:407:TRP:CD2  | 3:D3:255:VAL:HG22 | 2.54                     | 0.43              |
| 3:D7:289:LEU:HD22 | 3:D7:365:VAL:HG12 | 2.01                     | 0.43              |
| 2:E0:96:LYS:CE    | 3:E1:128:ASP:HB2  | 2.44                     | 0.43              |
| 3:E3:33:THR:HG23  | 3:E3:35:THR:HG23  | 1.98                     | 0.43              |
| 3:E5:20:PHE:HA    | 3:E5:230:SER:OG   | 2.19                     | 0.43              |
| 2:E6:115:VAL:HG12 | 2:E6:156:ARG:HE   | 1.82                     | 0.43              |
| 3:E9:105:HIS:HB3  | 3:E9:106:TYR:CD1  | 2.53                     | 0.43              |
| 2:F0:254:GLU:OE1  | 2:F0:352:LYS:NZ   | 2.40                     | 0.43              |
| 4:b:67:HIS:ND1    | 4:d:19:GLU:OE1    | 2.51                     | 0.43              |
| 4:e:71:LYS:CG     | 4:g:39:PRO:HD3    | 2.48                     | 0.43              |
| 4:m:10:LEU:HG     | 4:m:143:ILE:CG2   | 2.48                     | 0.43              |
| 5:w:15:ARG:HH12   | 5:w:91:PRO:C      | 2.24                     | 0.43              |
| 1:20:256:LEU:HD11 | 2:E8:31:GLN:CG    | 2.37                     | 0.43              |
| 1:21:256:LEU:HD21 | 2:F0:31:GLN:CA    | 2.49                     | 0.43              |
| 1:6:239:LEU:HD13  | 1:6:240:PRO:HD2   | 1.99                     | 0.43              |
| 2:A0:71:GLU:HB3   | 2:A0:98:ASP:HB2   | 2.00                     | 0.43              |
| 3:A1:72:THR:HG23  | 3:A1:73:MET:SD    | 2.58                     | 0.43              |
| 3:B1:103:LYS:HB2  | 3:B1:108:GLU:OE1  | 2.18                     | 0.43              |
| 2:B8:282:TYR:CE2  | 2:C2:85:HIS:CG    | 2.96                     | 0.43              |
| 3:B9:256:ASN:HD22 | 3:B9:350:LYS:HD2  | 1.84                     | 0.43              |
| 2:C0:265:ILE:HG13 | 2:C0:432:TYR:CZ   | 2.54                     | 0.43              |
| 3:C3:20:PHE:CD2   | 3:C3:233:MET:HE3  | 2.49                     | 0.43              |
| 2:C6:212:ILE:HD13 | 2:C6:215:ARG:HH22 | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D0:174:SER:HB3  | 2:D0:205:ASP:OD1  | 2.19                     | 0.43              |
| 2:D2:180:ALA:HB1  | 3:D3:256:ASN:ND2  | 2.33                     | 0.43              |
| 2:D2:425:LEU:HD12 | 2:D2:425:LEU:HA   | 1.92                     | 0.43              |
| 3:D7:378:PHE:HD1  | 3:D7:415:MET:HE3  | 1.83                     | 0.43              |
| 3:D9:283:ALA:HA   | 3:E3:55:THR:HB    | 2.00                     | 0.43              |
| 2:E0:64:ARG:HB3   | 2:E0:125:LEU:HD21 | 1.99                     | 0.43              |
| 2:E2:265:ILE:HG23 | 2:E2:432:TYR:HE1  | 1.83                     | 0.43              |
| 2:E4:238:LEU:HD13 | 2:E4:318:MET:HE3  | 2.00                     | 0.43              |
| 3:E7:349:MET:HB2  | 3:E7:349:MET:HE2  | 1.77                     | 0.43              |
| 2:E8:2:ARG:NE     | 2:E8:133:GLN:HE21 | 2.15                     | 0.43              |
| 2:E8:306:ASP:N    | 2:E8:386:GLU:OE2  | 2.51                     | 0.43              |
| 4:h:73:VAL:HG12   | 4:h:206:PHE:HB2   | 2.01                     | 0.43              |
| 5:k:27:ASP:HB2    | 4:m:23:LEU:HD11   | 2.01                     | 0.43              |
| 1:l:254:LYS:HB3   | 2:A6:364:PRO:CB   | 2.41                     | 0.43              |
| 2:A0:222:PRO:CD   | 3:A1:324:LYS:HB3  | 2.48                     | 0.43              |
| 2:A0:290:GLU:CB   | 2:A4:124:LYS:CE   | 2.97                     | 0.43              |
| 2:A0:356:ASN:OD1  | 2:A0:357:TYR:N    | 2.52                     | 0.43              |
| 2:A4:407:TRP:HH2  | 3:A5:258:ILE:HB   | 1.83                     | 0.43              |
| 3:A5:317:PHE:CE1  | 3:A5:365:VAL:HG22 | 2.53                     | 0.43              |
| 3:A9:208:TYR:HD1  | 2:B0:326:LYS:HE3  | 1.83                     | 0.43              |
| 3:A9:220:PRO:HD2  | 2:B0:326:LYS:CG   | 2.49                     | 0.43              |
| 3:C3:222:TYR:HA   | 3:C3:225:LEU:HB2  | 1.99                     | 0.43              |
| 2:C4:298:PRO:HA   | 2:C4:301:MET:HE1  | 2.00                     | 0.43              |
| 2:C6:66:VAL:HG12  | 2:C6:91:GLN:HB2   | 2.00                     | 0.43              |
| 2:C6:210:TYR:CD1  | 2:C6:222:PRO:HG2  | 2.53                     | 0.43              |
| 2:C6:334:THR:O    | 2:C6:337:THR:OG1  | 2.35                     | 0.43              |
| 3:D7:139:LEU:HD22 | 3:D7:188:SER:HB2  | 2.01                     | 0.43              |
| 3:E1:284:LEU:HD23 | 3:E1:362:LYS:HG2  | 2.01                     | 0.43              |
| 2:E4:64:ARG:HB3   | 2:E4:125:LEU:HD21 | 2.00                     | 0.43              |
| 3:E9:151:LEU:O    | 3:E9:155:VAL:HG12 | 2.19                     | 0.43              |
| 3:F1:13:GLY:HA2   | 3:F1:16:ILE:HG22  | 2.00                     | 0.43              |
| 4:f:18:ASN:HD22   | 4:f:45:MET:HA     | 1.82                     | 0.43              |
| 4:f:65:GLN:HE21   | 4:f:206:PHE:HZ    | 1.66                     | 0.43              |
| 4:r:63:ILE:O      | 4:r:63:ILE:HG13   | 2.17                     | 0.43              |
| 1:7:253:ALA:HA    | 2:B8:32:PRO:HG2   | 2.00                     | 0.43              |
| 2:A0:182:VAL:HG22 | 2:A0:185:TYR:HB2  | 2.00                     | 0.43              |
| 2:A0:290:GLU:CB   | 2:A4:124:LYS:HE2  | 2.48                     | 0.43              |
| 3:A1:172:SER:OG   | 3:A1:175:VAL:O    | 2.34                     | 0.43              |
| 2:A2:103:PHE:HD2  | 2:A2:413:MET:HE1  | 1.84                     | 0.43              |
| 2:A2:282:TYR:CD2  | 2:A6:60:LYS:HE3   | 2.53                     | 0.43              |
| 3:B3:125:GLU:HG2  | 3:B3:159:TYR:OH   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B4:338:LYS:HG2  | 2:B4:340:THR:HG22 | 2.00                     | 0.43              |
| 2:C0:416:GLY:O    | 2:C0:420:GLU:N    | 2.45                     | 0.43              |
| 2:C2:414:GLU:HG2  | 2:C2:417:GLU:OE2  | 2.19                     | 0.43              |
| 3:C3:309:ARG:NH1  | 3:C3:339:SER:O    | 2.52                     | 0.43              |
| 2:C6:158:SER:OG   | 2:C6:166:LYS:NZ   | 2.50                     | 0.43              |
| 2:D0:265:ILE:HG23 | 2:D0:432:TYR:CZ   | 2.54                     | 0.43              |
| 3:D3:175:VAL:HG12 | 2:D4:336:LYS:CG   | 2.49                     | 0.43              |
| 3:D3:291:GLN:CG   | 3:D7:122:LYS:HZ2  | 2.31                     | 0.43              |
| 3:D5:67:ASP:HB3   | 3:D5:73:MET:HE2   | 2.00                     | 0.43              |
| 3:D5:117:LEU:HA   | 3:D5:117:LEU:HD12 | 1.73                     | 0.43              |
| 3:D5:215:LEU:O    | 3:D5:216:LYS:HB2  | 2.18                     | 0.43              |
| 2:E2:265:ILE:HG23 | 2:E2:432:TYR:CE1  | 2.53                     | 0.43              |
| 4:f:68:LEU:HD21   | 4:f:132:LEU:HD11  | 2.01                     | 0.43              |
| 4:o:8:SER:HB2     | 4:o:147:HIS:HA    | 2.00                     | 0.43              |
| 4:r:170:VAL:HG23  | 4:r:183:LEU:HB2   | 2.00                     | 0.43              |
| 2:A0:172:TRP:HB3  | 2:A0:205:ASP:OD1  | 2.18                     | 0.43              |
| 2:A0:224:TYR:O    | 2:A0:228:ASN:ND2  | 2.50                     | 0.43              |
| 3:A1:308:GLY:HA3  | 3:A1:373:ALA:HB2  | 2.01                     | 0.43              |
| 2:A2:277:SER:OG   | 2:A2:278:ALA:N    | 2.51                     | 0.43              |
| 3:A7:4:ILE:HD11   | 3:A7:240:LEU:HD22 | 2.01                     | 0.43              |
| 2:A8:250:VAL:HG21 | 2:A8:352:LYS:HE3  | 2.00                     | 0.43              |
| 2:B0:30:ILE:HG21  | 2:B0:61:HIS:HD2   | 1.83                     | 0.43              |
| 3:B3:122:LYS:HD3  | 3:B3:122:LYS:HA   | 1.83                     | 0.43              |
| 2:B4:356:ASN:OD1  | 2:B4:357:TYR:N    | 2.52                     | 0.43              |
| 2:B8:285:GLN:HG3  | 2:B8:285:GLN:O    | 2.18                     | 0.43              |
| 2:C0:137:MET:HE2  | 2:C0:154:LEU:HD21 | 2.00                     | 0.43              |
| 3:C1:49:VAL:HG11  | 3:C1:241:ARG:HG2  | 2.01                     | 0.43              |
| 2:C2:417:GLU:OE2  | 2:C2:417:GLU:N    | 2.51                     | 0.43              |
| 2:C4:189:LEU:HD21 | 2:C4:418:PHE:HE1  | 1.83                     | 0.43              |
| 2:C6:135:PHE:CD2  | 2:C6:166:LYS:HG2  | 2.48                     | 0.43              |
| 3:C7:404:ASP:OD1  | 3:C7:405:GLU:N    | 2.49                     | 0.43              |
| 3:C9:174:LYS:NZ   | 2:D0:329:ASN:CG   | 2.77                     | 0.43              |
| 2:D0:84:ARG:HH22  | 4:n:94:ASN:ND2    | 2.12                     | 0.43              |
| 2:D0:98:ASP:OD1   | 2:D0:99:ALA:N     | 2.52                     | 0.43              |
| 3:D1:13:GLY:HA2   | 3:D1:16:ILE:HG22  | 2.00                     | 0.43              |
| 2:D2:221:ARG:NE   | 4:q:190:GLU:HB3   | 2.34                     | 0.43              |
| 2:D2:283:HIS:NE2  | 2:D6:85:HIS:O     | 2.40                     | 0.43              |
| 2:D4:221:ARG:C    | 3:D5:322:SER:OG   | 2.62                     | 0.43              |
| 3:D7:362:LYS:HZ2  | 3:D7:363:MET:HE2  | 1.84                     | 0.43              |
| 2:D8:214:ARG:HH11 | 2:D8:214:ARG:HG3  | 1.83                     | 0.43              |
| 2:E0:18:ASN:HD21  | 2:E0:78:VAL:HG22  | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E9:44:LEU:HB2   | 3:E9:47:ILE:HB    | 2.01                     | 0.43              |
| 4:f:152:LYS:HG3   | 4:f:153:GLU:N     | 2.33                     | 0.43              |
| 4:m:74:ALA:HB2    | 4:m:172:VAL:HG12  | 2.00                     | 0.43              |
| 4:n:142:GLU:HA    | 4:n:145:LYS:HG2   | 1.99                     | 0.43              |
| 4:t:36:ILE:HD13   | 4:t:36:ILE:HA     | 1.83                     | 0.43              |
| 1:3:257:PRO:HG3   | 2:B0:26:LEU:O     | 2.18                     | 0.43              |
| 1:4:240:PRO:C     | 4:g:154:TYR:HB3   | 2.44                     | 0.43              |
| 3:A1:244:GLY:HA2  | 3:A1:355:ASP:HB2  | 2.01                     | 0.43              |
| 3:A1:259:PRO:HB2  | 3:A1:260:PHE:CD2  | 2.54                     | 0.43              |
| 3:A1:291:GLN:HB3  | 3:A5:122:LYS:HE3  | 2.01                     | 0.43              |
| 2:A2:191:THR:HA   | 2:A2:194:LEU:HB3  | 2.01                     | 0.43              |
| 2:A2:208:ALA:HB2  | 2:A2:304:LYS:HB2  | 2.00                     | 0.43              |
| 2:A4:27:GLU:HG3   | 2:A4:361:THR:HG21 | 2.01                     | 0.43              |
| 2:A6:264:ARG:HG3  | 2:A6:264:ARG:HH11 | 1.84                     | 0.43              |
| 3:A7:73:MET:HB3   | 3:A7:73:MET:HE3   | 1.75                     | 0.43              |
| 3:A7:113:ILE:HG13 | 3:A7:117:LEU:HD23 | 2.01                     | 0.43              |
| 2:A8:73:THR:OG1   | 3:A9:46:ARG:CZ    | 2.67                     | 0.43              |
| 2:B2:10:GLY:HA2   | 2:B2:145:THR:HG23 | 2.00                     | 0.43              |
| 3:B3:403:MET:HE2  | 3:B3:403:MET:HB3  | 1.82                     | 0.43              |
| 2:B4:207:GLU:HA   | 2:B4:210:TYR:HB2  | 2.00                     | 0.43              |
| 3:B5:8:GLN:HE21   | 3:B5:65:LEU:HD11  | 1.84                     | 0.43              |
| 3:B5:66:MET:HE3   | 3:B5:147:MET:CE   | 2.49                     | 0.43              |
| 3:B7:141:GLY:O    | 3:B7:145:SER:OG   | 2.31                     | 0.43              |
| 2:B8:280:LYS:HA   | 2:B8:280:LYS:HD3  | 1.66                     | 0.43              |
| 2:B8:282:TYR:CE1  | 4:j:201:TRP:HZ2   | 2.37                     | 0.43              |
| 2:C0:338:LYS:HA   | 2:C0:338:LYS:HD2  | 1.93                     | 0.43              |
| 2:C4:76:ASP:OD1   | 2:C4:77:GLU:N     | 2.52                     | 0.43              |
| 2:C4:362:VAL:HG11 | 2:C4:369:ALA:C    | 2.43                     | 0.43              |
| 3:C5:73:MET:HE3   | 3:C5:92:PHE:HA    | 2.01                     | 0.43              |
| 2:C6:209:ILE:HB   | 2:C6:227:LEU:HD12 | 2.00                     | 0.43              |
| 2:C6:406:HIS:CE1  | 3:C7:259:PRO:O    | 2.72                     | 0.43              |
| 2:D2:91:GLN:OE1   | 2:D2:121:ARG:NH2  | 2.49                     | 0.43              |
| 3:D5:316:MET:HE3  | 3:D5:316:MET:HB2  | 1.78                     | 0.43              |
| 3:D7:229:VAL:HA   | 3:D7:300:MET:HE1  | 2.01                     | 0.43              |
| 2:E2:224:TYR:HD2  | 3:E3:245:GLN:HB3  | 1.84                     | 0.43              |
| 3:E3:211:CYS:HA   | 3:E3:215:LEU:HB2  | 2.00                     | 0.43              |
| 2:E6:180:ALA:HB3  | 2:E6:183:GLU:HB3  | 2.01                     | 0.43              |
| 3:E7:282:ARG:O    | 3:F1:55:THR:CG2   | 2.67                     | 0.43              |
| 3:E9:229:VAL:HG12 | 3:E9:233:MET:HE2  | 2.01                     | 0.43              |
| 2:F0:12:ALA:HB3   | 2:F0:140:ALA:HB2  | 2.00                     | 0.43              |
| 2:F0:154:LEU:HG   | 2:F0:197:HIS:HB3  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F1:149:THR:HA   | 3:F1:152:ILE:HD12 | 2.01                     | 0.43              |
| 4:q:99:MET:HE2    | 4:q:99:MET:HB3    | 1.80                     | 0.43              |
| 4:s:95:TYR:CZ     | 4:s:99:MET:HE2    | 2.53                     | 0.43              |
| 5:x:15:ARG:NH2    | 5:x:93:CYS:SG     | 2.85                     | 0.43              |
| 2:A0:274:PRO:HG2  | 2:A0:371:VAL:HG11 | 2.01                     | 0.43              |
| 3:A1:68:LEU:HD21  | 3:A1:147:MET:SD   | 2.59                     | 0.43              |
| 3:A1:218:THR:C    | 3:A1:219:THR:HG1  | 2.26                     | 0.43              |
| 3:A5:294:PHE:CD2  | 3:A5:333:VAL:HG21 | 2.54                     | 0.43              |
| 2:A6:36:MET:HA    | 2:A6:37:PRO:HD3   | 1.86                     | 0.43              |
| 3:B1:281:TYR:CD2  | 3:B5:87:PRO:HD3   | 2.53                     | 0.43              |
| 2:B4:264:ARG:H    | 2:B4:264:ARG:HG2  | 1.71                     | 0.43              |
| 2:B6:163:LYS:HD3  | 2:B6:163:LYS:HA   | 1.80                     | 0.43              |
| 2:B8:274:PRO:HG3  | 2:B8:286:LEU:HD12 | 1.99                     | 0.43              |
| 2:C0:54:SER:OG    | 2:C0:55:GLU:N     | 2.52                     | 0.43              |
| 2:C0:166:LYS:HE3  | 2:C0:166:LYS:HB2  | 1.88                     | 0.43              |
| 2:C6:132:LEU:HD13 | 2:C6:132:LEU:HA   | 1.89                     | 0.43              |
| 3:C7:28:HIS:NE2   | 3:C7:241:ARG:HD2  | 2.34                     | 0.43              |
| 3:C7:42:LEU:HD12  | 3:C7:243:PRO:CD   | 2.49                     | 0.43              |
| 2:C8:203:MET:HE3  | 2:C8:267:PHE:CD2  | 2.53                     | 0.43              |
| 2:D4:93:ILE:HG23  | 2:D4:117:LEU:HD23 | 2.01                     | 0.43              |
| 2:D4:250:VAL:HG22 | 2:D4:352:LYS:HZ1  | 1.83                     | 0.43              |
| 2:E2:216:ASN:O    | 2:E2:280:LYS:HE2  | 2.19                     | 0.43              |
| 3:E3:122:LYS:HD3  | 3:E3:122:LYS:HA   | 1.85                     | 0.43              |
| 2:F0:223:THR:OG1  | 2:F0:224:TYR:N    | 2.52                     | 0.43              |
| 3:F1:309:ARG:NH1  | 3:F1:341:PHE:O    | 2.49                     | 0.43              |
| 5:x:12:VAL:HG23   | 5:x:13:VAL:HG23   | 2.01                     | 0.43              |
| 3:A1:7:VAL:HG11   | 3:A1:151:LEU:HD23 | 2.00                     | 0.43              |
| 3:A1:66:MET:HA    | 3:A1:91:VAL:HG23  | 2.01                     | 0.43              |
| 2:A2:143:GLY:O    | 2:A2:186:ASN:ND2  | 2.52                     | 0.43              |
| 2:A6:265:ILE:HG23 | 2:A6:432:TYR:CZ   | 2.54                     | 0.43              |
| 2:B0:71:GLU:HG2   | 2:B0:73:THR:HG22  | 2.00                     | 0.43              |
| 2:B4:397:LEU:HD23 | 2:B4:397:LEU:HA   | 1.85                     | 0.43              |
| 2:B8:274:PRO:HB2  | 2:B8:276:ILE:HG12 | 2.01                     | 0.43              |
| 3:C1:257:LEU:HB3  | 3:C1:266:PHE:CE1  | 2.53                     | 0.43              |
| 2:C4:276:ILE:HD12 | 2:C4:281:ALA:HA   | 2.00                     | 0.43              |
| 3:C5:167:PHE:HD2  | 3:C5:233:MET:HE3  | 1.84                     | 0.43              |
| 3:C5:207:LEU:HB3  | 3:C5:225:LEU:CD1  | 2.46                     | 0.43              |
| 3:C7:19:LYS:HA    | 3:C7:19:LYS:HD3   | 1.82                     | 0.43              |
| 3:C7:311:LEU:HD12 | 3:C7:342:VAL:HG11 | 2.01                     | 0.43              |
| 2:C8:154:LEU:HB3  | 2:C8:197:HIS:HB3  | 2.01                     | 0.43              |
| 2:C8:337:THR:O    | 2:C8:339:ARG:NH1  | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C9:161:ASP:OD1  | 3:C9:161:ASP:N    | 2.47                     | 0.43              |
| 3:D3:113:ILE:HD12 | 3:D3:113:ILE:HA   | 1.91                     | 0.43              |
| 3:D7:27:GLU:OE1   | 3:D7:318:ARG:NH2  | 2.49                     | 0.43              |
| 3:D7:324:LYS:O    | 3:D7:328:GLU:N    | 2.32                     | 0.43              |
| 2:E0:96:LYS:CE    | 3:E1:128:ASP:OD2  | 2.67                     | 0.43              |
| 2:E0:179:THR:O    | 2:E0:180:ALA:HB2  | 2.19                     | 0.43              |
| 2:E2:392:ASP:O    | 2:E2:422:ARG:NH1  | 2.41                     | 0.43              |
| 3:E3:253:LEU:HD11 | 3:E3:368:VAL:HG21 | 2.00                     | 0.43              |
| 2:E6:302:MET:HB2  | 2:E6:302:MET:HE3  | 1.70                     | 0.43              |
| 3:E7:276:ARG:NH2  | 3:E7:279:GLN:OE1  | 2.40                     | 0.43              |
| 4:b:89:LEU:HB3    | 4:b:90:PRO:HD3    | 2.01                     | 0.43              |
| 4:f:7:ALA:HB3     | 4:f:161:TYR:HE1   | 1.83                     | 0.43              |
| 4:j:85:CYS:SG     | 4:j:167:VAL:HG22  | 2.59                     | 0.43              |
| 4:m:10:LEU:HB2    | 4:m:147:HIS:ND1   | 2.33                     | 0.43              |
| 4:o:18:ASN:HD21   | 4:o:46:ASP:H      | 1.65                     | 0.43              |
| 4:s:14:LYS:HD3    | 4:s:47:LEU:HD22   | 2.01                     | 0.43              |
| 2:A0:11:GLN:HG3   | 2:A0:74:VAL:HG11  | 2.01                     | 0.42              |
| 2:A0:232:ALA:HA   | 2:A0:235:ILE:HG22 | 2.00                     | 0.42              |
| 2:A2:306:ASP:HB3  | 2:A2:309:HIS:CE1  | 2.54                     | 0.42              |
| 2:A4:3:GLU:OE1    | 2:A4:132:LEU:HD13 | 2.19                     | 0.42              |
| 3:A7:206:ALA:HB2  | 3:A7:302:ALA:HB2  | 2.00                     | 0.42              |
| 2:A8:259:LEU:HD11 | 2:A8:316:CYS:HB2  | 2.01                     | 0.42              |
| 2:B0:73:THR:HB    | 3:B1:46:ARG:HE    | 1.81                     | 0.42              |
| 2:B0:339:ARG:HG3  | 2:B0:339:ARG:O    | 2.19                     | 0.42              |
| 2:B8:215:ARG:HH22 | 2:B8:299:ALA:C    | 2.27                     | 0.42              |
| 2:C2:311:LYS:H    | 2:C2:382:THR:HG1  | 1.65                     | 0.42              |
| 3:C3:262:ARG:HA   | 3:C3:262:ARG:HD2  | 1.76                     | 0.42              |
| 2:C4:25:CYS:HA    | 2:C4:30:ILE:HG12  | 2.00                     | 0.42              |
| 3:C5:10:GLY:O     | 3:C5:14:ASN:ND2   | 2.52                     | 0.42              |
| 2:D4:298:PRO:HG2  | 2:D4:308:ARG:NH1  | 2.34                     | 0.42              |
| 3:E1:113:ILE:HG12 | 3:E1:150:LEU:HD22 | 2.00                     | 0.42              |
| 3:E3:289:LEU:HD23 | 3:E3:289:LEU:HA   | 1.86                     | 0.42              |
| 3:E3:317:PHE:HB3  | 3:E3:321:MET:SD   | 2.59                     | 0.42              |
| 3:E3:403:MET:HE3  | 3:E3:403:MET:HB2  | 1.96                     | 0.42              |
| 2:E4:217:LEU:HD21 | 2:E4:367:ASP:CG   | 2.44                     | 0.42              |
| 3:E7:86:ARG:HG2   | 3:E7:88:ASP:H     | 1.84                     | 0.42              |
| 4:d:71:LYS:CD     | 4:f:39:PRO:HD3    | 2.48                     | 0.42              |
| 4:q:12:VAL:HG12   | 4:q:15:ARG:NH1    | 2.34                     | 0.42              |
| 1:16:241:PHE:CD2  | 3:E1:43:GLN:HG2   | 2.54                     | 0.42              |
| 1:16:256:LEU:HD13 | 2:E0:26:LEU:HD13  | 2.01                     | 0.42              |
| 1:17:241:PHE:CD2  | 3:E3:43:GLN:OE1   | 2.72                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:17:248:ARG:HH21 | 4:t:94:ASN:HD22   | 1.67                     | 0.42              |
| 1:23:257:PRO:HG2  | 2:C4:26:LEU:O     | 2.19                     | 0.42              |
| 1:9:243:ALA:C     | 3:C3:356:ILE:HD12 | 2.44                     | 0.42              |
| 2:A0:79:ARG:CG    | 2:A0:92:LEU:HD22  | 2.47                     | 0.42              |
| 3:A1:6:HIS:CD2    | 3:A1:134:GLN:HG3  | 2.53                     | 0.42              |
| 3:A3:180:VAL:O    | 3:A3:184:ASN:ND2  | 2.52                     | 0.42              |
| 2:A4:48:ALA:HB1   | 2:A4:243:ARG:O    | 2.19                     | 0.42              |
| 2:A4:103:PHE:H    | 2:A4:408:TYR:HE1  | 1.67                     | 0.42              |
| 3:A5:257:LEU:HD21 | 3:A5:314:SER:CB   | 2.49                     | 0.42              |
| 2:A8:10:GLY:O     | 2:A8:14:ILE:HG12  | 2.18                     | 0.42              |
| 3:A9:139:LEU:HA   | 3:A9:145:SER:HB2  | 2.01                     | 0.42              |
| 3:B5:6:HIS:HE2    | 3:B5:8:GLN:HB3    | 1.84                     | 0.42              |
| 3:B5:357:PRO:HB2  | 3:B5:361:LEU:O    | 2.19                     | 0.42              |
| 3:B7:294:PHE:HZ   | 3:B7:349:MET:HE1  | 1.84                     | 0.42              |
| 2:B8:164:LYS:HD3  | 2:B8:164:LYS:HA   | 1.71                     | 0.42              |
| 2:C0:168:ASN:HD22 | 2:C0:198:THR:HG21 | 1.83                     | 0.42              |
| 3:C3:263:LEU:HB3  | 3:C3:422:TYR:HE1  | 1.83                     | 0.42              |
| 3:C3:287:PRO:HB3  | 3:C3:329:GLN:HE21 | 1.84                     | 0.42              |
| 2:C4:2:ARG:NE     | 2:C4:2:ARG:HD2    | 2.08                     | 0.42              |
| 2:C4:268:MET:SD   | 2:C4:380:ASN:ND2  | 2.92                     | 0.42              |
| 3:C5:220:PRO:CD   | 2:C6:326:LYS:HD3  | 2.49                     | 0.42              |
| 2:C8:137:MET:HE1  | 2:C8:154:LEU:HD11 | 2.01                     | 0.42              |
| 2:D0:231:ILE:O    | 2:D0:235:ILE:HG12 | 2.19                     | 0.42              |
| 2:D2:194:LEU:O    | 2:D2:198:THR:HG22 | 2.20                     | 0.42              |
| 2:D2:259:LEU:HD21 | 2:D2:316:CYS:HB2  | 2.00                     | 0.42              |
| 2:D8:262:TYR:CB   | 2:D8:263:PRO:HD2  | 2.45                     | 0.42              |
| 3:D9:181:GLU:HB2  | 3:D9:182:PRO:HD3  | 2.01                     | 0.42              |
| 2:E2:70:LEU:HD12  | 2:E2:99:ALA:HB2   | 2.00                     | 0.42              |
| 3:E3:200:GLN:HB3  | 3:E3:268:ILE:HD11 | 2.01                     | 0.42              |
| 3:E5:208:TYR:CE1  | 3:E5:225:LEU:HD11 | 2.54                     | 0.42              |
| 3:E5:309:ARG:NH1  | 3:E5:341:PHE:O    | 2.49                     | 0.42              |
| 2:E6:282:TYR:CG   | 5:x:160:ARG:HD3   | 2.51                     | 0.42              |
| 3:E9:7:VAL:HG22   | 3:E9:64:ILE:HB    | 2.01                     | 0.42              |
| 4:b:97:ARG:NH2    | 4:d:7:ALA:N       | 2.67                     | 0.42              |
| 4:f:198:ARG:NH1   | 4:f:198:ARG:CG    | 2.82                     | 0.42              |
| 4:p:115:LEU:HD23  | 4:p:115:LEU:HA    | 1.85                     | 0.42              |
| 4:u:146:ARG:HH12  | 4:u:156:VAL:HG11  | 1.84                     | 0.42              |
| 5:x:133:VAL:HG11  | 5:x:157:TRP:HE1   | 1.84                     | 0.42              |
| 2:A0:242:LEU:HD21 | 2:A0:251:ASP:CB   | 2.49                     | 0.42              |
| 3:A1:47:ILE:HG12  | 3:A1:51:TYR:HB2   | 2.01                     | 0.42              |
| 3:A1:104:GLY:HA3  | 3:A1:146:GLY:HA3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A3:41:ASP:OD1   | 3:A3:41:ASP:N     | 2.53                     | 0.42              |
| 2:A4:250:VAL:HG23 | 2:A4:250:VAL:O    | 2.19                     | 0.42              |
| 3:A9:190:HIS:HB2  | 3:A9:414:ASN:HB3  | 2.00                     | 0.42              |
| 2:B2:69:ASP:OD1   | 2:B2:70:LEU:N     | 2.51                     | 0.42              |
| 3:B3:102:ALA:HB2  | 3:B3:398:TYR:HD1  | 1.84                     | 0.42              |
| 3:B5:117:LEU:HD12 | 3:B5:117:LEU:HA   | 1.84                     | 0.42              |
| 3:B9:7:VAL:HB     | 3:B9:135:ILE:HG13 | 2.01                     | 0.42              |
| 2:C0:411:GLU:OE1  | 2:C0:411:GLU:N    | 2.52                     | 0.42              |
| 3:C1:167:PHE:HE1  | 3:C1:200:GLN:NE2  | 2.17                     | 0.42              |
| 3:C1:177:ASP:HB3  | 2:C2:353:CYS:SG   | 2.58                     | 0.42              |
| 3:C3:200:GLN:HG3  | 3:C3:268:ILE:HD11 | 2.00                     | 0.42              |
| 2:C4:287:SER:N    | 2:C4:290:GLU:OE2  | 2.46                     | 0.42              |
| 2:C8:283:HIS:NE2  | 2:D2:85:HIS:O     | 2.48                     | 0.42              |
| 3:D5:155:VAL:HG13 | 3:D5:164:MET:SD   | 2.59                     | 0.42              |
| 3:D5:301:CYS:SG   | 3:D5:377:MET:HE2  | 2.59                     | 0.42              |
| 3:D5:392:LYS:HG2  | 3:D5:395:LEU:HD22 | 2.01                     | 0.42              |
| 3:D7:406:MET:CE   | 3:D7:406:MET:CA   | 2.86                     | 0.42              |
| 2:D8:251:ASP:H    | 2:D8:254:GLU:HG3  | 1.85                     | 0.42              |
| 3:D9:256:ASN:O    | 3:D9:312:THR:HG21 | 2.18                     | 0.42              |
| 2:E0:189:LEU:HD11 | 2:E0:418:PHE:HE1  | 1.84                     | 0.42              |
| 2:E0:208:ALA:O    | 2:E0:212:ILE:HG12 | 2.19                     | 0.42              |
| 3:E3:113:ILE:HA   | 3:E3:116:VAL:HG12 | 2.01                     | 0.42              |
| 2:E8:238:LEU:HD12 | 2:E8:238:LEU:HA   | 1.82                     | 0.42              |
| 3:F1:42:LEU:HD11  | 3:F1:243:PRO:HG3  | 2.00                     | 0.42              |
| 4:f:35:ASN:HD22   | 4:f:35:ASN:N      | 2.17                     | 0.42              |
| 4:g:75:LEU:O      | 4:g:170:VAL:HA    | 2.19                     | 0.42              |
| 4:m:201:TRP:CD1   | 4:m:201:TRP:H     | 2.37                     | 0.42              |
| 4:t:191:GLU:HB2   | 4:t:195:ALA:HB2   | 2.00                     | 0.42              |
| 1:12:250:GLU:HG3  | 1:12:251:TYR:CD1  | 2.54                     | 0.42              |
| 1:7:256:LEU:HD11  | 2:B8:31:GLN:CA    | 2.49                     | 0.42              |
| 3:A5:250:LEU:HD23 | 3:A5:250:LEU:HA   | 1.88                     | 0.42              |
| 3:A7:95:THR:OG1   | 3:A7:96:GLY:N     | 2.52                     | 0.42              |
| 2:B0:100:ALA:HA   | 3:B1:252:LYS:HZ2  | 1.82                     | 0.42              |
| 2:B2:36:MET:HE3   | 2:B2:36:MET:HB2   | 1.71                     | 0.42              |
| 2:B2:230:LEU:HD21 | 2:B2:368:LEU:HD11 | 2.00                     | 0.42              |
| 2:B6:286:LEU:O    | 2:B6:373:ARG:HD2  | 2.19                     | 0.42              |
| 2:B6:286:LEU:O    | 2:B6:373:ARG:NH1  | 2.37                     | 0.42              |
| 3:B7:213:ARG:HD3  | 3:B7:297:LYS:NZ   | 2.33                     | 0.42              |
| 3:B9:103:LYS:HA   | 3:B9:107:THR:HG22 | 2.01                     | 0.42              |
| 2:C2:372:MET:HE3  | 2:C2:372:MET:HB3  | 1.41                     | 0.42              |
| 3:C7:267:LEU:HD21 | 3:C7:374:ILE:CG2  | 2.48                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C8:306:ASP:HB3  | 2:C8:309:HIS:CE1  | 2.55                     | 0.42              |
| 3:C9:128:ASP:CG   | 3:C9:129:CYS:H    | 2.27                     | 0.42              |
| 3:C9:293:MET:SD   | 3:C9:365:VAL:HG11 | 2.58                     | 0.42              |
| 3:D5:68:LEU:HB3   | 3:D5:96:GLY:HA2   | 2.00                     | 0.42              |
| 2:D8:407:TRP:CG   | 3:D9:255:VAL:HG23 | 2.53                     | 0.42              |
| 2:D8:422:ARG:HA   | 2:D8:422:ARG:HD2  | 1.65                     | 0.42              |
| 3:D9:290:THR:HG21 | 3:D9:329:GLN:HB3  | 2.01                     | 0.42              |
| 3:E3:164:MET:H    | 3:E3:197:ASP:HB2  | 1.84                     | 0.42              |
| 3:E9:386:THR:O    | 3:E9:390:ARG:HG3  | 2.19                     | 0.42              |
| 2:F0:219:ILE:HG13 | 2:F0:222:PRO:HD3  | 2.00                     | 0.42              |
| 4:b:68:LEU:HD21   | 4:b:111:ILE:HD11  | 2.01                     | 0.42              |
| 4:f:110:ILE:O     | 4:f:131:TRP:HB2   | 2.20                     | 0.42              |
| 4:s:176:ASP:OD1   | 4:s:176:ASP:N     | 2.52                     | 0.42              |
| 1:10:254:LYS:H    | 1:10:254:LYS:HG2  | 1.65                     | 0.42              |
| 1:17:244:GLN:NE2  | 4:v:162:GLY:HA3   | 2.30                     | 0.42              |
| 1:6:247:TYR:CE2   | 2:B6:81:GLY:HA3   | 2.41                     | 0.42              |
| 2:A0:164:LYS:HD2  | 2:A0:164:LYS:HA   | 1.81                     | 0.42              |
| 3:A1:308:GLY:HA2  | 3:A1:426:GLN:NE2  | 2.35                     | 0.42              |
| 2:A2:306:ASP:HB3  | 2:A2:309:HIS:HE1  | 1.83                     | 0.42              |
| 2:A4:154:LEU:HD23 | 2:A4:154:LEU:HA   | 1.94                     | 0.42              |
| 3:A5:164:MET:HE2  | 3:A5:164:MET:HB2  | 1.82                     | 0.42              |
| 2:A6:291:ILE:HD12 | 2:A6:375:VAL:HG23 | 2.01                     | 0.42              |
| 3:A9:220:PRO:HG2  | 2:B0:326:LYS:CD   | 2.50                     | 0.42              |
| 3:B1:60:VAL:HA    | 3:B1:61:PRO:HD3   | 1.94                     | 0.42              |
| 3:B3:44:LEU:HG    | 3:B3:44:LEU:O     | 2.20                     | 0.42              |
| 2:B4:184:PRO:HA   | 2:B4:391:MET:HE1  | 2.00                     | 0.42              |
| 3:B9:128:ASP:OD1  | 3:B9:129:CYS:N    | 2.41                     | 0.42              |
| 2:C0:377:MET:HE3  | 2:C0:377:MET:HB3  | 1.95                     | 0.42              |
| 2:C2:173:PRO:O    | 2:C2:390:ARG:NH1  | 2.53                     | 0.42              |
| 3:C3:169:VAL:HG12 | 3:C3:202:ILE:HB   | 2.00                     | 0.42              |
| 3:C3:238:CYS:SG   | 3:C3:239:CYS:N    | 2.92                     | 0.42              |
| 2:C4:132:LEU:HB3  | 2:C4:164:LYS:NZ   | 2.33                     | 0.42              |
| 2:C4:209:ILE:CG2  | 2:C4:227:LEU:HD22 | 2.47                     | 0.42              |
| 2:C4:377:MET:SD   | 2:C4:379:SER:HB3  | 2.60                     | 0.42              |
| 3:C9:121:ARG:NH2  | 3:C9:158:GLU:OE2  | 2.51                     | 0.42              |
| 3:D3:291:GLN:HB3  | 3:D7:122:LYS:NZ   | 2.35                     | 0.42              |
| 2:D8:388:PHE:HB2  | 2:D8:429:GLU:OE2  | 2.19                     | 0.42              |
| 3:D9:287:PRO:HA   | 3:D9:290:THR:HG22 | 2.01                     | 0.42              |
| 2:E2:316:CYS:HA   | 2:E2:352:LYS:HB2  | 2.02                     | 0.42              |
| 3:E3:113:ILE:HD11 | 3:E3:151:LEU:HB2  | 2.01                     | 0.42              |
| 3:E7:1:MET:N      | 3:E7:128:ASP:OD2  | 2.46                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:25:SER:HB3   | 3:E7:30:ILE:HB    | 2.00                     | 0.42              |
| 3:E9:206:ALA:HB2  | 3:E9:302:ALA:HB2  | 2.01                     | 0.42              |
| 4:i:9:PRO:HG2     | 4:i:146:ARG:HD2   | 2.01                     | 0.42              |
| 4:j:88:LEU:HD12   | 4:j:88:LEU:HA     | 1.89                     | 0.42              |
| 4:p:72:SER:OG     | 4:p:199:TRP:NE1   | 2.46                     | 0.42              |
| 1:11:250:GLU:OE2  | 2:D0:225:THR:HG21 | 2.20                     | 0.42              |
| 1:14:256:LEU:HD21 | 2:D6:31:GLN:HG3   | 2.02                     | 0.42              |
| 1:6:256:LEU:HD11  | 2:B6:31:GLN:CA    | 2.48                     | 0.42              |
| 2:A0:9:VAL:HG22   | 2:A0:68:LEU:HD22  | 2.00                     | 0.42              |
| 2:A4:134:GLY:CA   | 2:A4:164:LYS:HZ3  | 2.32                     | 0.42              |
| 3:A9:92:PHE:O     | 3:A9:112:LEU:HD11 | 2.20                     | 0.42              |
| 2:B0:138:PHE:CZ   | 2:B0:235:ILE:HD12 | 2.54                     | 0.42              |
| 3:B3:12:CYS:HB3   | 3:B3:138:SER:OG   | 2.19                     | 0.42              |
| 2:B4:285:GLN:HB3  | 2:B8:56:THR:HA    | 2.02                     | 0.42              |
| 2:B6:5:ILE:HD12   | 2:B6:125:LEU:HD23 | 2.02                     | 0.42              |
| 2:B8:73:THR:OG1   | 3:B9:2:ARG:NH2    | 2.52                     | 0.42              |
| 2:C0:370:LYS:HE2  | 2:C0:370:LYS:HB2  | 1.87                     | 0.42              |
| 2:C2:105:ARG:HH21 | 2:C2:110:ILE:HG21 | 1.84                     | 0.42              |
| 2:C6:130:THR:HG22 | 2:C6:131:GLY:N    | 2.35                     | 0.42              |
| 2:D4:409:VAL:HG22 | 2:D4:415:GLU:HB2  | 2.00                     | 0.42              |
| 3:D5:139:LEU:HD22 | 3:D5:188:SER:HB2  | 2.01                     | 0.42              |
| 3:D7:186:THR:HG22 | 3:D7:411:ALA:HB1  | 2.02                     | 0.42              |
| 3:D9:6:HIS:HD2    | 3:D9:134:GLN:HE21 | 1.66                     | 0.42              |
| 3:E1:156:ARG:NH1  | 3:E1:162:ARG:O    | 2.53                     | 0.42              |
| 2:E4:194:LEU:O    | 2:E4:198:THR:HG22 | 2.20                     | 0.42              |
| 3:E5:67:ASP:OD1   | 3:E5:68:LEU:N     | 2.53                     | 0.42              |
| 3:E5:109:GLY:O    | 3:E5:113:ILE:HG12 | 2.19                     | 0.42              |
| 3:E7:216:LYS:HD3  | 3:E7:216:LYS:HA   | 1.82                     | 0.42              |
| 2:F0:99:ALA:O     | 2:F0:105:ARG:HD3  | 2.20                     | 0.42              |
| 3:F1:43:GLN:HA    | 3:F1:242:PHE:CE1  | 2.54                     | 0.42              |
| 4:e:67:HIS:CE1    | 4:g:20:GLU:HB3    | 2.53                     | 0.42              |
| 4:e:110:ILE:HB    | 4:e:131:TRP:CG    | 2.54                     | 0.42              |
| 4:g:56:LYS:O      | 4:g:126:ARG:NH2   | 2.52                     | 0.42              |
| 5:k:82:ASP:O      | 5:k:85:ARG:HG3    | 2.19                     | 0.42              |
| 4:s:2:SER:O       | 4:s:2:SER:OG      | 2.37                     | 0.42              |
| 4:s:19:GLU:HB3    | 4:s:40:PRO:HD2    | 2.02                     | 0.42              |
| 1:8:241:PHE:CZ    | 3:C1:356:ILE:HG23 | 2.41                     | 0.42              |
| 2:A2:370:LYS:HE3  | 2:A2:370:LYS:HB3  | 1.89                     | 0.42              |
| 3:A3:12:CYS:HB3   | 3:A3:138:SER:HB2  | 2.01                     | 0.42              |
| 2:A4:309:HIS:NE2  | 2:A4:386:GLU:OE1  | 2.53                     | 0.42              |
| 2:A8:68:LEU:HD23  | 2:A8:93:ILE:HB    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A9:73:MET:HE1   | 3:A9:90:PHE:CD1   | 2.55                     | 0.42              |
| 3:A9:321:MET:HB3  | 3:A9:363:MET:HE2  | 2.01                     | 0.42              |
| 2:B2:282:TYR:OH   | 2:B6:33:ASP:CG    | 2.62                     | 0.42              |
| 2:B2:319:TYR:N    | 2:B2:354:GLY:O    | 2.53                     | 0.42              |
| 3:B3:68:LEU:HG    | 3:B3:147:MET:HE2  | 2.02                     | 0.42              |
| 3:B3:117:LEU:HD23 | 3:B3:117:LEU:HA   | 1.82                     | 0.42              |
| 2:B4:36:MET:HA    | 2:B4:37:PRO:HD3   | 1.90                     | 0.42              |
| 3:B5:314:SER:OG   | 3:B5:315:ALA:N    | 2.51                     | 0.42              |
| 2:B6:269:LEU:HD21 | 2:B6:384:ILE:HD11 | 2.01                     | 0.42              |
| 2:C0:262:TYR:HB2  | 2:C0:265:ILE:HG22 | 2.01                     | 0.42              |
| 3:C5:239:CYS:SG   | 3:C5:248:SER:N    | 2.84                     | 0.42              |
| 2:C6:179:THR:OG1  | 3:C7:246:LEU:HD21 | 2.19                     | 0.42              |
| 3:C7:90:PHE:HB3   | 3:C7:92:PHE:CE1   | 2.54                     | 0.42              |
| 3:C7:281:TYR:O    | 3:D1:86:ARG:HD3   | 2.19                     | 0.42              |
| 2:D4:283:HIS:CD2  | 2:D8:60:LYS:HE2   | 2.55                     | 0.42              |
| 2:D4:283:HIS:NE2  | 2:D8:85:HIS:O     | 2.48                     | 0.42              |
| 3:D7:212:PHE:HE1  | 2:D8:326:LYS:CE   | 2.33                     | 0.42              |
| 2:D8:163:LYS:H    | 2:D8:163:LYS:CD   | 2.26                     | 0.42              |
| 2:E0:84:ARG:NH2   | 4:s:197:LEU:HD21  | 2.35                     | 0.42              |
| 2:E2:2:ARG:HD3    | 2:E2:2:ARG:HA     | 1.90                     | 0.42              |
| 3:F1:256:ASN:ND2  | 3:F1:350:LYS:HG3  | 2.35                     | 0.42              |
| 4:b:164:ARG:HG3   | 4:b:165:THR:HG23  | 2.02                     | 0.42              |
| 4:c:9:PRO:HA      | 4:c:12:VAL:HG22   | 2.02                     | 0.42              |
| 4:g:149:ARG:HD3   | 4:g:161:TYR:HD2   | 1.83                     | 0.42              |
| 4:h:11:ASN:HD22   | 4:h:14:LYS:HE2    | 1.85                     | 0.42              |
| 4:n:150:VAL:HG13  | 4:n:165:THR:HG23  | 2.02                     | 0.42              |
| 4:s:105:ASN:OD1   | 4:u:37:GLN:NE2    | 2.53                     | 0.42              |
| 4:v:183:LEU:HD11  | 4:v:199:TRP:HB2   | 2.01                     | 0.42              |
| 1:15:244:GLN:CD   | 4:t:162:GLY:HA3   | 2.44                     | 0.42              |
| 2:A0:136:LEU:HD23 | 2:A0:136:LEU:HA   | 1.89                     | 0.42              |
| 2:A0:428:LEU:HD12 | 2:A0:428:LEU:HA   | 1.91                     | 0.42              |
| 3:A1:21:TRP:CZ2   | 3:A1:63:ALA:HB2   | 2.54                     | 0.42              |
| 2:A4:36:MET:HA    | 2:A4:37:PRO:HD3   | 1.74                     | 0.42              |
| 3:A5:178:THR:O    | 3:A5:181:GLU:HG2  | 2.19                     | 0.42              |
| 2:A6:85:HIS:CE1   | 4:b:99:MET:HE1    | 2.44                     | 0.42              |
| 2:A8:306:ASP:HB3  | 2:A8:309:HIS:CE1  | 2.55                     | 0.42              |
| 3:B1:281:TYR:CE2  | 3:B5:87:PRO:HD3   | 2.55                     | 0.42              |
| 3:B3:152:ILE:HA   | 3:B3:155:VAL:HG12 | 2.00                     | 0.42              |
| 3:B5:139:LEU:HA   | 3:B5:145:SER:HB3  | 2.01                     | 0.42              |
| 2:B8:254:GLU:HG2  | 2:B8:352:LYS:HE2  | 2.00                     | 0.42              |
| 3:B9:15:GLN:O     | 3:B9:226:ASN:ND2  | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B9:101:TRP:H    | 3:B9:398:TYR:HE1  | 1.66                     | 0.42              |
| 3:B9:287:PRO:HA   | 3:B9:290:THR:HG22 | 2.02                     | 0.42              |
| 3:C3:275:SER:OG   | 3:C3:276:ARG:N    | 2.52                     | 0.42              |
| 2:C6:53:PHE:HB3   | 2:C6:61:HIS:HB3   | 2.01                     | 0.42              |
| 3:C7:167:PHE:CD2  | 3:C7:233:MET:HG2  | 2.55                     | 0.42              |
| 2:C8:311:LYS:HB3  | 2:C8:311:LYS:HE3  | 1.68                     | 0.42              |
| 2:D0:119:LEU:HD11 | 2:D0:157:LEU:HD22 | 2.01                     | 0.42              |
| 2:D0:205:ASP:O    | 2:D0:209:ILE:HG13 | 2.20                     | 0.42              |
| 3:D3:313:ALA:HB3  | 3:D3:349:MET:SD   | 2.60                     | 0.42              |
| 2:D4:301:MET:HE2  | 2:D4:301:MET:HB2  | 1.93                     | 0.42              |
| 3:D5:378:PHE:HD1  | 3:D5:415:MET:HE3  | 1.85                     | 0.42              |
| 2:D6:138:PHE:CZ   | 2:D6:235:ILE:HD12 | 2.53                     | 0.42              |
| 3:D7:150:LEU:HD21 | 3:D7:154:LYS:HE2  | 2.01                     | 0.42              |
| 3:D7:173:PRO:HB3  | 3:D7:380:ARG:HH21 | 1.84                     | 0.42              |
| 3:E3:113:ILE:O    | 3:E3:117:LEU:HB2  | 2.20                     | 0.42              |
| 3:E7:187:LEU:HD13 | 3:E7:403:MET:HE1  | 2.02                     | 0.42              |
| 2:E8:345:ASP:OD1  | 2:E8:346:TRP:N    | 2.53                     | 0.42              |
| 3:F1:205:GLU:OE1  | 3:F1:205:GLU:N    | 2.53                     | 0.42              |
| 4:e:99:MET:HE3    | 4:e:99:MET:HB2    | 1.59                     | 0.42              |
| 4:g:149:ARG:HG2   | 4:g:161:TYR:HD2   | 1.83                     | 0.42              |
| 5:k:156:ARG:HA    | 5:k:156:ARG:HD3   | 1.77                     | 0.42              |
| 4:m:148:PHE:O     | 4:m:149:ARG:HG2   | 2.20                     | 0.42              |
| 4:n:8:SER:HB2     | 4:n:147:HIS:ND1   | 2.35                     | 0.42              |
| 4:n:139:PRO:O     | 4:n:143:ILE:HG12  | 2.20                     | 0.42              |
| 4:q:72:SER:HB3    | 4:q:108:ILE:HG22  | 2.02                     | 0.42              |
| 1:18:241:PHE:HE2  | 3:E5:42:LEU:HB2   | 1.85                     | 0.42              |
| 1:22:246:CYS:SG   | 1:22:247:TYR:N    | 2.93                     | 0.42              |
| 3:A7:66:MET:HE1   | 3:A7:147:MET:CE   | 2.48                     | 0.42              |
| 2:A8:90:GLU:HB2   | 2:A8:121:ARG:NH2  | 2.34                     | 0.42              |
| 2:B0:5:ILE:HD12   | 2:B0:125:LEU:HD23 | 2.02                     | 0.42              |
| 2:B0:250:VAL:HG22 | 2:B0:352:LYS:NZ   | 2.35                     | 0.42              |
| 3:B1:237:THR:HA   | 3:B1:240:LEU:HD13 | 2.02                     | 0.42              |
| 2:B2:156:ARG:HA   | 2:B2:159:VAL:HG12 | 2.02                     | 0.42              |
| 2:B2:163:LYS:HD3  | 2:B2:163:LYS:N    | 2.35                     | 0.42              |
| 2:B2:422:ARG:HD2  | 2:B2:422:ARG:HA   | 1.93                     | 0.42              |
| 2:B4:185:TYR:CD2  | 2:B4:395:PHE:HE1  | 2.37                     | 0.42              |
| 2:B4:268:MET:HE2  | 2:B4:268:MET:HB3  | 1.96                     | 0.42              |
| 3:B5:150:LEU:CD2  | 3:B5:154:LYS:HD2  | 2.50                     | 0.42              |
| 2:C2:241:SER:OG   | 2:C2:250:VAL:O    | 2.24                     | 0.42              |
| 2:C2:259:LEU:HD23 | 2:C2:259:LEU:HA   | 1.92                     | 0.42              |
| 3:C7:133:PHE:HB2  | 3:C7:164:MET:HB3  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C9:167:PHE:CE1  | 3:C9:200:GLN:HG3  | 2.54                     | 0.42              |
| 3:C9:174:LYS:HG3  | 3:C9:175:VAL:N    | 2.34                     | 0.42              |
| 2:D0:203:MET:HE2  | 2:D0:267:PHE:CD1  | 2.55                     | 0.42              |
| 2:D0:221:ARG:HH11 | 2:D0:221:ARG:HD3  | 1.72                     | 0.42              |
| 2:D0:311:LYS:O    | 2:D0:382:THR:HG23 | 2.20                     | 0.42              |
| 3:D1:290:THR:HA   | 3:D1:293:MET:HE2  | 2.02                     | 0.42              |
| 2:D4:220:GLU:OE1  | 4:r:191:GLU:OE1   | 2.37                     | 0.42              |
| 3:D5:68:LEU:HD12  | 3:D5:143:THR:HG22 | 2.02                     | 0.42              |
| 3:D5:77:ARG:HH22  | 3:D5:92:PHE:HZ    | 1.68                     | 0.42              |
| 3:D5:117:LEU:CD2  | 3:D5:154:LYS:HD2  | 2.47                     | 0.42              |
| 3:D7:273:LEU:HD23 | 3:D7:273:LEU:HA   | 1.88                     | 0.42              |
| 2:E6:316:CYS:CB   | 2:E6:352:LYS:HG3  | 2.50                     | 0.42              |
| 2:E6:345:ASP:OD1  | 2:E6:346:TRP:N    | 2.52                     | 0.42              |
| 2:E8:173:PRO:HG2  | 2:E8:391:MET:HE3  | 2.01                     | 0.42              |
| 3:E9:293:MET:SD   | 3:E9:367:PHE:HB2  | 2.60                     | 0.42              |
| 3:E9:399:THR:HA   | 3:E9:403:MET:HB2  | 2.01                     | 0.42              |
| 3:F1:47:ILE:HD12  | 3:F1:47:ILE:HA    | 1.93                     | 0.42              |
| 4:b:78:ALA:HB3    | 4:b:112:PHE:CE1   | 2.52                     | 0.42              |
| 5:l:18:GLN:CG     | 4:n:146:ARG:NH1   | 2.83                     | 0.42              |
| 4:m:18:ASN:CB     | 4:m:45:MET:HG3    | 2.50                     | 0.42              |
| 1:2:244:GLN:NE2   | 4:e:163:SER:N     | 2.68                     | 0.42              |
| 3:A1:10:GLY:O     | 3:A1:14:ASN:ND2   | 2.43                     | 0.42              |
| 3:A1:239:CYS:HB3  | 3:A1:248:SER:O    | 2.19                     | 0.42              |
| 2:A2:141:VAL:HG11 | 2:A2:172:TRP:CE3  | 2.54                     | 0.42              |
| 2:A4:112:LYS:HA   | 2:A4:115:VAL:HG12 | 2.00                     | 0.42              |
| 3:A5:201:VAL:HG11 | 3:A5:374:ILE:HD11 | 2.02                     | 0.42              |
| 2:A6:125:LEU:HD23 | 2:A6:125:LEU:HA   | 1.92                     | 0.42              |
| 2:A8:163:LYS:HA   | 2:A8:163:LYS:HE3  | 2.02                     | 0.42              |
| 2:B0:149:LEU:HD23 | 2:B0:149:LEU:HA   | 1.92                     | 0.42              |
| 2:B0:259:LEU:HD11 | 2:B0:316:CYS:HB2  | 2.01                     | 0.42              |
| 3:B1:181:GLU:HB2  | 3:B1:182:PRO:HD3  | 2.02                     | 0.42              |
| 3:B7:35:THR:HG22  | 4:g:83:PRO:HG3    | 2.01                     | 0.42              |
| 2:B8:215:ARG:HH12 | 2:B8:299:ALA:HB1  | 1.85                     | 0.42              |
| 3:C1:20:PHE:CE1   | 3:C1:24:ILE:HG13  | 2.55                     | 0.42              |
| 3:C1:181:GLU:HB2  | 3:C1:182:PRO:HD3  | 2.00                     | 0.42              |
| 3:C3:173:PRO:HA   | 3:C3:380:ARG:HH21 | 1.85                     | 0.42              |
| 2:C4:93:ILE:HD12  | 2:C4:114:ILE:HG13 | 2.02                     | 0.42              |
| 2:C6:103:PHE:HB3  | 2:C6:189:LEU:HD23 | 2.02                     | 0.42              |
| 2:C6:187:SER:O    | 2:C6:191:THR:HG23 | 2.20                     | 0.42              |
| 3:C9:113:ILE:HG12 | 3:C9:150:LEU:HD22 | 2.02                     | 0.42              |
| 2:D2:121:ARG:HD2  | 2:D2:121:ARG:HA   | 1.77                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D2:174:SER:HB2  | 2:D2:177:VAL:O    | 2.19                     | 0.42              |
| 3:D3:169:VAL:HG12 | 3:D3:202:ILE:HB   | 2.01                     | 0.42              |
| 3:D3:385:PHE:HE2  | 3:D3:412:GLU:HB2  | 1.84                     | 0.42              |
| 3:E3:46:ARG:CG    | 3:E3:46:ARG:NH2   | 2.82                     | 0.42              |
| 3:E5:2:ARG:HD3    | 3:E5:240:LEU:HD23 | 2.01                     | 0.42              |
| 2:F0:152:LEU:HD11 | 2:F0:156:ARG:HH11 | 1.85                     | 0.42              |
| 4:a:96:TYR:CZ     | 4:c:6:PHE:CE2     | 3.08                     | 0.42              |
| 4:e:97:ARG:NH1    | 4:g:161:TYR:CE1   | 2.88                     | 0.42              |
| 4:o:18:ASN:ND2    | 4:o:46:ASP:H      | 2.18                     | 0.42              |
| 4:o:48:ILE:HD12   | 4:o:48:ILE:HA     | 1.89                     | 0.42              |
| 4:r:9:PRO:HA      | 4:r:12:VAL:HG22   | 2.02                     | 0.42              |
| 4:s:94:ASN:O      | 4:s:98:THR:HG22   | 2.20                     | 0.42              |
| 4:t:67:HIS:CG     | 4:v:19:GLU:OE1    | 2.73                     | 0.42              |
| 4:v:48:ILE:HD12   | 4:v:48:ILE:HA     | 1.90                     | 0.42              |
| 5:x:66:LYS:HG3    | 5:x:67:ALA:N      | 2.35                     | 0.42              |
| 3:A1:117:LEU:HD13 | 3:A1:154:LYS:HZ2  | 1.82                     | 0.41              |
| 3:A1:274:THR:HG21 | 3:A1:282:ARG:HD2  | 2.02                     | 0.41              |
| 2:A4:363:VAL:HA   | 2:A4:364:PRO:HD3  | 1.95                     | 0.41              |
| 3:A5:181:GLU:HB2  | 3:A5:182:PRO:HD3  | 2.02                     | 0.41              |
| 2:A8:12:ALA:HB3   | 2:A8:140:ALA:HB2  | 2.01                     | 0.41              |
| 2:A8:221:ARG:HB3  | 3:A9:322:SER:CB   | 2.50                     | 0.41              |
| 3:A9:232:ALA:HB1  | 3:A9:268:ILE:HG21 | 2.02                     | 0.41              |
| 2:B4:25:CYS:SG    | 2:B4:86:LEU:HD11  | 2.59                     | 0.41              |
| 2:B4:154:LEU:HB3  | 2:B4:197:HIS:HB3  | 2.02                     | 0.41              |
| 2:B4:277:SER:OG   | 2:B4:278:ALA:N    | 2.53                     | 0.41              |
| 2:B4:284:GLU:OE2  | 2:B8:88:HIS:CD2   | 2.73                     | 0.41              |
| 2:B6:239:THR:OG1  | 2:B6:243:ARG:NH1  | 2.52                     | 0.41              |
| 2:B6:397:LEU:HD23 | 2:B6:397:LEU:HA   | 1.88                     | 0.41              |
| 2:B8:282:TYR:HE2  | 2:C2:85:HIS:CB    | 2.32                     | 0.41              |
| 3:B9:165:GLU:OE2  | 3:B9:200:GLN:NE2  | 2.52                     | 0.41              |
| 3:C1:167:PHE:HE1  | 3:C1:200:GLN:HE21 | 1.67                     | 0.41              |
| 2:C4:23:LEU:HD11  | 2:C4:233:GLN:OE1  | 2.20                     | 0.41              |
| 3:C5:32:PRO:HD3   | 3:C5:81:PHE:CZ    | 2.55                     | 0.41              |
| 2:D2:136:LEU:CD2  | 2:D2:235:ILE:HD11 | 2.48                     | 0.41              |
| 2:D2:241:SER:OG   | 2:D2:250:VAL:O    | 2.30                     | 0.41              |
| 3:D3:207:LEU:HB3  | 3:D3:225:LEU:HG   | 2.01                     | 0.41              |
| 2:D8:1:MET:N      | 2:D8:3:GLU:OE2    | 2.39                     | 0.41              |
| 3:E7:232:ALA:HB2  | 3:E7:270:PHE:HB2  | 2.02                     | 0.41              |
| 3:F1:382:SER:HA   | 3:F1:415:MET:HE1  | 2.02                     | 0.41              |
| 5:l:15:ARG:HG2    | 5:l:24:VAL:HB     | 2.01                     | 0.41              |
| 5:l:101:LEU:HA    | 5:l:104:LYS:HG2   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:12:241:PHE:CE1  | 3:D3:356:ILE:CG2  | 3.02                     | 0.41              |
| 1:17:248:ARG:NH2  | 4:t:94:ASN:HD22   | 2.18                     | 0.41              |
| 1:3:255:PRO:HG2   | 2:B0:364:PRO:HG2  | 2.02                     | 0.41              |
| 2:A0:73:THR:O     | 3:A1:46:ARG:NH1   | 2.53                     | 0.41              |
| 3:A3:172:SER:HB3  | 3:A3:205:GLU:HG2  | 2.03                     | 0.41              |
| 3:A5:409:THR:HA   | 3:A5:412:GLU:HG3  | 2.02                     | 0.41              |
| 2:A6:69:ASP:OD1   | 2:A6:70:LEU:N     | 2.54                     | 0.41              |
| 2:A8:107:HIS:CE1  | 2:A8:151:CYS:HB3  | 2.55                     | 0.41              |
| 2:A8:221:ARG:C    | 3:A9:322:SER:OG   | 2.63                     | 0.41              |
| 2:B0:33:ASP:HB2   | 4:d:102:GLY:O     | 2.20                     | 0.41              |
| 3:B3:241:ARG:HH11 | 3:B3:241:ARG:HD2  | 1.73                     | 0.41              |
| 2:B6:345:ASP:OD1  | 2:B6:346:TRP:N    | 2.53                     | 0.41              |
| 3:B7:383:ASP:HA   | 3:B7:386:THR:HG22 | 2.00                     | 0.41              |
| 2:B8:192:HIS:ND1  | 2:B8:424:ASP:OD2  | 2.48                     | 0.41              |
| 2:C2:170:CYS:HB2  | 2:C2:203:MET:HE1  | 2.02                     | 0.41              |
| 3:C5:121:ARG:NH1  | 3:C5:158:GLU:OE1  | 2.45                     | 0.41              |
| 3:C5:286:VAL:N    | 3:C5:287:PRO:HD2  | 2.35                     | 0.41              |
| 2:C6:231:ILE:HD13 | 2:C6:302:MET:HE1  | 2.01                     | 0.41              |
| 3:C7:248:SER:HA   | 3:C7:252:LYS:HD3  | 2.02                     | 0.41              |
| 2:C8:121:ARG:HA   | 2:C8:121:ARG:HD2  | 1.87                     | 0.41              |
| 3:C9:19:LYS:HA    | 3:C9:19:LYS:HD3   | 1.83                     | 0.41              |
| 3:C9:128:ASP:OD1  | 3:C9:129:CYS:N    | 2.47                     | 0.41              |
| 3:D1:293:MET:HE2  | 3:D1:293:MET:HB3  | 1.77                     | 0.41              |
| 3:D3:117:LEU:HD11 | 3:D3:154:LYS:HD3  | 2.02                     | 0.41              |
| 2:D6:154:LEU:HB3  | 2:D6:197:HIS:HB3  | 2.02                     | 0.41              |
| 2:E2:11:GLN:HE22  | 3:E3:246:LEU:HD12 | 1.84                     | 0.41              |
| 2:E4:403:ALA:HA   | 3:E5:260:PHE:CE1  | 2.56                     | 0.41              |
| 3:E5:180:VAL:HB   | 3:E5:183:TYR:HB2  | 2.03                     | 0.41              |
| 3:E5:286:VAL:HG23 | 3:E5:287:PRO:HD3  | 2.00                     | 0.41              |
| 3:E7:347:ASN:C    | 3:E7:347:ASN:HD22 | 2.28                     | 0.41              |
| 2:E8:71:GLU:HB3   | 2:E8:98:ASP:HB2   | 2.01                     | 0.41              |
| 3:E9:113:ILE:HG13 | 3:E9:150:LEU:HD22 | 2.01                     | 0.41              |
| 3:E9:128:ASP:OD1  | 3:E9:128:ASP:N    | 2.50                     | 0.41              |
| 3:E9:167:PHE:CZ   | 3:E9:233:MET:HG2  | 2.55                     | 0.41              |
| 3:E9:259:PRO:HB2  | 3:E9:260:PHE:HD1  | 1.86                     | 0.41              |
| 3:F1:156:ARG:HD3  | 3:F1:164:MET:HE3  | 2.01                     | 0.41              |
| 3:F1:187:LEU:HD11 | 3:F1:408:PHE:CE1  | 2.55                     | 0.41              |
| 4:a:49:LEU:HD21   | 4:a:177:GLY:H     | 1.85                     | 0.41              |
| 4:f:68:LEU:HB2    | 4:f:206:PHE:HD2   | 1.84                     | 0.41              |
| 4:g:187:SER:OG    | 4:g:188:GLY:N     | 2.52                     | 0.41              |
| 1:9:243:ALA:CB    | 3:C3:356:ILE:CD1  | 2.99                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A0:27:GLU:OE2   | 2:A0:236:SER:OG   | 2.37                     | 0.41              |
| 2:A0:172:TRP:CZ2  | 2:A0:391:MET:HG3  | 2.56                     | 0.41              |
| 2:A0:216:ASN:HD22 | 2:A0:275:ILE:HG13 | 1.86                     | 0.41              |
| 2:A0:259:LEU:HD21 | 2:A0:316:CYS:HB2  | 2.02                     | 0.41              |
| 3:A1:43:GLN:HA    | 3:A1:242:PHE:HE1  | 1.84                     | 0.41              |
| 3:A3:271:ALA:HB3  | 3:A3:365:VAL:HG22 | 2.01                     | 0.41              |
| 2:A4:264:ARG:HD3  | 2:A4:431:ASP:OD2  | 2.19                     | 0.41              |
| 2:A6:271:SER:OG   | 2:A6:377:MET:HB3  | 2.20                     | 0.41              |
| 2:B4:250:VAL:HG13 | 2:B4:318:MET:HE1  | 2.01                     | 0.41              |
| 2:B6:5:ILE:HG12   | 2:B6:132:LEU:HD11 | 2.02                     | 0.41              |
| 3:B7:152:ILE:HG22 | 3:B7:195:ASN:HB3  | 2.02                     | 0.41              |
| 3:C1:391:ARG:HE   | 3:C1:391:ARG:HB3  | 1.78                     | 0.41              |
| 2:C2:210:TYR:CE1  | 2:C2:227:LEU:HD21 | 2.56                     | 0.41              |
| 3:C3:190:HIS:HB2  | 3:C3:414:ASN:ND2  | 2.29                     | 0.41              |
| 2:C4:208:ALA:O    | 2:C4:212:ILE:HG12 | 2.19                     | 0.41              |
| 2:C8:166:LYS:HE3  | 2:C8:166:LYS:HB3  | 1.95                     | 0.41              |
| 2:C8:210:TYR:HB3  | 3:C9:324:LYS:NZ   | 2.36                     | 0.41              |
| 2:C8:215:ARG:HH22 | 2:C8:300:SER:HB2  | 1.84                     | 0.41              |
| 2:C8:288:VAL:HG21 | 2:C8:323:VAL:HG23 | 2.03                     | 0.41              |
| 2:C8:407:TRP:HH2  | 3:C9:254:ALA:HB1  | 1.85                     | 0.41              |
| 2:D2:99:ALA:HA    | 2:D2:110:ILE:HD11 | 2.02                     | 0.41              |
| 2:D4:258:ASN:ND2  | 2:D4:352:LYS:HD3  | 2.35                     | 0.41              |
| 2:D4:279:GLU:OE2  | 4:r:198:ARG:HG2   | 2.20                     | 0.41              |
| 3:D5:156:ARG:NH2  | 3:D5:197:ASP:HB2  | 2.35                     | 0.41              |
| 3:D5:283:ALA:HB2  | 3:D9:53:GLU:O     | 2.21                     | 0.41              |
| 3:D7:299:MET:HE1  | 3:D7:367:PHE:HD2  | 1.84                     | 0.41              |
| 2:D8:282:TYR:HB2  | 4:t:202:ARG:NH1   | 2.35                     | 0.41              |
| 2:E0:214:ARG:NH1  | 2:E0:220:GLU:OE2  | 2.52                     | 0.41              |
| 2:E2:176:GLN:HB3  | 3:E3:331:LEU:CD1  | 2.50                     | 0.41              |
| 2:E4:109:THR:HG23 | 2:E4:411:GLU:OE1  | 2.20                     | 0.41              |
| 2:E6:230:LEU:HD21 | 2:E6:368:LEU:HD11 | 2.01                     | 0.41              |
| 3:E7:8:GLN:OE1    | 3:E7:17:GLY:HA3   | 2.20                     | 0.41              |
| 3:E7:362:LYS:HD2  | 3:E7:363:MET:HB2  | 2.02                     | 0.41              |
| 3:F1:44:LEU:HD21  | 5:x:48:GLN:OE1    | 2.20                     | 0.41              |
| 3:F1:112:LEU:HG   | 3:F1:112:LEU:O    | 2.21                     | 0.41              |
| 4:a:192:GLY:O     | 4:a:193:ASP:HB2   | 2.20                     | 0.41              |
| 4:j:84:LYS:HD2    | 4:j:84:LYS:HA     | 1.93                     | 0.41              |
| 2:A8:210:TYR:CD2  | 3:A9:324:LYS:HG3  | 2.55                     | 0.41              |
| 2:A8:225:THR:O    | 2:A8:229:ARG:HG2  | 2.21                     | 0.41              |
| 3:A9:33:THR:HG23  | 3:A9:35:THR:HG23  | 2.03                     | 0.41              |
| 3:A9:316:MET:HE2  | 3:A9:366:THR:HG23 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B1:238:CYS:HB3  | 3:B1:318:ARG:NH1  | 2.35                     | 0.41              |
| 2:B2:3:GLU:OE1    | 2:B2:64:ARG:NE    | 2.53                     | 0.41              |
| 2:B2:298:PRO:HB3  | 2:B2:307:PRO:HD2  | 2.02                     | 0.41              |
| 3:B5:377:MET:HE2  | 3:B5:377:MET:HB3  | 1.93                     | 0.41              |
| 3:B7:128:ASP:OD1  | 3:B7:129:CYS:N    | 2.41                     | 0.41              |
| 3:B7:175:VAL:HG11 | 2:B8:332:VAL:HG13 | 2.02                     | 0.41              |
| 2:B8:84:ARG:HH21  | 4:h:197:LEU:HD11  | 1.85                     | 0.41              |
| 2:C0:274:PRO:HD2  | 2:C0:374:ALA:HA   | 2.02                     | 0.41              |
| 2:C6:154:LEU:HG   | 2:C6:197:HIS:HB3  | 2.01                     | 0.41              |
| 2:C6:215:ARG:HB2  | 2:C6:215:ARG:HH11 | 1.85                     | 0.41              |
| 3:C9:220:PRO:HG2  | 2:D0:326:LYS:CD   | 2.51                     | 0.41              |
| 2:D2:163:LYS:HE3  | 2:D2:163:LYS:HB3  | 1.79                     | 0.41              |
| 3:D3:317:PHE:HB3  | 3:D3:321:MET:SD   | 2.60                     | 0.41              |
| 2:D4:28:HIS:CE1   | 2:D4:243:ARG:HD2  | 2.56                     | 0.41              |
| 2:D4:180:ALA:HB3  | 2:D4:183:GLU:HG3  | 2.00                     | 0.41              |
| 2:D4:278:ALA:HB1  | 4:r:200:ASP:HB3   | 2.01                     | 0.41              |
| 2:D6:221:ARG:HB3  | 3:D7:322:SER:CB   | 2.51                     | 0.41              |
| 3:E1:395:LEU:O    | 3:E1:395:LEU:HG   | 2.21                     | 0.41              |
| 3:E3:165:GLU:OE1  | 3:E3:200:GLN:NE2  | 2.53                     | 0.41              |
| 2:E4:132:LEU:HG   | 2:E4:164:LYS:HZ3  | 1.85                     | 0.41              |
| 4:d:170:VAL:HG22  | 4:d:185:ILE:HD11  | 2.01                     | 0.41              |
| 1:5:242:ASN:OD1   | 4:h:154:TYR:CG    | 2.73                     | 0.41              |
| 3:A3:113:ILE:HA   | 3:A3:116:VAL:HG22 | 2.01                     | 0.41              |
| 2:A4:207:GLU:HA   | 2:A4:210:TYR:CD2  | 2.55                     | 0.41              |
| 3:B1:249:ASP:H    | 3:B1:252:LYS:CB   | 2.33                     | 0.41              |
| 3:B3:211:CYS:SG   | 3:B3:217:LEU:HB2  | 2.61                     | 0.41              |
| 2:B4:272:TYR:HD2  | 2:B4:275:ILE:HD11 | 1.86                     | 0.41              |
| 3:B7:375:GLN:HE22 | 3:B7:419:VAL:HA   | 1.85                     | 0.41              |
| 3:B9:46:ARG:HE    | 3:B9:46:ARG:HB2   | 1.39                     | 0.41              |
| 2:C0:76:ASP:HA    | 2:C0:79:ARG:HD2   | 2.02                     | 0.41              |
| 2:C0:254:GLU:HA   | 2:C0:257:THR:HG22 | 2.03                     | 0.41              |
| 2:C4:141:VAL:HG11 | 2:C4:172:TRP:CE3  | 2.56                     | 0.41              |
| 3:C5:105:HIS:ND1  | 3:C5:150:LEU:HB2  | 2.36                     | 0.41              |
| 2:C8:274:PRO:HB2  | 2:C8:276:ILE:HG12 | 2.01                     | 0.41              |
| 2:D2:69:ASP:O     | 2:D2:94:SER:HA    | 2.20                     | 0.41              |
| 2:D2:404:PHE:CZ   | 3:D3:312:THR:HG21 | 2.55                     | 0.41              |
| 2:D6:174:SER:HB2  | 2:D6:177:VAL:O    | 2.20                     | 0.41              |
| 3:E3:192:LEU:HD21 | 3:E3:199:VAL:HG21 | 2.03                     | 0.41              |
| 3:E5:281:TYR:HD2  | 3:E9:86:ARG:HA    | 1.84                     | 0.41              |
| 2:E6:203:MET:SD   | 2:E6:267:PHE:HD2  | 2.44                     | 0.41              |
| 3:F1:258:ILE:HG13 | 3:F1:258:ILE:O    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:d:28:LYS:HD3    | 4:d:28:LYS:HA     | 1.68                     | 0.41              |
| 4:f:10:LEU:HG     | 4:f:143:ILE:HG22  | 2.02                     | 0.41              |
| 1:23:254:LYS:HB3  | 2:C4:364:PRO:HD2  | 2.02                     | 0.41              |
| 1:7:242:ASN:OD1   | 1:7:242:ASN:N     | 2.53                     | 0.41              |
| 3:A1:24:ILE:HD13  | 3:A1:24:ILE:HA    | 1.98                     | 0.41              |
| 2:A2:119:LEU:HD23 | 2:A2:119:LEU:HA   | 1.85                     | 0.41              |
| 2:A2:212:ILE:HG23 | 2:A2:275:ILE:HD12 | 2.03                     | 0.41              |
| 2:A4:288:VAL:HG21 | 2:A4:323:VAL:HG13 | 2.02                     | 0.41              |
| 3:A5:5:VAL:HB     | 3:A5:133:PHE:CD1  | 2.56                     | 0.41              |
| 3:A5:216:LYS:HA   | 3:A5:216:LYS:HD2  | 1.91                     | 0.41              |
| 3:A7:6:HIS:CD2    | 3:A7:8:GLN:HG3    | 2.55                     | 0.41              |
| 3:A7:173:PRO:HB3  | 3:A7:380:ARG:HD2  | 2.03                     | 0.41              |
| 2:A8:6:SER:OG     | 2:A8:8:HIS:NE2    | 2.45                     | 0.41              |
| 3:B5:253:LEU:O    | 3:B5:257:LEU:HB2  | 2.20                     | 0.41              |
| 2:B6:342:GLN:OE1  | 2:B6:342:GLN:HA   | 2.20                     | 0.41              |
| 3:B7:156:ARG:NH1  | 3:B7:197:ASP:OD1  | 2.53                     | 0.41              |
| 2:B8:174:SER:OG   | 2:B8:205:ASP:OD1  | 2.37                     | 0.41              |
| 2:B8:185:TYR:HE1  | 2:B8:398:MET:HG2  | 1.85                     | 0.41              |
| 3:B9:12:CYS:SG    | 3:B9:169:VAL:HG21 | 2.61                     | 0.41              |
| 3:B9:141:GLY:O    | 3:B9:145:SER:OG   | 2.30                     | 0.41              |
| 2:C2:417:GLU:HA   | 2:C2:420:GLU:HG3  | 2.01                     | 0.41              |
| 2:C4:210:TYR:CD1  | 2:C4:227:LEU:HD21 | 2.56                     | 0.41              |
| 3:C5:190:HIS:HA   | 3:C5:193:VAL:HG22 | 2.03                     | 0.41              |
| 2:C6:282:TYR:CB   | 4:n:202:ARG:HD2   | 2.51                     | 0.41              |
| 3:C7:165:GLU:HG3  | 3:C7:198:GLU:HG3  | 2.02                     | 0.41              |
| 3:C9:166:THR:OG1  | 3:C9:199:VAL:HG22 | 2.20                     | 0.41              |
| 2:D0:278:ALA:O    | 4:p:202:ARG:NH2   | 2.53                     | 0.41              |
| 3:D1:117:LEU:HA   | 3:D1:117:LEU:HD13 | 1.97                     | 0.41              |
| 3:D3:117:LEU:HA   | 3:D3:117:LEU:HD23 | 1.84                     | 0.41              |
| 3:D3:397:TRP:CG   | 2:D4:257:THR:HG1  | 2.38                     | 0.41              |
| 3:D7:27:GLU:HA    | 3:D7:359:LYS:HD2  | 2.02                     | 0.41              |
| 3:D9:24:ILE:HD13  | 3:D9:24:ILE:HA    | 1.93                     | 0.41              |
| 3:D9:239:CYS:SG   | 3:D9:247:ASN:HB3  | 2.61                     | 0.41              |
| 2:E6:209:ILE:HD13 | 2:E6:231:ILE:HD11 | 2.01                     | 0.41              |
| 2:F0:392:ASP:OD1  | 2:F0:422:ARG:NE   | 2.51                     | 0.41              |
| 3:F1:172:SER:HB2  | 3:F1:205:GLU:CD   | 2.46                     | 0.41              |
| 4:a:129:MET:HG2   | 4:a:131:TRP:CZ2   | 2.55                     | 0.41              |
| 4:e:110:ILE:O     | 4:e:131:TRP:HB2   | 2.19                     | 0.41              |
| 4:t:181:GLN:NE2   | 4:t:200:ASP:OD1   | 2.54                     | 0.41              |
| 2:A2:91:GLN:HA    | 2:A2:121:ARG:NH1  | 2.33                     | 0.41              |
| 3:A3:12:CYS:CB    | 3:A3:138:SER:HB2  | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A3:412:GLU:OE1  | 3:A3:416:ASN:ND2  | 2.53                     | 0.41              |
| 2:A4:115:VAL:HG21 | 2:A4:152:LEU:HG   | 2.02                     | 0.41              |
| 3:A5:2:ARG:NH2    | 3:A5:249:ASP:OD2  | 2.53                     | 0.41              |
| 3:A5:316:MET:HE3  | 3:A5:316:MET:HB3  | 1.91                     | 0.41              |
| 2:A6:27:GLU:HG3   | 2:A6:361:THR:HG21 | 2.03                     | 0.41              |
| 2:A6:188:VAL:HG23 | 2:A6:391:MET:HE3  | 2.03                     | 0.41              |
| 2:A6:340:THR:HG23 | 2:A6:341:ILE:HG13 | 2.02                     | 0.41              |
| 3:A7:140:GLY:O    | 3:A7:184:ASN:ND2  | 2.50                     | 0.41              |
| 3:A9:63:ALA:O     | 3:A9:89:ASN:ND2   | 2.54                     | 0.41              |
| 3:A9:200:GLN:HB3  | 3:A9:268:ILE:HD11 | 2.01                     | 0.41              |
| 3:B1:263:LEU:HD23 | 3:B1:263:LEU:H    | 1.85                     | 0.41              |
| 2:B2:221:ARG:HG3  | 2:B2:221:ARG:HH11 | 1.86                     | 0.41              |
| 2:B2:221:ARG:HH11 | 2:B2:221:ARG:CG   | 2.33                     | 0.41              |
| 3:B3:114:ASP:OD1  | 3:B3:114:ASP:N    | 2.54                     | 0.41              |
| 3:B3:128:ASP:OD1  | 3:B3:128:ASP:N    | 2.53                     | 0.41              |
| 3:B5:200:GLN:HB3  | 3:B5:268:ILE:HD11 | 2.02                     | 0.41              |
| 3:C1:148:GLY:O    | 3:C1:152:ILE:HG13 | 2.21                     | 0.41              |
| 2:C2:425:LEU:HA   | 2:C2:425:LEU:HD23 | 1.80                     | 0.41              |
| 2:C4:192:HIS:ND1  | 2:C4:424:ASP:OD2  | 2.49                     | 0.41              |
| 3:C5:221:THR:O    | 3:C5:225:LEU:HD23 | 2.19                     | 0.41              |
| 3:C7:238:CYS:SG   | 3:C7:239:CYS:N    | 2.94                     | 0.41              |
| 3:C7:325:GLU:HA   | 3:C7:328:GLU:HG2  | 2.02                     | 0.41              |
| 3:C9:228:LEU:HA   | 3:C9:228:LEU:HD23 | 1.84                     | 0.41              |
| 2:D0:425:LEU:HD12 | 2:D0:425:LEU:HA   | 1.93                     | 0.41              |
| 3:D1:66:MET:HE1   | 3:D1:151:LEU:HD22 | 2.03                     | 0.41              |
| 3:D3:187:LEU:HD21 | 3:D3:408:PHE:CD1  | 2.56                     | 0.41              |
| 3:D3:383:ASP:HA   | 3:D3:386:THR:HG22 | 2.02                     | 0.41              |
| 3:D5:309:ARG:HH11 | 3:D5:309:ARG:HD2  | 1.53                     | 0.41              |
| 3:D7:117:LEU:HD23 | 3:D7:121:ARG:NH2  | 2.36                     | 0.41              |
| 3:E5:396:HIS:HA   | 3:E5:399:THR:HG22 | 2.02                     | 0.41              |
| 2:E6:364:PRO:HD3  | 5:x:161:PHE:CZ    | 2.55                     | 0.41              |
| 2:E8:189:LEU:HD21 | 2:E8:418:PHE:CD1  | 2.56                     | 0.41              |
| 2:E8:213:CYS:HA   | 2:E8:217:LEU:HB3  | 2.03                     | 0.41              |
| 2:F0:231:ILE:O    | 2:F0:235:ILE:HG12 | 2.21                     | 0.41              |
| 4:b:115:LEU:HD21  | 4:b:145:LYS:CE    | 2.50                     | 0.41              |
| 5:k:57:TYR:HE1    | 5:k:61:ASN:HD22   | 1.66                     | 0.41              |
| 4:o:73:VAL:HG12   | 4:o:109:GLU:HB3   | 2.03                     | 0.41              |
| 4:o:184:PRO:HB2   | 4:o:189:LEU:HB2   | 2.03                     | 0.41              |
| 4:r:8:SER:OG      | 4:r:11:ASN:ND2    | 2.54                     | 0.41              |
| 4:u:146:ARG:NH1   | 4:u:156:VAL:HG11  | 2.36                     | 0.41              |
| 1:23:256:LEU:HA   | 1:23:257:PRO:HD3  | 1.96                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A2:137:MET:HB3  | 2:A2:168:ASN:HA   | 2.02                     | 0.41              |
| 3:A3:112:LEU:HD12 | 3:A3:112:LEU:HA   | 1.92                     | 0.41              |
| 2:A6:262:TYR:HB3  | 2:A6:263:PRO:HD2  | 2.02                     | 0.41              |
| 3:A7:114:ASP:OD1  | 3:A7:115:SER:N    | 2.54                     | 0.41              |
| 3:B1:382:SER:OG   | 3:B1:412:GLU:OE2  | 2.33                     | 0.41              |
| 2:B2:180:ALA:O    | 3:B3:347:ASN:ND2  | 2.54                     | 0.41              |
| 2:B4:359:PRO:HA   | 2:B4:360:PRO:HD3  | 1.96                     | 0.41              |
| 3:B9:107:THR:HG21 | 3:B9:401:GLU:OE1  | 2.21                     | 0.41              |
| 2:C0:396:ASP:CG   | 2:C0:422:ARG:HH21 | 2.28                     | 0.41              |
| 3:C1:128:ASP:OD1  | 3:C1:129:CYS:N    | 2.52                     | 0.41              |
| 3:C1:211:CYS:HA   | 3:C1:215:LEU:HB2  | 2.03                     | 0.41              |
| 3:C7:256:ASN:HD21 | 3:C7:350:LYS:HD3  | 1.86                     | 0.41              |
| 2:D0:96:LYS:HD2   | 2:D0:96:LYS:HA    | 1.88                     | 0.41              |
| 3:D1:375:GLN:HG3  | 3:D1:419:VAL:HG13 | 2.02                     | 0.41              |
| 2:D4:30:ILE:HG22  | 2:D4:36:MET:HB3   | 2.03                     | 0.41              |
| 3:D5:32:PRO:HD3   | 3:D5:81:PHE:CZ    | 2.54                     | 0.41              |
| 2:D8:100:ALA:HB1  | 3:D9:252:LYS:HA   | 2.02                     | 0.41              |
| 3:D9:35:THR:HG22  | 4:r:83:PRO:HG3    | 2.03                     | 0.41              |
| 2:E4:98:ASP:OD1   | 2:E4:99:ALA:N     | 2.52                     | 0.41              |
| 2:F0:320:ARG:HG2  | 2:F0:360:PRO:HG3  | 2.03                     | 0.41              |
| 4:b:92:LEU:HA     | 4:b:92:LEU:HD23   | 1.82                     | 0.41              |
| 4:i:55:LEU:HD21   | 4:i:111:ILE:HD13  | 2.02                     | 0.41              |
| 4:j:146:ARG:NH1   | 4:j:156:VAL:HG11  | 2.36                     | 0.41              |
| 5:l:163:LYS:HE2   | 5:l:163:LYS:HB2   | 1.80                     | 0.41              |
| 4:o:88:LEU:HD11   | 4:o:185:ILE:HD13  | 2.02                     | 0.41              |
| 4:s:184:PRO:HB2   | 4:s:189:LEU:HB2   | 2.02                     | 0.41              |
| 4:u:172:VAL:O     | 4:u:180:ALA:N     | 2.51                     | 0.41              |
| 5:w:158:ASP:OD1   | 5:w:160:ARG:NE    | 2.53                     | 0.41              |
| 1:5:256:LEU:CD2   | 2:B4:31:GLN:HA    | 2.47                     | 0.41              |
| 2:A0:210:TYR:HD1  | 2:A0:210:TYR:HA   | 1.76                     | 0.41              |
| 2:A0:269:LEU:HD23 | 2:A0:303:ALA:HB3  | 2.02                     | 0.41              |
| 3:A1:365:VAL:HG22 | 3:A1:366:THR:N    | 2.35                     | 0.41              |
| 2:A4:372:MET:HE3  | 2:A4:372:MET:HB3  | 1.78                     | 0.41              |
| 3:A5:229:VAL:O    | 3:A5:233:MET:HG3  | 2.21                     | 0.41              |
| 3:A5:326:VAL:O    | 3:A5:330:MET:HG2  | 2.21                     | 0.41              |
| 2:A6:370:LYS:HE3  | 2:A6:370:LYS:HB3  | 1.83                     | 0.41              |
| 3:A7:190:HIS:HB2  | 3:A7:414:ASN:ND2  | 2.34                     | 0.41              |
| 3:A7:259:PRO:HG2  | 3:A7:311:LEU:CD2  | 2.49                     | 0.41              |
| 3:A9:192:LEU:HD21 | 3:A9:199:VAL:HG21 | 2.02                     | 0.41              |
| 3:A9:217:LEU:HD23 | 3:A9:217:LEU:HA   | 1.91                     | 0.41              |
| 2:B0:73:THR:CA    | 3:B1:46:ARG:HH11  | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:5:ILE:HG12   | 2:B2:132:LEU:HD11 | 2.03                     | 0.41              |
| 2:B2:181:VAL:HG11 | 3:B3:256:ASN:O    | 2.21                     | 0.41              |
| 2:B4:311:LYS:H    | 2:B4:382:THR:CG2  | 2.34                     | 0.41              |
| 2:B6:215:ARG:NH2  | 2:B6:299:ALA:O    | 2.53                     | 0.41              |
| 2:B6:392:ASP:HA   | 2:B6:422:ARG:HH12 | 1.86                     | 0.41              |
| 2:B6:392:ASP:CG   | 2:B6:422:ARG:HH22 | 2.23                     | 0.41              |
| 3:B7:13:GLY:HA2   | 3:B7:136:THR:HG22 | 2.03                     | 0.41              |
| 3:B7:192:LEU:HD21 | 3:B7:199:VAL:HG21 | 2.03                     | 0.41              |
| 2:B8:69:ASP:OD1   | 2:B8:70:LEU:N     | 2.54                     | 0.41              |
| 2:B8:283:HIS:CE1  | 2:C2:89:PRO:HD3   | 2.56                     | 0.41              |
| 2:C0:181:VAL:H    | 3:C1:256:ASN:HD21 | 1.69                     | 0.41              |
| 2:C0:275:ILE:HD12 | 2:C0:368:LEU:HD11 | 2.02                     | 0.41              |
| 2:C2:53:PHE:O     | 2:C2:64:ARG:NH2   | 2.54                     | 0.41              |
| 2:C2:207:GLU:HA   | 2:C2:210:TYR:HB2  | 2.03                     | 0.41              |
| 3:C3:316:MET:HE1  | 3:C3:368:VAL:HG13 | 2.03                     | 0.41              |
| 2:C4:105:ARG:HG2  | 2:C4:411:GLU:HG2  | 2.03                     | 0.41              |
| 2:C4:356:ASN:OD1  | 2:C4:357:TYR:N    | 2.51                     | 0.41              |
| 3:C5:282:ARG:NH1  | 3:C5:288:GLU:OE2  | 2.54                     | 0.41              |
| 2:C6:282:TYR:HB2  | 4:n:202:ARG:CD    | 2.50                     | 0.41              |
| 3:C7:417:ASP:O    | 3:C7:420:SER:OG   | 2.27                     | 0.41              |
| 3:C9:22:GLU:HG3   | 3:C9:81:PHE:CD2   | 2.56                     | 0.41              |
| 3:C9:190:HIS:HA   | 3:C9:193:VAL:HG12 | 2.03                     | 0.41              |
| 2:D0:88:HIS:CD2   | 2:D0:90:GLU:HB3   | 2.55                     | 0.41              |
| 2:D0:207:GLU:HA   | 2:D0:210:TYR:HB2  | 2.03                     | 0.41              |
| 2:D0:278:ALA:CB   | 4:p:200:ASP:HB3   | 2.47                     | 0.41              |
| 3:D1:128:ASP:CG   | 3:D1:129:CYS:H    | 2.28                     | 0.41              |
| 2:D2:122:ILE:HD13 | 2:D2:122:ILE:HA   | 1.95                     | 0.41              |
| 2:D2:176:GLN:OE1  | 3:D3:331:LEU:HD21 | 2.20                     | 0.41              |
| 3:D3:173:PRO:HD2  | 3:D3:205:GLU:HG3  | 2.02                     | 0.41              |
| 3:D3:191:GLN:HA   | 3:D3:194:GLU:HG2  | 2.03                     | 0.41              |
| 2:D6:79:ARG:O     | 2:D6:84:ARG:HG2   | 2.21                     | 0.41              |
| 2:D6:123:ARG:HH11 | 2:D6:123:ARG:HG3  | 1.86                     | 0.41              |
| 2:D6:270:SER:HB2  | 2:D6:302:MET:HB2  | 2.03                     | 0.41              |
| 2:D6:272:TYR:HD2  | 2:D6:275:ILE:HG23 | 1.86                     | 0.41              |
| 3:D7:20:PHE:HA    | 3:D7:230:SER:HB2  | 2.03                     | 0.41              |
| 3:D7:220:PRO:HG2  | 2:D8:326:LYS:HD2  | 2.03                     | 0.41              |
| 3:D7:228:LEU:HD23 | 3:D7:228:LEU:HA   | 1.97                     | 0.41              |
| 2:D8:12:ALA:CB    | 2:D8:140:ALA:HB2  | 2.50                     | 0.41              |
| 2:D8:392:ASP:OD1  | 2:D8:422:ARG:NH2  | 2.49                     | 0.41              |
| 2:E0:50:ASN:O     | 2:E0:64:ARG:NH2   | 2.54                     | 0.41              |
| 2:E0:105:ARG:HH12 | 3:E1:251:ARG:HD3  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E1:113:ILE:HD11 | 3:E1:151:LEU:HD13 | 2.02                     | 0.41              |
| 3:E1:207:LEU:HB3  | 3:E1:225:LEU:HD22 | 2.02                     | 0.41              |
| 2:E2:363:VAL:HA   | 2:E2:364:PRO:HD3  | 1.94                     | 0.41              |
| 2:E4:276:ILE:HD11 | 2:E4:280:LYS:HG2  | 2.03                     | 0.41              |
| 3:E5:326:VAL:O    | 3:E5:330:MET:HG2  | 2.20                     | 0.41              |
| 3:E5:403:MET:HB2  | 3:E5:403:MET:HE3  | 1.69                     | 0.41              |
| 3:E7:2:ARG:HD2    | 3:E7:240:LEU:HD23 | 2.03                     | 0.41              |
| 3:E7:28:HIS:HA    | 3:E7:43:GLN:HG2   | 2.02                     | 0.41              |
| 3:E7:341:PHE:CZ   | 3:E7:349:MET:HE1  | 2.56                     | 0.41              |
| 2:E8:141:VAL:HG11 | 2:E8:172:TRP:CZ3  | 2.56                     | 0.41              |
| 2:E8:212:ILE:HD13 | 2:E8:212:ILE:HA   | 1.95                     | 0.41              |
| 2:E8:339:ARG:HD2  | 2:E8:339:ARG:HA   | 1.82                     | 0.41              |
| 2:F0:313:MET:HE3  | 2:F0:346:TRP:HZ2  | 1.86                     | 0.41              |
| 3:F1:19:LYS:HZ1   | 3:F1:227:HIS:HB2  | 1.85                     | 0.41              |
| 3:F1:133:PHE:HZ   | 3:F1:159:TYR:HD2  | 1.68                     | 0.41              |
| 3:F1:314:SER:HB3  | 3:F1:368:VAL:HG13 | 2.03                     | 0.41              |
| 3:F1:330:MET:HG2  | 3:F1:349:MET:HG2  | 2.02                     | 0.41              |
| 4:a:88:LEU:O      | 4:a:88:LEU:HD23   | 2.19                     | 0.41              |
| 4:e:95:TYR:CZ     | 4:e:99:MET:HE1    | 2.56                     | 0.41              |
| 4:f:35:ASN:N      | 4:f:35:ASN:ND2    | 2.69                     | 0.41              |
| 4:i:55:LEU:HD21   | 4:i:111:ILE:CD1   | 2.51                     | 0.41              |
| 4:m:10:LEU:HD12   | 4:m:147:HIS:CD2   | 2.56                     | 0.41              |
| 4:n:172:VAL:HG21  | 4:n:199:TRP:HE1   | 1.86                     | 0.41              |
| 4:t:63:ILE:HA     | 4:t:64:PRO:HD3    | 1.92                     | 0.41              |
| 5:w:83:PHE:O      | 5:w:87:ARG:HB2    | 2.21                     | 0.41              |
| 1:8:250:GLU:CD    | 2:C0:229:ARG:HH21 | 2.28                     | 0.41              |
| 2:A0:301:MET:HE1  | 2:A0:304:LYS:N    | 2.35                     | 0.41              |
| 3:A1:136:THR:HG22 | 3:A1:167:PHE:HD2  | 1.85                     | 0.41              |
| 3:A3:113:ILE:HA   | 3:A3:113:ILE:HD13 | 1.97                     | 0.41              |
| 2:A4:210:TYR:CG   | 3:A5:324:LYS:HE2  | 2.56                     | 0.41              |
| 2:A6:132:LEU:H    | 2:A6:132:LEU:HD23 | 1.86                     | 0.41              |
| 2:B0:95:GLY:C     | 2:B0:96:LYS:HG2   | 2.45                     | 0.41              |
| 3:B1:248:SER:HA   | 3:B1:252:LYS:HG2  | 2.02                     | 0.41              |
| 2:B4:274:PRO:HG3  | 2:B4:286:LEU:CD1  | 2.50                     | 0.41              |
| 3:B9:50:PHE:CE2   | 3:B9:241:ARG:HD3  | 2.55                     | 0.41              |
| 2:C0:387:VAL:HG13 | 2:C0:388:PHE:CD1  | 2.56                     | 0.41              |
| 3:C3:103:LYS:HB3  | 3:C3:103:LYS:HE2  | 1.86                     | 0.41              |
| 3:C5:213:ARG:HH22 | 3:C5:297:LYS:HG3  | 1.85                     | 0.41              |
| 2:C8:340:THR:O    | 2:C8:340:THR:HG22 | 2.21                     | 0.41              |
| 2:D2:230:LEU:HD21 | 2:D2:368:LEU:HD11 | 2.02                     | 0.41              |
| 2:D4:8:HIS:CE1    | 2:D4:138:PHE:CD2  | 3.08                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D6:204:LEU:HD13 | 2:D6:231:ILE:HD12 | 2.02                     | 0.41              |
| 3:E5:12:CYS:CB    | 3:E5:138:SER:HB2  | 2.47                     | 0.41              |
| 3:E5:25:SER:HB3   | 3:E5:30:ILE:HB    | 2.03                     | 0.41              |
| 3:E5:261:PRO:O    | 3:E5:264:HIS:ND1  | 2.50                     | 0.41              |
| 2:E6:352:LYS:HA   | 2:E6:352:LYS:HD3  | 1.87                     | 0.41              |
| 2:E8:191:THR:CG2  | 2:E8:425:LEU:HD21 | 2.50                     | 0.41              |
| 3:F1:205:GLU:HA   | 3:F1:208:TYR:HB2  | 2.03                     | 0.41              |
| 4:b:78:ALA:HB1    | 4:b:85:CYS:SG     | 2.61                     | 0.41              |
| 4:g:13:GLU:HG3    | 4:g:14:LYS:N      | 2.36                     | 0.41              |
| 4:h:119:ARG:HD2   | 4:h:119:ARG:HA    | 1.90                     | 0.41              |
| 5:k:38:PHE:HE1    | 5:k:106:ILE:HG22  | 1.86                     | 0.41              |
| 5:l:39:ALA:O      | 5:l:75:SER:HA     | 2.21                     | 0.41              |
| 4:n:8:SER:HA      | 4:n:9:PRO:HD3     | 1.87                     | 0.41              |
| 4:p:10:LEU:HD23   | 4:p:147:HIS:CE1   | 2.56                     | 0.41              |
| 1:16:253:ALA:N    | 2:E0:82:THR:HG21  | 2.35                     | 0.40              |
| 1:5:257:PRO:HA    | 1:5:258:PRO:HD3   | 1.99                     | 0.40              |
| 1:8:243:ALA:HB1   | 3:C1:357:PRO:HD3  | 2.03                     | 0.40              |
| 2:A2:15:GLN:HB3   | 2:A2:228:ASN:HD21 | 1.85                     | 0.40              |
| 2:A8:73:THR:OG1   | 3:A9:46:ARG:NH2   | 2.54                     | 0.40              |
| 3:A9:257:LEU:O    | 3:A9:259:PRO:HD3  | 2.21                     | 0.40              |
| 3:A9:392:LYS:HD3  | 3:A9:395:LEU:HG   | 2.02                     | 0.40              |
| 2:B2:177:VAL:HG12 | 3:B3:331:LEU:CB   | 2.51                     | 0.40              |
| 2:B2:318:MET:HE3  | 2:B2:318:MET:HB3  | 1.84                     | 0.40              |
| 2:B4:69:ASP:OD1   | 2:B4:70:LEU:N     | 2.53                     | 0.40              |
| 2:B8:167:LEU:HD22 | 2:B8:200:VAL:HB   | 2.02                     | 0.40              |
| 2:C2:306:ASP:OD1  | 2:C2:308:ARG:HG2  | 2.21                     | 0.40              |
| 2:C6:88:HIS:HA    | 2:C6:89:PRO:HD3   | 1.97                     | 0.40              |
| 3:C9:220:PRO:CG   | 2:D0:326:LYS:NZ   | 2.71                     | 0.40              |
| 3:C9:238:CYS:SG   | 3:C9:318:ARG:NE   | 2.90                     | 0.40              |
| 3:C9:246:LEU:HD12 | 3:C9:246:LEU:HA   | 1.93                     | 0.40              |
| 2:D2:6:SER:OG     | 2:D2:8:HIS:NE2    | 2.54                     | 0.40              |
| 2:D2:434:GLU:HA   | 2:D2:437:ILE:HD12 | 2.03                     | 0.40              |
| 3:D3:289:LEU:CD2  | 3:D3:365:VAL:HG23 | 2.50                     | 0.40              |
| 2:D4:298:PRO:HG2  | 2:D4:308:ARG:HH12 | 1.85                     | 0.40              |
| 2:D6:4:VAL:HG12   | 2:D6:133:GLN:HB3  | 2.02                     | 0.40              |
| 3:E3:153:SER:HB2  | 3:E3:191:GLN:HE22 | 1.86                     | 0.40              |
| 3:E3:292:GLN:HG2  | 3:E3:298:ASN:ND2  | 2.36                     | 0.40              |
| 3:E5:139:LEU:HA   | 3:E5:145:SER:HB2  | 2.03                     | 0.40              |
| 2:E6:324:VAL:HA   | 2:E6:325:PRO:HD3  | 1.89                     | 0.40              |
| 3:E7:117:LEU:HD11 | 3:E7:154:LYS:HB3  | 2.03                     | 0.40              |
| 2:E8:157:LEU:HD23 | 2:E8:157:LEU:HA   | 1.96                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E9:259:PRO:HB2  | 3:E9:260:PHE:CD1  | 2.56                     | 0.40              |
| 4:a:183:LEU:O     | 4:a:185:ILE:N     | 2.53                     | 0.40              |
| 4:b:144:LEU:HD23  | 4:b:144:LEU:HA    | 1.95                     | 0.40              |
| 4:f:129:MET:SD    | 4:f:131:TRP:NE1   | 2.93                     | 0.40              |
| 4:f:154:TYR:HE1   | 4:f:158:THR:HG22  | 1.86                     | 0.40              |
| 4:g:25:GLN:NE2    | 4:g:36:ILE:HG12   | 2.35                     | 0.40              |
| 5:k:94:SER:OG     | 5:k:95:VAL:N      | 2.51                     | 0.40              |
| 5:l:27:ASP:OD2    | 4:n:23:LEU:CD2    | 2.69                     | 0.40              |
| 4:p:15:ARG:HG2    | 4:p:45:MET:HE1    | 2.02                     | 0.40              |
| 4:p:52:GLU:H      | 4:p:52:GLU:CD     | 2.29                     | 0.40              |
| 5:w:38:PHE:HB2    | 5:w:130:LEU:HB3   | 2.03                     | 0.40              |
| 5:x:90:MET:HA     | 5:x:91:PRO:HD3    | 1.96                     | 0.40              |
| 2:A0:88:HIS:CE1   | 2:A0:90:GLU:HG3   | 2.57                     | 0.40              |
| 2:A2:172:TRP:N    | 2:A2:204:LEU:O    | 2.48                     | 0.40              |
| 3:A3:167:PHE:CE2  | 3:A3:233:MET:HG3  | 2.56                     | 0.40              |
| 3:A5:297:LYS:HB3  | 3:A5:297:LYS:HE3  | 1.94                     | 0.40              |
| 3:A5:392:LYS:HG3  | 3:A5:392:LYS:O    | 2.21                     | 0.40              |
| 3:A9:326:VAL:O    | 3:A9:330:MET:HG2  | 2.21                     | 0.40              |
| 2:B6:250:VAL:CG1  | 2:B6:318:MET:HE1  | 2.51                     | 0.40              |
| 3:C1:164:MET:H    | 3:C1:197:ASP:HB3  | 1.85                     | 0.40              |
| 3:C3:20:PHE:HB2   | 3:C3:233:MET:HE3  | 2.03                     | 0.40              |
| 3:C3:21:TRP:CH2   | 3:C3:61:PRO:HB3   | 2.56                     | 0.40              |
| 3:C5:313:ALA:HA   | 3:C5:369:GLY:HA2  | 2.02                     | 0.40              |
| 2:C6:191:THR:HA   | 2:C6:194:LEU:HB3  | 2.03                     | 0.40              |
| 2:C8:323:VAL:CG1  | 2:C8:355:ILE:HG23 | 2.48                     | 0.40              |
| 3:C9:170:PHE:CD1  | 3:C9:171:PRO:HD2  | 2.55                     | 0.40              |
| 3:D1:66:MET:CE    | 3:D1:151:LEU:HD22 | 2.51                     | 0.40              |
| 2:D4:313:MET:HE2  | 2:D4:313:MET:HB3  | 1.92                     | 0.40              |
| 3:D5:124:ALA:HA   | 3:D5:130:LEU:HD12 | 2.03                     | 0.40              |
| 2:D6:425:LEU:HD12 | 2:D6:425:LEU:HA   | 1.98                     | 0.40              |
| 3:D7:192:LEU:HD21 | 3:D7:199:VAL:HG11 | 2.04                     | 0.40              |
| 2:D8:238:LEU:CD1  | 2:D8:255:PHE:HE2  | 2.33                     | 0.40              |
| 2:D8:285:GLN:HB2  | 2:E2:56:THR:CA    | 2.24                     | 0.40              |
| 3:E3:28:HIS:ND1   | 3:E3:43:GLN:O     | 2.53                     | 0.40              |
| 3:E3:87:PRO:HA    | 3:E3:90:PHE:HD1   | 1.86                     | 0.40              |
| 2:E8:11:GLN:HG3   | 2:E8:74:VAL:HG21  | 2.04                     | 0.40              |
| 2:E8:70:LEU:HD21  | 2:E8:114:ILE:HG21 | 2.03                     | 0.40              |
| 2:E8:322:ASP:O    | 2:E8:373:ARG:NE   | 2.54                     | 0.40              |
| 4:a:64:PRO:HD2    | 4:a:67:HIS:CE1    | 2.57                     | 0.40              |
| 4:f:6:PHE:O       | 4:f:15:ARG:NH1    | 2.54                     | 0.40              |
| 4:f:67:HIS:CG     | 4:h:19:GLU:OE2    | 2.74                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:g:106:GLN:NE2   | 4:g:109:GLU:OE1   | 2.54                     | 0.40              |
| 4:j:94:ASN:O      | 4:j:98:THR:HG22   | 2.21                     | 0.40              |
| 4:n:167:VAL:HA    | 4:n:168:PRO:HA    | 1.77                     | 0.40              |
| 4:q:73:VAL:HA     | 4:q:109:GLU:O     | 2.21                     | 0.40              |
| 4:s:88:LEU:HD22   | 4:s:185:ILE:HG21  | 2.03                     | 0.40              |
| 1:18:245:SER:HB3  | 1:18:248:ARG:HD3  | 2.03                     | 0.40              |
| 2:A0:5:ILE:HG23   | 2:A0:5:ILE:HD12   | 1.82                     | 0.40              |
| 2:A8:107:HIS:HE1  | 2:A8:151:CYS:SG   | 2.44                     | 0.40              |
| 3:A9:16:ILE:HG22  | 3:A9:226:ASN:CG   | 2.47                     | 0.40              |
| 3:B1:249:ASP:H    | 3:B1:252:LYS:HB2  | 1.86                     | 0.40              |
| 3:B3:47:ILE:HD12  | 3:B3:47:ILE:HA    | 1.98                     | 0.40              |
| 2:B4:221:ARG:O    | 4:h:189:LEU:HD23  | 2.21                     | 0.40              |
| 3:B5:324:LYS:HB2  | 3:B5:324:LYS:HE3  | 1.64                     | 0.40              |
| 3:B7:11:GLN:HA    | 3:B7:72:THR:HG21  | 2.03                     | 0.40              |
| 2:C0:414:GLU:N    | 2:C0:414:GLU:OE2  | 2.54                     | 0.40              |
| 3:C1:86:ARG:HD2   | 3:C1:88:ASP:HB2   | 2.04                     | 0.40              |
| 2:C2:101:ASN:C    | 2:C2:186:ASN:HD21 | 2.29                     | 0.40              |
| 2:C2:119:LEU:HD23 | 2:C2:119:LEU:HA   | 1.83                     | 0.40              |
| 3:C3:128:ASP:N    | 3:C3:128:ASP:OD1  | 2.53                     | 0.40              |
| 3:C5:391:ARG:O    | 2:C6:262:TYR:OH   | 2.40                     | 0.40              |
| 3:D3:176:SER:HB2  | 2:D4:349:THR:CG2  | 2.51                     | 0.40              |
| 3:D5:318:ARG:HB3  | 3:D5:357:PRO:HA   | 2.02                     | 0.40              |
| 3:D5:321:MET:HE3  | 3:D5:326:VAL:HG21 | 2.04                     | 0.40              |
| 2:D8:11:GLN:NE2   | 3:D9:245:GLN:O    | 2.55                     | 0.40              |
| 2:D8:203:MET:HE2  | 2:D8:267:PHE:HB3  | 2.03                     | 0.40              |
| 2:D8:401:LYS:NZ   | 3:D9:344:TRP:HB3  | 2.37                     | 0.40              |
| 3:E1:291:GLN:OE1  | 3:E5:122:LYS:HE2  | 2.20                     | 0.40              |
| 2:E2:1:MET:N      | 2:E2:3:GLU:OE2    | 2.43                     | 0.40              |
| 3:E3:215:LEU:HD23 | 3:E3:215:LEU:HA   | 1.96                     | 0.40              |
| 3:E9:207:LEU:HD13 | 3:E9:225:LEU:HB3  | 2.02                     | 0.40              |
| 3:E9:311:LEU:HD12 | 3:E9:342:VAL:HG11 | 2.02                     | 0.40              |
| 3:F1:6:HIS:CD2    | 3:F1:134:GLN:HE21 | 2.40                     | 0.40              |
| 4:j:126:ARG:NH1   | 4:j:133:SER:HB3   | 2.36                     | 0.40              |
| 4:n:92:LEU:HD21   | 4:n:110:ILE:HG13  | 2.03                     | 0.40              |
| 4:o:26:ALA:HB2    | 4:o:36:ILE:HG21   | 2.02                     | 0.40              |
| 4:o:96:TYR:HA     | 4:o:108:ILE:HD11  | 2.02                     | 0.40              |
| 4:r:28:LYS:HA     | 4:r:28:LYS:HD3    | 1.80                     | 0.40              |
| 5:x:96:GLU:OE1    | 5:x:99:SER:N      | 2.55                     | 0.40              |
| 2:A0:221:ARG:CB   | 3:A1:325:GLU:HB3  | 2.51                     | 0.40              |
| 3:A1:282:ARG:HA   | 3:A5:86:ARG:HH12  | 1.86                     | 0.40              |
| 2:A2:279:GLU:HG2  | 4:b:197:LEU:O     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A5:406:MET:HA   | 3:A5:409:THR:HG22 | 2.04                     | 0.40              |
| 3:A7:281:TYR:CZ   | 3:B1:83:GLN:O     | 2.74                     | 0.40              |
| 3:A7:362:LYS:HA   | 3:A7:362:LYS:HE2  | 2.04                     | 0.40              |
| 3:A9:156:ARG:HH21 | 3:A9:164:MET:HB2  | 1.87                     | 0.40              |
| 2:B2:262:TYR:CB   | 2:B2:263:PRO:HD2  | 2.49                     | 0.40              |
| 3:B3:46:ARG:HE    | 3:B3:46:ARG:HB2   | 1.56                     | 0.40              |
| 2:B6:407:TRP:HZ2  | 3:B7:258:ILE:HD11 | 1.87                     | 0.40              |
| 3:B9:139:LEU:HA   | 3:B9:145:SER:HB3  | 2.04                     | 0.40              |
| 2:C2:209:ILE:HA   | 2:C2:212:ILE:HG22 | 2.03                     | 0.40              |
| 2:C6:395:PHE:HZ   | 2:C6:418:PHE:HB3  | 1.85                     | 0.40              |
| 2:C8:164:LYS:O    | 2:C8:166:LYS:NZ   | 2.54                     | 0.40              |
| 3:D1:316:MET:HG3  | 3:D1:352:SER:OG   | 2.21                     | 0.40              |
| 3:D5:321:MET:HE2  | 3:D5:353:VAL:HG13 | 2.03                     | 0.40              |
| 3:D7:176:SER:HB3  | 3:D7:181:GLU:OE1  | 2.22                     | 0.40              |
| 2:E0:155:GLU:HG3  | 2:E0:197:HIS:NE2  | 2.36                     | 0.40              |
| 2:E0:282:TYR:HB3  | 2:E4:60:LYS:CE    | 2.52                     | 0.40              |
| 2:E2:96:LYS:HE3   | 3:E3:1:MET:H2     | 1.86                     | 0.40              |
| 3:E3:46:ARG:HH21  | 3:E3:46:ARG:HG2   | 1.87                     | 0.40              |
| 3:E3:295:ASP:OD2  | 3:E3:297:LYS:HG2  | 2.21                     | 0.40              |
| 2:E4:276:ILE:HG23 | 2:E4:281:ALA:HB2  | 2.03                     | 0.40              |
| 2:E8:211:ASP:OD1  | 2:E8:211:ASP:N    | 2.53                     | 0.40              |
| 2:F0:60:LYS:O     | 2:F0:61:HIS:ND1   | 2.54                     | 0.40              |
| 2:F0:112:LYS:HB3  | 2:F0:112:LYS:HE3  | 1.85                     | 0.40              |
| 3:F1:363:MET:HE2  | 3:F1:363:MET:HB2  | 1.97                     | 0.40              |
| 4:d:18:ASN:CB     | 4:d:45:MET:HG2    | 2.51                     | 0.40              |
| 4:i:184:PRO:HB2   | 4:i:189:LEU:HB2   | 2.04                     | 0.40              |
| 5:l:34:VAL:HA     | 5:l:70:GLU:O      | 2.22                     | 0.40              |
| 5:l:59:THR:O      | 5:l:63:SER:OG     | 2.33                     | 0.40              |
| 4:p:63:ILE:HB     | 4:p:67:HIS:HD2    | 1.86                     | 0.40              |
| 4:t:110:ILE:O     | 4:t:131:TRP:HB2   | 2.20                     | 0.40              |
| 4:t:154:TYR:HE1   | 4:t:158:THR:HG22  | 1.86                     | 0.40              |
| 1:16:254:LYS:H    | 1:16:254:LYS:HG2  | 1.66                     | 0.40              |
| 1:18:250:GLU:OE1  | 2:E4:229:ARG:NH2  | 2.54                     | 0.40              |
| 1:7:243:ALA:HB3   | 3:B9:356:ILE:HG23 | 2.03                     | 0.40              |
| 2:A2:156:ARG:HD3  | 2:A2:156:ARG:HA   | 1.67                     | 0.40              |
| 2:A2:356:ASN:OD1  | 2:A2:357:TYR:N    | 2.54                     | 0.40              |
| 3:A3:86:ARG:HA    | 3:A3:87:PRO:HD3   | 1.97                     | 0.40              |
| 2:A8:28:HIS:HD2   | 2:A8:53:PHE:HE2   | 1.70                     | 0.40              |
| 2:B0:9:VAL:HG13   | 2:B0:139:ASN:HB3  | 2.04                     | 0.40              |
| 2:B0:69:ASP:OD1   | 2:B0:70:LEU:N     | 2.55                     | 0.40              |
| 2:B6:430:LYS:HB3  | 2:B6:430:LYS:HE3  | 1.88                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B8:73:THR:HG23  | 3:B9:46:ARG:HH12  | 1.85                     | 0.40              |
| 2:C2:214:ARG:O    | 2:C2:214:ARG:NH1  | 2.54                     | 0.40              |
| 3:C5:258:ILE:HA   | 3:C5:259:PRO:HD3  | 1.94                     | 0.40              |
| 3:C7:253:LEU:HD12 | 3:C7:253:LEU:HA   | 1.86                     | 0.40              |
| 2:D2:93:ILE:HG23  | 2:D2:117:LEU:HD23 | 2.03                     | 0.40              |
| 2:D2:138:PHE:HZ   | 2:D2:235:ILE:HD13 | 1.86                     | 0.40              |
| 2:D2:217:LEU:HD11 | 2:D2:275:ILE:CG2  | 2.50                     | 0.40              |
| 2:D4:11:GLN:HE22  | 3:D5:246:LEU:CD1  | 2.35                     | 0.40              |
| 2:D8:207:GLU:HA   | 2:D8:210:TYR:HB2  | 2.03                     | 0.40              |
| 2:E2:430:LYS:HE2  | 2:E2:430:LYS:HB3  | 1.74                     | 0.40              |
| 3:E9:272:PRO:HD2  | 3:E9:361:LEU:HD13 | 2.04                     | 0.40              |
| 4:a:68:LEU:HD21   | 4:a:111:ILE:HD11  | 2.02                     | 0.40              |
| 4:f:68:LEU:HB2    | 4:f:206:PHE:CD2   | 2.57                     | 0.40              |
| 4:j:57:ASN:HB3    | 4:j:132:LEU:HD23  | 2.04                     | 0.40              |
| 5:l:27:ASP:HB2    | 4:n:23:LEU:HD11   | 2.04                     | 0.40              |
| 4:s:72:SER:HB3    | 4:s:108:ILE:HG22  | 2.04                     | 0.40              |
| 4:s:204:THR:O     | 4:s:204:THR:OG1   | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed    | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|----------|---------|----------|-------------|-----|
| 1   | 0     | 20/351 (6%) | 19 (95%) | 1 (5%)  | 0        | 100         | 100 |
| 1   | 1     | 20/351 (6%) | 18 (90%) | 2 (10%) | 0        | 100         | 100 |
| 1   | 10    | 20/351 (6%) | 17 (85%) | 3 (15%) | 0        | 100         | 100 |
| 1   | 11    | 20/351 (6%) | 16 (80%) | 4 (20%) | 0        | 100         | 100 |
| 1   | 12    | 20/351 (6%) | 19 (95%) | 1 (5%)  | 0        | 100         | 100 |
| 1   | 13    | 20/351 (6%) | 18 (90%) | 2 (10%) | 0        | 100         | 100 |
| 1   | 14    | 20/351 (6%) | 19 (95%) | 1 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 15    | 20/351 (6%)   | 18 (90%)  | 2 (10%) | 0        | 100         | 100 |
| 1   | 16    | 20/351 (6%)   | 20 (100%) | 0       | 0        | 100         | 100 |
| 1   | 17    | 20/351 (6%)   | 20 (100%) | 0       | 0        | 100         | 100 |
| 1   | 18    | 20/351 (6%)   | 18 (90%)  | 2 (10%) | 0        | 100         | 100 |
| 1   | 19    | 20/351 (6%)   | 19 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 1   | 2     | 20/351 (6%)   | 18 (90%)  | 2 (10%) | 0        | 100         | 100 |
| 1   | 20    | 20/351 (6%)   | 17 (85%)  | 3 (15%) | 0        | 100         | 100 |
| 1   | 21    | 20/351 (6%)   | 18 (90%)  | 1 (5%)  | 1 (5%)   | 1           | 16  |
| 1   | 22    | 18/351 (5%)   | 16 (89%)  | 2 (11%) | 0        | 100         | 100 |
| 1   | 23    | 18/351 (5%)   | 15 (83%)  | 3 (17%) | 0        | 100         | 100 |
| 1   | 3     | 20/351 (6%)   | 18 (90%)  | 1 (5%)  | 1 (5%)   | 1           | 16  |
| 1   | 4     | 20/351 (6%)   | 20 (100%) | 0       | 0        | 100         | 100 |
| 1   | 5     | 20/351 (6%)   | 19 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 1   | 6     | 20/351 (6%)   | 19 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 1   | 7     | 20/351 (6%)   | 20 (100%) | 0       | 0        | 100         | 100 |
| 1   | 8     | 20/351 (6%)   | 19 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 1   | 9     | 20/351 (6%)   | 18 (90%)  | 2 (10%) | 0        | 100         | 100 |
| 2   | A0    | 424/453 (94%) | 398 (94%) | 26 (6%) | 0        | 100         | 100 |
| 2   | A2    | 424/453 (94%) | 405 (96%) | 18 (4%) | 1 (0%)   | 43          | 78  |
| 2   | A4    | 424/453 (94%) | 393 (93%) | 31 (7%) | 0        | 100         | 100 |
| 2   | A6    | 424/453 (94%) | 402 (95%) | 22 (5%) | 0        | 100         | 100 |
| 2   | A8    | 424/453 (94%) | 403 (95%) | 21 (5%) | 0        | 100         | 100 |
| 2   | B0    | 424/453 (94%) | 400 (94%) | 24 (6%) | 0        | 100         | 100 |
| 2   | B2    | 424/453 (94%) | 405 (96%) | 19 (4%) | 0        | 100         | 100 |
| 2   | B4    | 424/453 (94%) | 408 (96%) | 16 (4%) | 0        | 100         | 100 |
| 2   | B6    | 424/453 (94%) | 405 (96%) | 19 (4%) | 0        | 100         | 100 |
| 2   | B8    | 424/453 (94%) | 400 (94%) | 24 (6%) | 0        | 100         | 100 |
| 2   | C0    | 424/453 (94%) | 402 (95%) | 21 (5%) | 1 (0%)   | 43          | 78  |
| 2   | C2    | 424/453 (94%) | 399 (94%) | 24 (6%) | 1 (0%)   | 43          | 78  |
| 2   | C4    | 424/453 (94%) | 386 (91%) | 37 (9%) | 1 (0%)   | 43          | 78  |
| 2   | C6    | 424/453 (94%) | 397 (94%) | 27 (6%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | C8    | 424/453 (94%) | 396 (93%) | 28 (7%) | 0        | 100         | 100 |
| 2   | D0    | 424/453 (94%) | 401 (95%) | 23 (5%) | 0        | 100         | 100 |
| 2   | D2    | 424/453 (94%) | 404 (95%) | 20 (5%) | 0        | 100         | 100 |
| 2   | D4    | 424/453 (94%) | 409 (96%) | 15 (4%) | 0        | 100         | 100 |
| 2   | D6    | 424/453 (94%) | 408 (96%) | 16 (4%) | 0        | 100         | 100 |
| 2   | D8    | 424/453 (94%) | 407 (96%) | 17 (4%) | 0        | 100         | 100 |
| 2   | E0    | 424/453 (94%) | 403 (95%) | 21 (5%) | 0        | 100         | 100 |
| 2   | E2    | 424/453 (94%) | 402 (95%) | 22 (5%) | 0        | 100         | 100 |
| 2   | E4    | 424/453 (94%) | 399 (94%) | 25 (6%) | 0        | 100         | 100 |
| 2   | E6    | 424/453 (94%) | 399 (94%) | 24 (6%) | 1 (0%)   | 43          | 78  |
| 2   | E8    | 424/453 (94%) | 402 (95%) | 22 (5%) | 0        | 100         | 100 |
| 2   | F0    | 424/453 (94%) | 401 (95%) | 23 (5%) | 0        | 100         | 100 |
| 3   | A1    | 424/449 (94%) | 397 (94%) | 27 (6%) | 0        | 100         | 100 |
| 3   | A3    | 424/449 (94%) | 399 (94%) | 24 (6%) | 1 (0%)   | 43          | 78  |
| 3   | A5    | 424/449 (94%) | 388 (92%) | 34 (8%) | 2 (0%)   | 24          | 63  |
| 3   | A7    | 424/449 (94%) | 397 (94%) | 26 (6%) | 1 (0%)   | 43          | 78  |
| 3   | A9    | 424/449 (94%) | 400 (94%) | 23 (5%) | 1 (0%)   | 43          | 78  |
| 3   | B1    | 424/449 (94%) | 401 (95%) | 22 (5%) | 1 (0%)   | 43          | 78  |
| 3   | B3    | 424/449 (94%) | 400 (94%) | 22 (5%) | 2 (0%)   | 24          | 63  |
| 3   | B5    | 424/449 (94%) | 394 (93%) | 28 (7%) | 2 (0%)   | 24          | 63  |
| 3   | B7    | 424/449 (94%) | 396 (93%) | 28 (7%) | 0        | 100         | 100 |
| 3   | B9    | 424/449 (94%) | 407 (96%) | 17 (4%) | 0        | 100         | 100 |
| 3   | C1    | 424/449 (94%) | 401 (95%) | 23 (5%) | 0        | 100         | 100 |
| 3   | C3    | 424/449 (94%) | 396 (93%) | 27 (6%) | 1 (0%)   | 43          | 78  |
| 3   | C5    | 424/449 (94%) | 402 (95%) | 22 (5%) | 0        | 100         | 100 |
| 3   | C7    | 424/449 (94%) | 396 (93%) | 28 (7%) | 0        | 100         | 100 |
| 3   | C9    | 424/449 (94%) | 396 (93%) | 27 (6%) | 1 (0%)   | 43          | 78  |
| 3   | D1    | 424/449 (94%) | 399 (94%) | 24 (6%) | 1 (0%)   | 43          | 78  |
| 3   | D3    | 424/449 (94%) | 395 (93%) | 28 (7%) | 1 (0%)   | 43          | 78  |
| 3   | D5    | 424/449 (94%) | 396 (93%) | 28 (7%) | 0        | 100         | 100 |
| 3   | D7    | 424/449 (94%) | 399 (94%) | 24 (6%) | 1 (0%)   | 43          | 78  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | D9    | 424/449 (94%) | 402 (95%) | 22 (5%) | 0        | 100         | 100 |
| 3   | E1    | 424/449 (94%) | 402 (95%) | 22 (5%) | 0        | 100         | 100 |
| 3   | E3    | 424/449 (94%) | 402 (95%) | 21 (5%) | 1 (0%)   | 43          | 78  |
| 3   | E5    | 424/449 (94%) | 392 (92%) | 32 (8%) | 0        | 100         | 100 |
| 3   | E7    | 424/449 (94%) | 397 (94%) | 26 (6%) | 1 (0%)   | 43          | 78  |
| 3   | E9    | 424/449 (94%) | 388 (92%) | 36 (8%) | 0        | 100         | 100 |
| 3   | F1    | 424/449 (94%) | 389 (92%) | 34 (8%) | 1 (0%)   | 43          | 78  |
| 4   | a     | 146/220 (66%) | 135 (92%) | 11 (8%) | 0        | 100         | 100 |
| 4   | b     | 146/220 (66%) | 137 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 4   | c     | 197/220 (90%) | 188 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 4   | d     | 197/220 (90%) | 179 (91%) | 18 (9%) | 0        | 100         | 100 |
| 4   | e     | 197/220 (90%) | 183 (93%) | 13 (7%) | 1 (0%)   | 24          | 63  |
| 4   | f     | 197/220 (90%) | 184 (93%) | 13 (7%) | 0        | 100         | 100 |
| 4   | g     | 197/220 (90%) | 185 (94%) | 11 (6%) | 1 (0%)   | 24          | 63  |
| 4   | h     | 197/220 (90%) | 183 (93%) | 14 (7%) | 0        | 100         | 100 |
| 4   | i     | 197/220 (90%) | 186 (94%) | 11 (6%) | 0        | 100         | 100 |
| 4   | j     | 197/220 (90%) | 184 (93%) | 13 (7%) | 0        | 100         | 100 |
| 4   | m     | 197/220 (90%) | 180 (91%) | 17 (9%) | 0        | 100         | 100 |
| 4   | n     | 197/220 (90%) | 186 (94%) | 11 (6%) | 0        | 100         | 100 |
| 4   | o     | 197/220 (90%) | 179 (91%) | 18 (9%) | 0        | 100         | 100 |
| 4   | p     | 197/220 (90%) | 182 (92%) | 15 (8%) | 0        | 100         | 100 |
| 4   | q     | 197/220 (90%) | 187 (95%) | 10 (5%) | 0        | 100         | 100 |
| 4   | r     | 197/220 (90%) | 185 (94%) | 12 (6%) | 0        | 100         | 100 |
| 4   | s     | 197/220 (90%) | 179 (91%) | 18 (9%) | 0        | 100         | 100 |
| 4   | t     | 197/220 (90%) | 184 (93%) | 13 (7%) | 0        | 100         | 100 |
| 4   | u     | 197/220 (90%) | 189 (96%) | 7 (4%)  | 1 (0%)   | 24          | 63  |
| 4   | v     | 197/220 (90%) | 183 (93%) | 14 (7%) | 0        | 100         | 100 |
| 5   | k     | 133/189 (70%) | 127 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 5   | l     | 133/189 (70%) | 128 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 5   | w     | 139/189 (74%) | 133 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 5   | x     | 139/189 (74%) | 129 (93%) | 10 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|-----------|----------|-------------|----|
| All | All   | 26906/37032 (73%) | 25298 (94%) | 1580 (6%) | 28 (0%)  | 49          | 83 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A3    | 179 | VAL  |
| 3   | A5    | 55  | THR  |
| 3   | A7    | 55  | THR  |
| 3   | B3    | 55  | THR  |
| 3   | C3    | 179 | VAL  |
| 3   | D1    | 179 | VAL  |
| 3   | D3    | 55  | THR  |
| 1   | 3     | 251 | TYR  |
| 3   | B1    | 55  | THR  |
| 3   | B5    | 55  | THR  |
| 3   | A9    | 179 | VAL  |
| 2   | C4    | 89  | PRO  |
| 3   | C9    | 55  | THR  |
| 3   | E3    | 55  | THR  |
| 2   | E6    | 81  | GLY  |
| 4   | e     | 60  | ASN  |
| 3   | B5    | 336 | LYS  |
| 2   | C2    | 58  | ALA  |
| 3   | D7    | 320 | ARG  |
| 3   | E7    | 55  | THR  |
| 3   | F1    | 171 | PRO  |
| 1   | 21    | 253 | ALA  |
| 3   | B3    | 128 | ASP  |
| 2   | C0    | 83  | TYR  |
| 4   | u     | 154 | TYR  |
| 2   | A2    | 32  | PRO  |
| 4   | g     | 51  | PRO  |
| 3   | A5    | 259 | 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   | 0     | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 1     | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 10    | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 11    | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 12    | 20/304 (7%)   | 18 (90%)   | 2 (10%)  | 7           | 24  |
| 1   | 13    | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 14    | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 15    | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 16    | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 17    | 20/304 (7%)   | 18 (90%)   | 2 (10%)  | 7           | 24  |
| 1   | 18    | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 19    | 20/304 (7%)   | 17 (85%)   | 3 (15%)  | 3           | 12  |
| 1   | 2     | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 20    | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 21    | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 22    | 18/304 (6%)   | 17 (94%)   | 1 (6%)   | 19          | 40  |
| 1   | 23    | 18/304 (6%)   | 18 (100%)  | 0        | 100         | 100 |
| 1   | 3     | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 4     | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 5     | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 6     | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 7     | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 1   | 8     | 20/304 (7%)   | 19 (95%)   | 1 (5%)   | 22          | 43  |
| 1   | 9     | 20/304 (7%)   | 20 (100%)  | 0        | 100         | 100 |
| 2   | A0    | 359/379 (95%) | 351 (98%)  | 8 (2%)   | 45          | 64  |
| 2   | A2    | 359/379 (95%) | 355 (99%)  | 4 (1%)   | 65          | 76  |
| 2   | A4    | 359/379 (95%) | 346 (96%)  | 13 (4%)  | 31          | 52  |
| 2   | A6    | 359/379 (95%) | 348 (97%)  | 11 (3%)  | 35          | 56  |
| 2   | A8    | 359/379 (95%) | 358 (100%) | 1 (0%)   | 86          | 86  |
| 2   | B0    | 359/379 (95%) | 351 (98%)  | 8 (2%)   | 45          | 64  |
| 2   | B2    | 359/379 (95%) | 350 (98%)  | 9 (2%)   | 42          | 63  |
| 2   | B4    | 359/379 (95%) | 353 (98%)  | 6 (2%)   | 53          | 69  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 2   | B6    | 359/379 (95%) | 356 (99%)  | 3 (1%)   | 73          | 80 |
| 2   | B8    | 359/379 (95%) | 352 (98%)  | 7 (2%)   | 50          | 67 |
| 2   | C0    | 359/379 (95%) | 353 (98%)  | 6 (2%)   | 53          | 69 |
| 2   | C2    | 359/379 (95%) | 355 (99%)  | 4 (1%)   | 65          | 76 |
| 2   | C4    | 359/379 (95%) | 355 (99%)  | 4 (1%)   | 65          | 76 |
| 2   | C6    | 359/379 (95%) | 351 (98%)  | 8 (2%)   | 45          | 64 |
| 2   | C8    | 359/379 (95%) | 350 (98%)  | 9 (2%)   | 42          | 63 |
| 2   | D0    | 359/379 (95%) | 354 (99%)  | 5 (1%)   | 59          | 72 |
| 2   | D2    | 359/379 (95%) | 350 (98%)  | 9 (2%)   | 42          | 63 |
| 2   | D4    | 359/379 (95%) | 349 (97%)  | 10 (3%)  | 38          | 60 |
| 2   | D6    | 359/379 (95%) | 355 (99%)  | 4 (1%)   | 65          | 76 |
| 2   | D8    | 359/379 (95%) | 350 (98%)  | 9 (2%)   | 42          | 63 |
| 2   | E0    | 359/379 (95%) | 356 (99%)  | 3 (1%)   | 73          | 80 |
| 2   | E2    | 359/379 (95%) | 352 (98%)  | 7 (2%)   | 50          | 67 |
| 2   | E4    | 359/379 (95%) | 356 (99%)  | 3 (1%)   | 73          | 80 |
| 2   | E6    | 359/379 (95%) | 353 (98%)  | 6 (2%)   | 53          | 69 |
| 2   | E8    | 359/379 (95%) | 358 (100%) | 1 (0%)   | 86          | 86 |
| 2   | F0    | 359/379 (95%) | 353 (98%)  | 6 (2%)   | 53          | 69 |
| 3   | A1    | 364/381 (96%) | 362 (100%) | 2 (0%)   | 81          | 83 |
| 3   | A3    | 364/381 (96%) | 361 (99%)  | 3 (1%)   | 73          | 80 |
| 3   | A5    | 364/381 (96%) | 356 (98%)  | 8 (2%)   | 45          | 64 |
| 3   | A7    | 364/381 (96%) | 360 (99%)  | 4 (1%)   | 65          | 76 |
| 3   | A9    | 364/381 (96%) | 358 (98%)  | 6 (2%)   | 55          | 70 |
| 3   | B1    | 364/381 (96%) | 359 (99%)  | 5 (1%)   | 59          | 72 |
| 3   | B3    | 364/381 (96%) | 361 (99%)  | 3 (1%)   | 73          | 80 |
| 3   | B5    | 364/381 (96%) | 356 (98%)  | 8 (2%)   | 45          | 64 |
| 3   | B7    | 364/381 (96%) | 359 (99%)  | 5 (1%)   | 59          | 72 |
| 3   | B9    | 364/381 (96%) | 358 (98%)  | 6 (2%)   | 55          | 70 |
| 3   | C1    | 364/381 (96%) | 358 (98%)  | 6 (2%)   | 55          | 70 |
| 3   | C3    | 364/381 (96%) | 358 (98%)  | 6 (2%)   | 55          | 70 |
| 3   | C5    | 364/381 (96%) | 358 (98%)  | 6 (2%)   | 55          | 70 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 3   | C7    | 364/381 (96%) | 357 (98%)  | 7 (2%)   | 50          | 67 |
| 3   | C9    | 364/381 (96%) | 357 (98%)  | 7 (2%)   | 50          | 67 |
| 3   | D1    | 364/381 (96%) | 353 (97%)  | 11 (3%)  | 36          | 57 |
| 3   | D3    | 364/381 (96%) | 357 (98%)  | 7 (2%)   | 50          | 67 |
| 3   | D5    | 364/381 (96%) | 351 (96%)  | 13 (4%)  | 31          | 52 |
| 3   | D7    | 364/381 (96%) | 357 (98%)  | 7 (2%)   | 50          | 67 |
| 3   | D9    | 364/381 (96%) | 356 (98%)  | 8 (2%)   | 45          | 64 |
| 3   | E1    | 364/381 (96%) | 358 (98%)  | 6 (2%)   | 55          | 70 |
| 3   | E3    | 364/381 (96%) | 353 (97%)  | 11 (3%)  | 36          | 57 |
| 3   | E5    | 364/381 (96%) | 361 (99%)  | 3 (1%)   | 73          | 80 |
| 3   | E7    | 364/381 (96%) | 360 (99%)  | 4 (1%)   | 65          | 76 |
| 3   | E9    | 364/381 (96%) | 362 (100%) | 2 (0%)   | 81          | 83 |
| 3   | F1    | 364/381 (96%) | 357 (98%)  | 7 (2%)   | 50          | 67 |
| 4   | a     | 130/190 (68%) | 128 (98%)  | 2 (2%)   | 57          | 72 |
| 4   | b     | 130/190 (68%) | 128 (98%)  | 2 (2%)   | 57          | 72 |
| 4   | c     | 174/190 (92%) | 168 (97%)  | 6 (3%)   | 32          | 54 |
| 4   | d     | 174/190 (92%) | 165 (95%)  | 9 (5%)   | 21          | 42 |
| 4   | e     | 174/190 (92%) | 170 (98%)  | 4 (2%)   | 44          | 64 |
| 4   | f     | 174/190 (92%) | 170 (98%)  | 4 (2%)   | 44          | 64 |
| 4   | g     | 174/190 (92%) | 172 (99%)  | 2 (1%)   | 65          | 76 |
| 4   | h     | 174/190 (92%) | 171 (98%)  | 3 (2%)   | 53          | 69 |
| 4   | i     | 174/190 (92%) | 173 (99%)  | 1 (1%)   | 78          | 83 |
| 4   | j     | 174/190 (92%) | 172 (99%)  | 2 (1%)   | 65          | 76 |
| 4   | m     | 174/190 (92%) | 172 (99%)  | 2 (1%)   | 65          | 76 |
| 4   | n     | 174/190 (92%) | 169 (97%)  | 5 (3%)   | 37          | 58 |
| 4   | o     | 174/190 (92%) | 167 (96%)  | 7 (4%)   | 28          | 49 |
| 4   | p     | 174/190 (92%) | 171 (98%)  | 3 (2%)   | 53          | 69 |
| 4   | q     | 174/190 (92%) | 169 (97%)  | 5 (3%)   | 37          | 58 |
| 4   | r     | 174/190 (92%) | 168 (97%)  | 6 (3%)   | 32          | 54 |
| 4   | s     | 174/190 (92%) | 170 (98%)  | 4 (2%)   | 44          | 64 |
| 4   | t     | 174/190 (92%) | 173 (99%)  | 1 (1%)   | 78          | 83 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 4   | u     | 174/190 (92%)     | 170 (98%)   | 4 (2%)   | 44          | 64 |
| 4   | v     | 174/190 (92%)     | 168 (97%)   | 6 (3%)   | 32          | 54 |
| 5   | k     | 122/164 (74%)     | 116 (95%)   | 6 (5%)   | 22          | 43 |
| 5   | l     | 122/164 (74%)     | 119 (98%)   | 3 (2%)   | 42          | 63 |
| 5   | w     | 127/164 (77%)     | 122 (96%)   | 5 (4%)   | 28          | 49 |
| 5   | x     | 127/164 (77%)     | 123 (97%)   | 4 (3%)   | 35          | 56 |
| All | All   | 23164/31512 (74%) | 22724 (98%) | 440 (2%) | 49          | 67 |

All (440) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 252 | VAL  |
| 1   | 11    | 246 | CYS  |
| 1   | 12    | 248 | ARG  |
| 1   | 12    | 256 | LEU  |
| 1   | 14    | 256 | LEU  |
| 1   | 15    | 252 | VAL  |
| 1   | 16    | 254 | LYS  |
| 1   | 17    | 248 | ARG  |
| 1   | 17    | 252 | VAL  |
| 1   | 18    | 256 | LEU  |
| 1   | 19    | 238 | THR  |
| 1   | 19    | 248 | ARG  |
| 1   | 19    | 256 | LEU  |
| 1   | 21    | 256 | LEU  |
| 1   | 22    | 248 | ARG  |
| 1   | 4     | 248 | ARG  |
| 1   | 5     | 248 | ARG  |
| 1   | 6     | 254 | LYS  |
| 1   | 8     | 237 | PRO  |
| 2   | A0    | 119 | LEU  |
| 2   | A0    | 163 | LYS  |
| 2   | A0    | 231 | ILE  |
| 2   | A0    | 285 | GLN  |
| 2   | A0    | 370 | LYS  |
| 2   | A0    | 397 | LEU  |
| 2   | A0    | 401 | LYS  |
| 2   | A0    | 430 | LYS  |
| 3   | A1    | 179 | VAL  |
| 3   | A1    | 379 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A2    | 15  | GLN  |
| 2   | A2    | 372 | MET  |
| 2   | A2    | 401 | LYS  |
| 2   | A2    | 402 | ARG  |
| 3   | A3    | 11  | GLN  |
| 3   | A3    | 174 | LYS  |
| 3   | A3    | 298 | ASN  |
| 2   | A4    | 4   | VAL  |
| 2   | A4    | 7   | ILE  |
| 2   | A4    | 15  | GLN  |
| 2   | A4    | 60  | LYS  |
| 2   | A4    | 163 | LYS  |
| 2   | A4    | 251 | ASP  |
| 2   | A4    | 257 | THR  |
| 2   | A4    | 275 | ILE  |
| 2   | A4    | 328 | VAL  |
| 2   | A4    | 338 | LYS  |
| 2   | A4    | 353 | CYS  |
| 2   | A4    | 370 | LYS  |
| 2   | A4    | 372 | MET  |
| 3   | A5    | 11  | GLN  |
| 3   | A5    | 114 | ASP  |
| 3   | A5    | 125 | GLU  |
| 3   | A5    | 225 | LEU  |
| 3   | A5    | 320 | ARG  |
| 3   | A5    | 362 | LYS  |
| 3   | A5    | 379 | LYS  |
| 3   | A5    | 391 | ARG  |
| 2   | A6    | 60  | LYS  |
| 2   | A6    | 77  | GLU  |
| 2   | A6    | 163 | LYS  |
| 2   | A6    | 254 | GLU  |
| 2   | A6    | 308 | ARG  |
| 2   | A6    | 323 | VAL  |
| 2   | A6    | 326 | LYS  |
| 2   | A6    | 370 | LYS  |
| 2   | A6    | 401 | LYS  |
| 2   | A6    | 413 | MET  |
| 2   | A6    | 430 | LYS  |
| 3   | A7    | 11  | GLN  |
| 3   | A7    | 247 | ASN  |
| 3   | A7    | 297 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A7    | 336 | LYS  |
| 2   | A8    | 164 | LYS  |
| 3   | A9    | 113 | ILE  |
| 3   | A9    | 174 | LYS  |
| 3   | A9    | 221 | THR  |
| 3   | A9    | 324 | LYS  |
| 3   | A9    | 379 | LYS  |
| 3   | A9    | 391 | ARG  |
| 2   | B0    | 92  | LEU  |
| 2   | B0    | 96  | LYS  |
| 2   | B0    | 98  | ASP  |
| 2   | B0    | 156 | ARG  |
| 2   | B0    | 163 | LYS  |
| 2   | B0    | 336 | LYS  |
| 2   | B0    | 338 | LYS  |
| 2   | B0    | 372 | MET  |
| 3   | B1    | 193 | VAL  |
| 3   | B1    | 252 | LYS  |
| 3   | B1    | 280 | GLN  |
| 3   | B1    | 350 | LYS  |
| 3   | B1    | 362 | LYS  |
| 2   | B2    | 2   | ARG  |
| 2   | B2    | 156 | ARG  |
| 2   | B2    | 163 | LYS  |
| 2   | B2    | 196 | GLU  |
| 2   | B2    | 297 | GLU  |
| 2   | B2    | 338 | LYS  |
| 2   | B2    | 393 | HIS  |
| 2   | B2    | 401 | LYS  |
| 2   | B2    | 430 | LYS  |
| 3   | B3    | 122 | LYS  |
| 3   | B3    | 280 | GLN  |
| 3   | B3    | 336 | LYS  |
| 2   | B4    | 163 | LYS  |
| 2   | B4    | 224 | TYR  |
| 2   | B4    | 227 | LEU  |
| 2   | B4    | 253 | THR  |
| 2   | B4    | 264 | ARG  |
| 2   | B4    | 336 | LYS  |
| 3   | B5    | 16  | ILE  |
| 3   | B5    | 155 | VAL  |
| 3   | B5    | 162 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B5    | 252 | LYS  |
| 3   | B5    | 298 | ASN  |
| 3   | B5    | 324 | LYS  |
| 3   | B5    | 336 | LYS  |
| 3   | B5    | 391 | ARG  |
| 2   | B6    | 77  | GLU  |
| 2   | B6    | 326 | LYS  |
| 2   | B6    | 339 | ARG  |
| 3   | B7    | 11  | GLN  |
| 3   | B7    | 147 | MET  |
| 3   | B7    | 154 | LYS  |
| 3   | B7    | 256 | ASN  |
| 3   | B7    | 324 | LYS  |
| 2   | B8    | 11  | GLN  |
| 2   | B8    | 60  | LYS  |
| 2   | B8    | 96  | LYS  |
| 2   | B8    | 113 | GLU  |
| 2   | B8    | 124 | LYS  |
| 2   | B8    | 181 | VAL  |
| 2   | B8    | 397 | LEU  |
| 3   | B9    | 2   | ARG  |
| 3   | B9    | 46  | ARG  |
| 3   | B9    | 122 | LYS  |
| 3   | B9    | 157 | GLU  |
| 3   | B9    | 177 | ASP  |
| 3   | B9    | 379 | LYS  |
| 2   | C0    | 96  | LYS  |
| 2   | C0    | 112 | LYS  |
| 2   | C0    | 154 | LEU  |
| 2   | C0    | 217 | LEU  |
| 2   | C0    | 221 | ARG  |
| 2   | C0    | 326 | LYS  |
| 3   | C1    | 83  | GLN  |
| 3   | C1    | 174 | LYS  |
| 3   | C1    | 297 | LYS  |
| 3   | C1    | 320 | ARG  |
| 3   | C1    | 324 | LYS  |
| 3   | C1    | 362 | LYS  |
| 2   | C2    | 96  | LYS  |
| 2   | C2    | 163 | LYS  |
| 2   | C2    | 181 | VAL  |
| 2   | C2    | 372 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C3    | 95  | THR  |
| 3   | C3    | 178 | THR  |
| 3   | C3    | 297 | LYS  |
| 3   | C3    | 330 | MET  |
| 3   | C3    | 359 | LYS  |
| 3   | C3    | 388 | MET  |
| 2   | C4    | 2   | ARG  |
| 2   | C4    | 115 | VAL  |
| 2   | C4    | 280 | LYS  |
| 2   | C4    | 326 | LYS  |
| 3   | C5    | 42  | LEU  |
| 3   | C5    | 83  | GLN  |
| 3   | C5    | 154 | LYS  |
| 3   | C5    | 174 | LYS  |
| 3   | C5    | 297 | LYS  |
| 3   | C5    | 405 | GLU  |
| 2   | C6    | 36  | MET  |
| 2   | C6    | 85  | HIS  |
| 2   | C6    | 112 | LYS  |
| 2   | C6    | 132 | LEU  |
| 2   | C6    | 336 | LYS  |
| 2   | C6    | 338 | LYS  |
| 2   | C6    | 339 | ARG  |
| 2   | C6    | 401 | LYS  |
| 3   | C7    | 42  | LEU  |
| 3   | C7    | 88  | ASP  |
| 3   | C7    | 174 | LYS  |
| 3   | C7    | 276 | ARG  |
| 3   | C7    | 324 | LYS  |
| 3   | C7    | 334 | GLN  |
| 3   | C7    | 379 | LYS  |
| 2   | C8    | 96  | LYS  |
| 2   | C8    | 163 | LYS  |
| 2   | C8    | 224 | TYR  |
| 2   | C8    | 311 | LYS  |
| 2   | C8    | 338 | LYS  |
| 2   | C8    | 342 | GLN  |
| 2   | C8    | 352 | LYS  |
| 2   | C8    | 401 | LYS  |
| 2   | C8    | 433 | GLU  |
| 3   | C9    | 16  | ILE  |
| 3   | C9    | 154 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C9    | 164 | MET  |
| 3   | C9    | 336 | LYS  |
| 3   | C9    | 343 | GLU  |
| 3   | C9    | 390 | ARG  |
| 3   | C9    | 424 | GLN  |
| 2   | D0    | 7   | ILE  |
| 2   | D0    | 156 | ARG  |
| 2   | D0    | 339 | ARG  |
| 2   | D0    | 401 | LYS  |
| 2   | D0    | 409 | VAL  |
| 3   | D1    | 46  | ARG  |
| 3   | D1    | 77  | ARG  |
| 3   | D1    | 99  | ASN  |
| 3   | D1    | 121 | ARG  |
| 3   | D1    | 134 | GLN  |
| 3   | D1    | 154 | LYS  |
| 3   | D1    | 213 | ARG  |
| 3   | D1    | 276 | ARG  |
| 3   | D1    | 376 | GLU  |
| 3   | D1    | 391 | ARG  |
| 3   | D1    | 406 | MET  |
| 2   | D2    | 92  | LEU  |
| 2   | D2    | 155 | GLU  |
| 2   | D2    | 163 | LYS  |
| 2   | D2    | 264 | ARG  |
| 2   | D2    | 297 | GLU  |
| 2   | D2    | 311 | LYS  |
| 2   | D2    | 339 | ARG  |
| 2   | D2    | 370 | LYS  |
| 2   | D2    | 401 | LYS  |
| 3   | D3    | 113 | ILE  |
| 3   | D3    | 191 | GLN  |
| 3   | D3    | 213 | ARG  |
| 3   | D3    | 343 | GLU  |
| 3   | D3    | 362 | LYS  |
| 3   | D3    | 391 | ARG  |
| 3   | D3    | 406 | MET  |
| 2   | D4    | 123 | ARG  |
| 2   | D4    | 141 | VAL  |
| 2   | D4    | 163 | LYS  |
| 2   | D4    | 181 | VAL  |
| 2   | D4    | 248 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D4    | 252 | VAL  |
| 2   | D4    | 285 | GLN  |
| 2   | D4    | 311 | LYS  |
| 2   | D4    | 430 | LYS  |
| 2   | D4    | 437 | ILE  |
| 3   | D5    | 2   | ARG  |
| 3   | D5    | 46  | ARG  |
| 3   | D5    | 112 | LEU  |
| 3   | D5    | 129 | CYS  |
| 3   | D5    | 209 | ASP  |
| 3   | D5    | 217 | LEU  |
| 3   | D5    | 229 | VAL  |
| 3   | D5    | 246 | LEU  |
| 3   | D5    | 316 | MET  |
| 3   | D5    | 343 | GLU  |
| 3   | D5    | 352 | SER  |
| 3   | D5    | 391 | ARG  |
| 3   | D5    | 410 | GLU  |
| 2   | D6    | 96  | LYS  |
| 2   | D6    | 163 | LYS  |
| 2   | D6    | 297 | GLU  |
| 2   | D6    | 430 | LYS  |
| 3   | D7    | 122 | LYS  |
| 3   | D7    | 154 | LYS  |
| 3   | D7    | 164 | MET  |
| 3   | D7    | 174 | LYS  |
| 3   | D7    | 390 | ARG  |
| 3   | D7    | 391 | ARG  |
| 3   | D7    | 406 | MET  |
| 2   | D8    | 92  | LEU  |
| 2   | D8    | 96  | LYS  |
| 2   | D8    | 141 | VAL  |
| 2   | D8    | 163 | LYS  |
| 2   | D8    | 214 | ARG  |
| 2   | D8    | 297 | GLU  |
| 2   | D8    | 326 | LYS  |
| 2   | D8    | 372 | MET  |
| 2   | D8    | 430 | LYS  |
| 3   | D9    | 2   | ARG  |
| 3   | D9    | 19  | LYS  |
| 3   | D9    | 32  | PRO  |
| 3   | D9    | 48  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D9    | 128 | ASP  |
| 3   | D9    | 215 | LEU  |
| 3   | D9    | 276 | ARG  |
| 3   | D9    | 405 | GLU  |
| 2   | E0    | 96  | LYS  |
| 2   | E0    | 163 | LYS  |
| 2   | E0    | 221 | ARG  |
| 3   | E1    | 11  | GLN  |
| 3   | E1    | 122 | LYS  |
| 3   | E1    | 215 | LEU  |
| 3   | E1    | 297 | LYS  |
| 3   | E1    | 328 | GLU  |
| 3   | E1    | 391 | ARG  |
| 2   | E2    | 89  | PRO  |
| 2   | E2    | 160 | ASP  |
| 2   | E2    | 163 | LYS  |
| 2   | E2    | 184 | PRO  |
| 2   | E2    | 338 | LYS  |
| 2   | E2    | 397 | LEU  |
| 2   | E2    | 430 | LYS  |
| 3   | E3    | 11  | GLN  |
| 3   | E3    | 46  | ARG  |
| 3   | E3    | 130 | LEU  |
| 3   | E3    | 174 | LYS  |
| 3   | E3    | 247 | ASN  |
| 3   | E3    | 276 | ARG  |
| 3   | E3    | 320 | ARG  |
| 3   | E3    | 324 | LYS  |
| 3   | E3    | 362 | LYS  |
| 3   | E3    | 391 | ARG  |
| 3   | E3    | 406 | MET  |
| 2   | E4    | 256 | GLN  |
| 2   | E4    | 280 | LYS  |
| 2   | E4    | 401 | LYS  |
| 3   | E5    | 11  | GLN  |
| 3   | E5    | 297 | LYS  |
| 3   | E5    | 390 | ARG  |
| 2   | E6    | 124 | LYS  |
| 2   | E6    | 280 | LYS  |
| 2   | E6    | 285 | GLN  |
| 2   | E6    | 326 | LYS  |
| 2   | E6    | 338 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E6    | 401 | LYS  |
| 3   | E7    | 174 | LYS  |
| 3   | E7    | 217 | LEU  |
| 3   | E7    | 291 | GLN  |
| 3   | E7    | 320 | ARG  |
| 2   | E8    | 283 | HIS  |
| 3   | E9    | 122 | LYS  |
| 3   | E9    | 379 | LYS  |
| 2   | F0    | 96  | LYS  |
| 2   | F0    | 227 | LEU  |
| 2   | F0    | 280 | LYS  |
| 2   | F0    | 336 | LYS  |
| 2   | F0    | 370 | LYS  |
| 2   | F0    | 401 | LYS  |
| 3   | F1    | 91  | VAL  |
| 3   | F1    | 122 | LYS  |
| 3   | F1    | 125 | GLU  |
| 3   | F1    | 177 | ASP  |
| 3   | F1    | 252 | LYS  |
| 3   | F1    | 324 | LYS  |
| 3   | F1    | 384 | GLN  |
| 4   | a     | 66  | SER  |
| 4   | a     | 196 | LEU  |
| 4   | b     | 69  | LYS  |
| 4   | b     | 176 | ASP  |
| 4   | c     | 36  | ILE  |
| 4   | c     | 52  | GLU  |
| 4   | c     | 69  | LYS  |
| 4   | c     | 151 | MET  |
| 4   | c     | 191 | GLU  |
| 4   | c     | 202 | ARG  |
| 4   | d     | 28  | LYS  |
| 4   | d     | 35  | ASN  |
| 4   | d     | 101 | GLU  |
| 4   | d     | 117 | ARG  |
| 4   | d     | 151 | MET  |
| 4   | d     | 152 | LYS  |
| 4   | d     | 155 | GLU  |
| 4   | d     | 191 | GLU  |
| 4   | d     | 202 | ARG  |
| 4   | e     | 69  | LYS  |
| 4   | e     | 107 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | e     | 120 | GLU  |
| 4   | e     | 153 | GLU  |
| 4   | f     | 35  | ASN  |
| 4   | f     | 36  | ILE  |
| 4   | f     | 56  | LYS  |
| 4   | f     | 69  | LYS  |
| 4   | g     | 13  | GLU  |
| 4   | g     | 24  | MET  |
| 4   | h     | 28  | LYS  |
| 4   | h     | 97  | ARG  |
| 4   | h     | 198 | ARG  |
| 4   | i     | 36  | ILE  |
| 4   | j     | 178 | ARG  |
| 4   | j     | 202 | ARG  |
| 5   | k     | 25  | ARG  |
| 5   | k     | 52  | VAL  |
| 5   | k     | 78  | LYS  |
| 5   | k     | 98  | LYS  |
| 5   | k     | 103 | LYS  |
| 5   | k     | 153 | VAL  |
| 5   | l     | 52  | VAL  |
| 5   | l     | 153 | VAL  |
| 5   | l     | 163 | LYS  |
| 4   | m     | 28  | LYS  |
| 4   | m     | 99  | MET  |
| 4   | n     | 17  | LEU  |
| 4   | n     | 28  | LYS  |
| 4   | n     | 38  | LEU  |
| 4   | n     | 48  | ILE  |
| 4   | n     | 202 | ARG  |
| 4   | o     | 3   | GLN  |
| 4   | o     | 24  | MET  |
| 4   | o     | 63  | ILE  |
| 4   | o     | 91  | PHE  |
| 4   | o     | 117 | ARG  |
| 4   | o     | 164 | ARG  |
| 4   | o     | 202 | ARG  |
| 4   | p     | 56  | LYS  |
| 4   | p     | 152 | LYS  |
| 4   | p     | 185 | ILE  |
| 4   | q     | 48  | ILE  |
| 4   | q     | 56  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | q     | 97  | ARG  |
| 4   | q     | 117 | ARG  |
| 4   | q     | 202 | ARG  |
| 4   | r     | 24  | MET  |
| 4   | r     | 117 | ARG  |
| 4   | r     | 152 | LYS  |
| 4   | r     | 156 | VAL  |
| 4   | r     | 202 | ARG  |
| 4   | r     | 203 | ASN  |
| 4   | s     | 24  | MET  |
| 4   | s     | 63  | ILE  |
| 4   | s     | 152 | LYS  |
| 4   | s     | 202 | ARG  |
| 4   | t     | 173 | ILE  |
| 4   | u     | 3   | GLN  |
| 4   | u     | 28  | LYS  |
| 4   | u     | 119 | ARG  |
| 4   | u     | 125 | HIS  |
| 4   | v     | 3   | GLN  |
| 4   | v     | 69  | LYS  |
| 4   | v     | 84  | LYS  |
| 4   | v     | 94  | ASN  |
| 4   | v     | 197 | LEU  |
| 4   | v     | 202 | ARG  |
| 5   | w     | 25  | ARG  |
| 5   | w     | 58  | LYS  |
| 5   | w     | 65  | GLU  |
| 5   | w     | 78  | LYS  |
| 5   | w     | 156 | ARG  |
| 5   | x     | 85  | ARG  |
| 5   | x     | 89  | LEU  |
| 5   | x     | 110 | ARG  |
| 5   | x     | 162 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (355) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 242 | ASN  |
| 1   | 0     | 244 | GLN  |
| 1   | 1     | 244 | GLN  |
| 1   | 12    | 242 | ASN  |
| 1   | 13    | 244 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 17    | 242 | ASN  |
| 1   | 18    | 244 | GLN  |
| 1   | 2     | 242 | ASN  |
| 1   | 2     | 244 | GLN  |
| 1   | 20    | 244 | GLN  |
| 1   | 23    | 242 | ASN  |
| 1   | 3     | 242 | ASN  |
| 1   | 4     | 242 | ASN  |
| 2   | A0    | 102 | ASN  |
| 2   | A0    | 228 | ASN  |
| 2   | A0    | 285 | GLN  |
| 3   | A1    | 43  | GLN  |
| 3   | A1    | 89  | ASN  |
| 3   | A1    | 247 | ASN  |
| 3   | A1    | 256 | ASN  |
| 3   | A1    | 348 | ASN  |
| 3   | A1    | 375 | GLN  |
| 3   | A1    | 396 | HIS  |
| 3   | A1    | 426 | GLN  |
| 2   | A2    | 85  | HIS  |
| 2   | A2    | 101 | ASN  |
| 2   | A2    | 102 | ASN  |
| 2   | A2    | 128 | ASN  |
| 2   | A2    | 206 | ASN  |
| 2   | A2    | 216 | ASN  |
| 2   | A2    | 256 | GLN  |
| 2   | A2    | 358 | GLN  |
| 2   | A2    | 393 | HIS  |
| 3   | A3    | 89  | ASN  |
| 3   | A3    | 94  | GLN  |
| 3   | A3    | 256 | ASN  |
| 3   | A3    | 347 | ASN  |
| 3   | A3    | 348 | ASN  |
| 3   | A3    | 414 | ASN  |
| 3   | A3    | 426 | GLN  |
| 2   | A4    | 186 | ASN  |
| 3   | A5    | 43  | GLN  |
| 3   | A5    | 100 | ASN  |
| 3   | A5    | 191 | GLN  |
| 3   | A5    | 280 | GLN  |
| 3   | A5    | 329 | GLN  |
| 3   | A5    | 348 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A6    | 11  | GLN  |
| 2   | A6    | 31  | GLN  |
| 2   | A6    | 102 | ASN  |
| 2   | A6    | 128 | ASN  |
| 2   | A6    | 256 | GLN  |
| 2   | A6    | 283 | HIS  |
| 2   | A6    | 342 | GLN  |
| 2   | A6    | 380 | ASN  |
| 3   | A7    | 131 | GLN  |
| 3   | A7    | 191 | GLN  |
| 3   | A7    | 195 | ASN  |
| 3   | A7    | 204 | ASN  |
| 3   | A7    | 247 | ASN  |
| 2   | A8    | 11  | GLN  |
| 2   | A8    | 91  | GLN  |
| 2   | A8    | 102 | ASN  |
| 2   | A8    | 107 | HIS  |
| 2   | A8    | 329 | ASN  |
| 2   | A8    | 380 | ASN  |
| 2   | A8    | 393 | HIS  |
| 3   | A9    | 137 | HIS  |
| 3   | A9    | 190 | HIS  |
| 3   | A9    | 279 | GLN  |
| 3   | A9    | 332 | ASN  |
| 2   | B0    | 11  | GLN  |
| 2   | B0    | 233 | GLN  |
| 2   | B0    | 283 | HIS  |
| 3   | B1    | 94  | GLN  |
| 2   | B2    | 11  | GLN  |
| 2   | B2    | 15  | GLN  |
| 2   | B2    | 31  | GLN  |
| 2   | B2    | 35  | GLN  |
| 2   | B2    | 91  | GLN  |
| 2   | B2    | 101 | ASN  |
| 2   | B2    | 226 | ASN  |
| 2   | B2    | 256 | GLN  |
| 3   | B3    | 6   | HIS  |
| 3   | B3    | 11  | GLN  |
| 3   | B3    | 100 | ASN  |
| 3   | B3    | 131 | GLN  |
| 3   | B3    | 134 | GLN  |
| 3   | B3    | 195 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B3    | 307 | HIS  |
| 3   | B3    | 347 | ASN  |
| 3   | B3    | 348 | ASN  |
| 2   | B4    | 31  | GLN  |
| 2   | B4    | 256 | GLN  |
| 2   | B4    | 266 | HIS  |
| 2   | B4    | 285 | GLN  |
| 3   | B5    | 14  | ASN  |
| 3   | B5    | 52  | ASN  |
| 3   | B5    | 83  | GLN  |
| 3   | B5    | 99  | ASN  |
| 3   | B5    | 191 | GLN  |
| 3   | B5    | 298 | ASN  |
| 3   | B5    | 329 | GLN  |
| 3   | B5    | 334 | GLN  |
| 3   | B5    | 347 | ASN  |
| 3   | B5    | 348 | ASN  |
| 2   | B6    | 168 | ASN  |
| 2   | B6    | 256 | GLN  |
| 3   | B7    | 105 | HIS  |
| 3   | B7    | 256 | ASN  |
| 3   | B7    | 307 | HIS  |
| 3   | B7    | 396 | HIS  |
| 2   | B8    | 11  | GLN  |
| 2   | B8    | 50  | ASN  |
| 2   | B8    | 107 | HIS  |
| 2   | B8    | 133 | GLN  |
| 2   | B8    | 176 | GLN  |
| 2   | B8    | 216 | ASN  |
| 2   | B8    | 226 | ASN  |
| 2   | B8    | 258 | ASN  |
| 2   | B8    | 406 | HIS  |
| 3   | B9    | 8   | GLN  |
| 3   | B9    | 191 | GLN  |
| 3   | B9    | 227 | HIS  |
| 3   | B9    | 245 | GLN  |
| 3   | B9    | 426 | GLN  |
| 2   | C0    | 11  | GLN  |
| 2   | C0    | 139 | ASN  |
| 2   | C0    | 258 | ASN  |
| 2   | C0    | 285 | GLN  |
| 2   | C0    | 293 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C0    | 406 | HIS  |
| 3   | C1    | 89  | ASN  |
| 3   | C1    | 195 | ASN  |
| 3   | C1    | 337 | ASN  |
| 2   | C2    | 11  | GLN  |
| 2   | C2    | 256 | GLN  |
| 2   | C2    | 380 | ASN  |
| 2   | C2    | 406 | HIS  |
| 3   | C3    | 14  | ASN  |
| 3   | C3    | 137 | HIS  |
| 3   | C3    | 191 | GLN  |
| 3   | C3    | 195 | ASN  |
| 3   | C3    | 292 | GLN  |
| 3   | C3    | 335 | ASN  |
| 2   | C4    | 31  | GLN  |
| 2   | C4    | 101 | ASN  |
| 2   | C4    | 133 | GLN  |
| 3   | C5    | 43  | GLN  |
| 3   | C5    | 105 | HIS  |
| 3   | C5    | 131 | GLN  |
| 3   | C5    | 291 | GLN  |
| 3   | C5    | 335 | ASN  |
| 3   | C5    | 337 | ASN  |
| 2   | C6    | 28  | HIS  |
| 2   | C6    | 168 | ASN  |
| 3   | C7    | 8   | GLN  |
| 3   | C7    | 131 | GLN  |
| 3   | C7    | 245 | GLN  |
| 3   | C7    | 332 | ASN  |
| 2   | C8    | 28  | HIS  |
| 2   | C8    | 101 | ASN  |
| 2   | C8    | 206 | ASN  |
| 3   | C9    | 11  | GLN  |
| 3   | C9    | 94  | GLN  |
| 3   | C9    | 99  | ASN  |
| 3   | C9    | 131 | GLN  |
| 3   | C9    | 245 | GLN  |
| 3   | C9    | 264 | HIS  |
| 3   | C9    | 334 | GLN  |
| 3   | C9    | 384 | GLN  |
| 3   | C9    | 414 | ASN  |
| 3   | C9    | 426 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D0    | 18  | ASN  |
| 2   | D0    | 102 | ASN  |
| 2   | D0    | 133 | GLN  |
| 2   | D0    | 139 | ASN  |
| 2   | D0    | 168 | ASN  |
| 2   | D0    | 206 | ASN  |
| 2   | D0    | 258 | ASN  |
| 2   | D0    | 283 | HIS  |
| 3   | D1    | 43  | GLN  |
| 3   | D1    | 337 | ASN  |
| 3   | D1    | 414 | ASN  |
| 3   | D1    | 424 | GLN  |
| 2   | D2    | 11  | GLN  |
| 2   | D2    | 88  | HIS  |
| 2   | D2    | 258 | ASN  |
| 2   | D2    | 293 | ASN  |
| 2   | D2    | 380 | ASN  |
| 3   | D3    | 134 | GLN  |
| 3   | D3    | 195 | ASN  |
| 3   | D3    | 332 | ASN  |
| 3   | D3    | 347 | ASN  |
| 3   | D3    | 384 | GLN  |
| 3   | D3    | 396 | HIS  |
| 2   | D4    | 8   | HIS  |
| 2   | D4    | 11  | GLN  |
| 2   | D4    | 18  | ASN  |
| 2   | D4    | 206 | ASN  |
| 2   | D4    | 216 | ASN  |
| 2   | D4    | 380 | ASN  |
| 3   | D5    | 137 | HIS  |
| 3   | D5    | 191 | GLN  |
| 3   | D5    | 195 | ASN  |
| 3   | D5    | 256 | ASN  |
| 3   | D5    | 298 | ASN  |
| 3   | D5    | 347 | ASN  |
| 3   | D5    | 348 | ASN  |
| 2   | D6    | 31  | GLN  |
| 2   | D6    | 91  | GLN  |
| 2   | D6    | 102 | ASN  |
| 2   | D6    | 176 | GLN  |
| 2   | D6    | 186 | ASN  |
| 2   | D6    | 192 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D7    | 99  | ASN  |
| 3   | D7    | 191 | GLN  |
| 3   | D7    | 292 | GLN  |
| 3   | D7    | 348 | ASN  |
| 3   | D7    | 375 | GLN  |
| 3   | D7    | 426 | GLN  |
| 2   | D8    | 101 | ASN  |
| 2   | D8    | 102 | ASN  |
| 2   | D8    | 356 | ASN  |
| 3   | D9    | 6   | HIS  |
| 3   | D9    | 8   | GLN  |
| 3   | D9    | 14  | ASN  |
| 3   | D9    | 52  | ASN  |
| 3   | D9    | 204 | ASN  |
| 3   | D9    | 279 | GLN  |
| 3   | D9    | 280 | GLN  |
| 3   | D9    | 291 | GLN  |
| 2   | E0    | 18  | ASN  |
| 2   | E0    | 102 | ASN  |
| 2   | E0    | 258 | ASN  |
| 2   | E0    | 356 | ASN  |
| 3   | E1    | 14  | ASN  |
| 3   | E1    | 43  | GLN  |
| 3   | E1    | 191 | GLN  |
| 3   | E1    | 247 | ASN  |
| 3   | E1    | 298 | ASN  |
| 2   | E2    | 11  | GLN  |
| 2   | E2    | 216 | ASN  |
| 2   | E2    | 228 | ASN  |
| 2   | E2    | 258 | ASN  |
| 3   | E3    | 6   | HIS  |
| 3   | E3    | 131 | GLN  |
| 3   | E3    | 247 | ASN  |
| 2   | E4    | 11  | GLN  |
| 2   | E4    | 31  | GLN  |
| 2   | E4    | 50  | ASN  |
| 2   | E4    | 128 | ASN  |
| 2   | E4    | 197 | HIS  |
| 2   | E4    | 285 | GLN  |
| 2   | E4    | 342 | GLN  |
| 3   | E5    | 11  | GLN  |
| 3   | E5    | 245 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E5    | 256 | ASN  |
| 3   | E5    | 329 | GLN  |
| 3   | E5    | 423 | GLN  |
| 2   | E6    | 35  | GLN  |
| 2   | E6    | 101 | ASN  |
| 2   | E6    | 216 | ASN  |
| 2   | E6    | 226 | ASN  |
| 2   | E6    | 358 | GLN  |
| 3   | E7    | 43  | GLN  |
| 3   | E7    | 292 | GLN  |
| 3   | E7    | 347 | ASN  |
| 3   | E7    | 348 | ASN  |
| 3   | E7    | 375 | GLN  |
| 3   | E7    | 414 | ASN  |
| 2   | E8    | 8   | HIS  |
| 2   | E8    | 128 | ASN  |
| 3   | E9    | 99  | ASN  |
| 3   | E9    | 204 | ASN  |
| 3   | E9    | 256 | ASN  |
| 3   | E9    | 335 | ASN  |
| 3   | E9    | 348 | ASN  |
| 3   | E9    | 396 | HIS  |
| 2   | F0    | 18  | ASN  |
| 2   | F0    | 31  | GLN  |
| 2   | F0    | 258 | ASN  |
| 3   | F1    | 15  | GLN  |
| 3   | F1    | 134 | GLN  |
| 3   | F1    | 279 | GLN  |
| 3   | F1    | 291 | GLN  |
| 3   | F1    | 337 | ASN  |
| 3   | F1    | 347 | ASN  |
| 4   | a     | 100 | ASN  |
| 4   | b     | 60  | ASN  |
| 4   | b     | 94  | ASN  |
| 4   | b     | 105 | ASN  |
| 4   | c     | 18  | ASN  |
| 4   | c     | 65  | GLN  |
| 4   | c     | 106 | GLN  |
| 4   | d     | 35  | ASN  |
| 4   | d     | 60  | ASN  |
| 4   | d     | 181 | GLN  |
| 4   | d     | 203 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | e     | 37  | GLN  |
| 4   | e     | 106 | GLN  |
| 4   | f     | 18  | ASN  |
| 4   | f     | 37  | GLN  |
| 4   | f     | 94  | ASN  |
| 4   | f     | 125 | HIS  |
| 4   | g     | 25  | GLN  |
| 4   | g     | 37  | GLN  |
| 4   | g     | 106 | GLN  |
| 4   | h     | 11  | ASN  |
| 4   | h     | 37  | GLN  |
| 4   | h     | 106 | GLN  |
| 4   | h     | 147 | HIS  |
| 4   | i     | 3   | GLN  |
| 4   | i     | 94  | ASN  |
| 4   | j     | 3   | GLN  |
| 4   | j     | 18  | ASN  |
| 4   | j     | 59  | ASN  |
| 5   | k     | 17  | GLN  |
| 5   | k     | 28  | HIS  |
| 5   | k     | 113 | ASN  |
| 5   | k     | 148 | GLN  |
| 5   | l     | 17  | GLN  |
| 5   | l     | 18  | GLN  |
| 4   | m     | 11  | ASN  |
| 4   | m     | 35  | ASN  |
| 4   | m     | 94  | ASN  |
| 4   | m     | 147 | HIS  |
| 4   | n     | 18  | ASN  |
| 4   | n     | 94  | ASN  |
| 4   | n     | 105 | ASN  |
| 4   | o     | 125 | HIS  |
| 4   | o     | 181 | GLN  |
| 4   | p     | 18  | ASN  |
| 4   | p     | 67  | HIS  |
| 4   | p     | 105 | ASN  |
| 4   | p     | 203 | ASN  |
| 4   | q     | 37  | GLN  |
| 4   | q     | 60  | ASN  |
| 4   | q     | 181 | GLN  |
| 4   | s     | 25  | GLN  |
| 4   | s     | 59  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | t     | 11  | ASN  |
| 4   | t     | 94  | ASN  |
| 4   | t     | 181 | GLN  |
| 4   | u     | 59  | ASN  |
| 4   | u     | 67  | HIS  |
| 4   | u     | 100 | ASN  |
| 4   | u     | 181 | GLN  |
| 4   | v     | 18  | ASN  |
| 4   | v     | 65  | GLN  |
| 4   | v     | 94  | ASN  |
| 4   | v     | 203 | ASN  |
| 5   | w     | 155 | GLN  |
| 5   | x     | 55  | GLN  |
| 5   | x     | 147 | GLN  |

### 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.

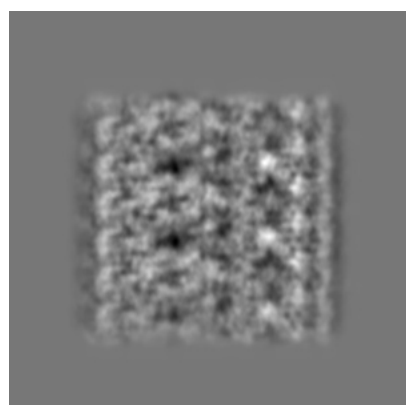
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26018. These allow visual inspection of the internal detail of the map and identification of artifacts.

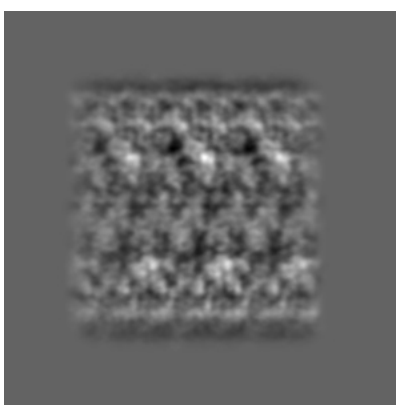
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 6.1.1 Primary map



X



Y

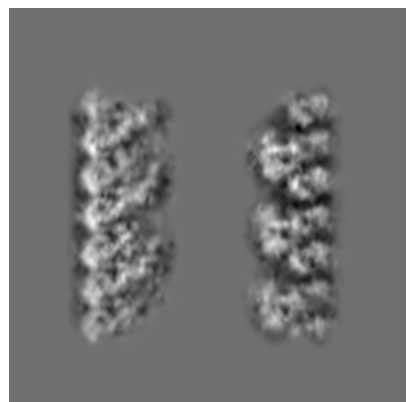


Z

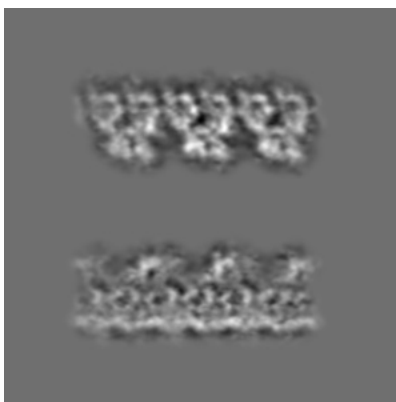
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 108



Y Index: 108

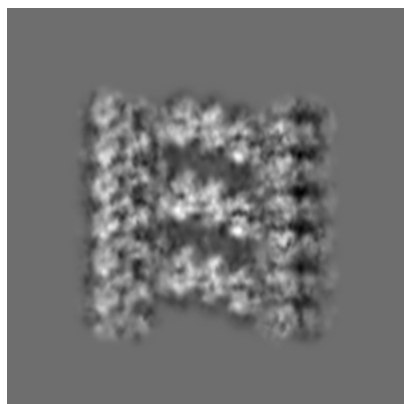


Z Index: 108

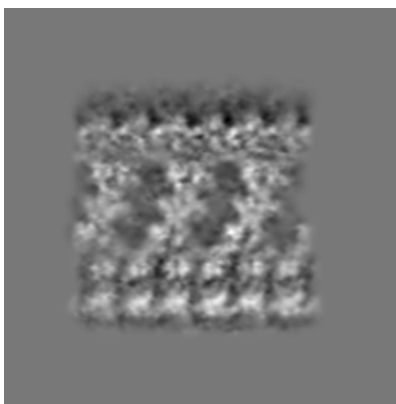
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 137



Y Index: 139

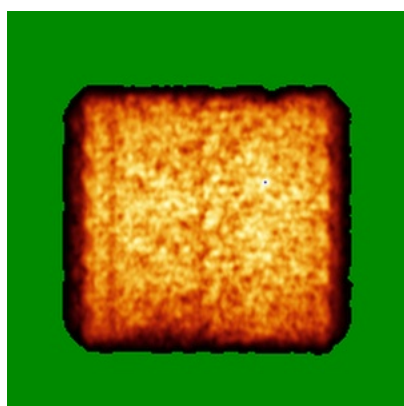


Z Index: 114

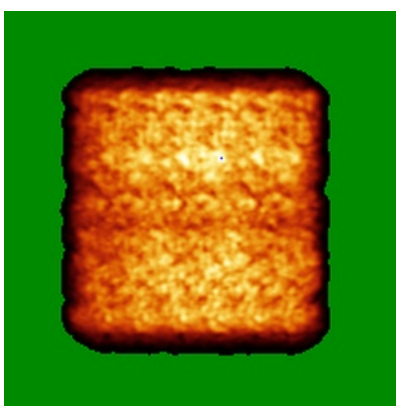
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y

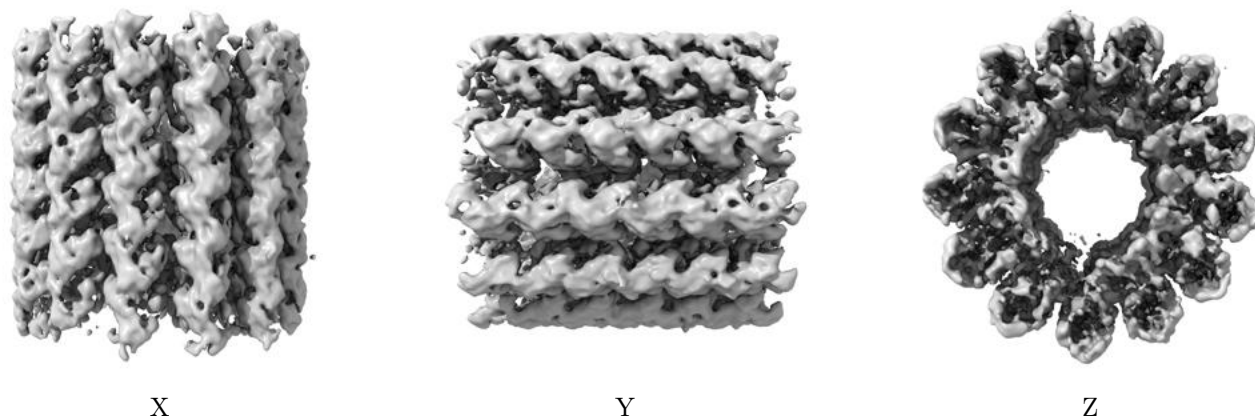


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

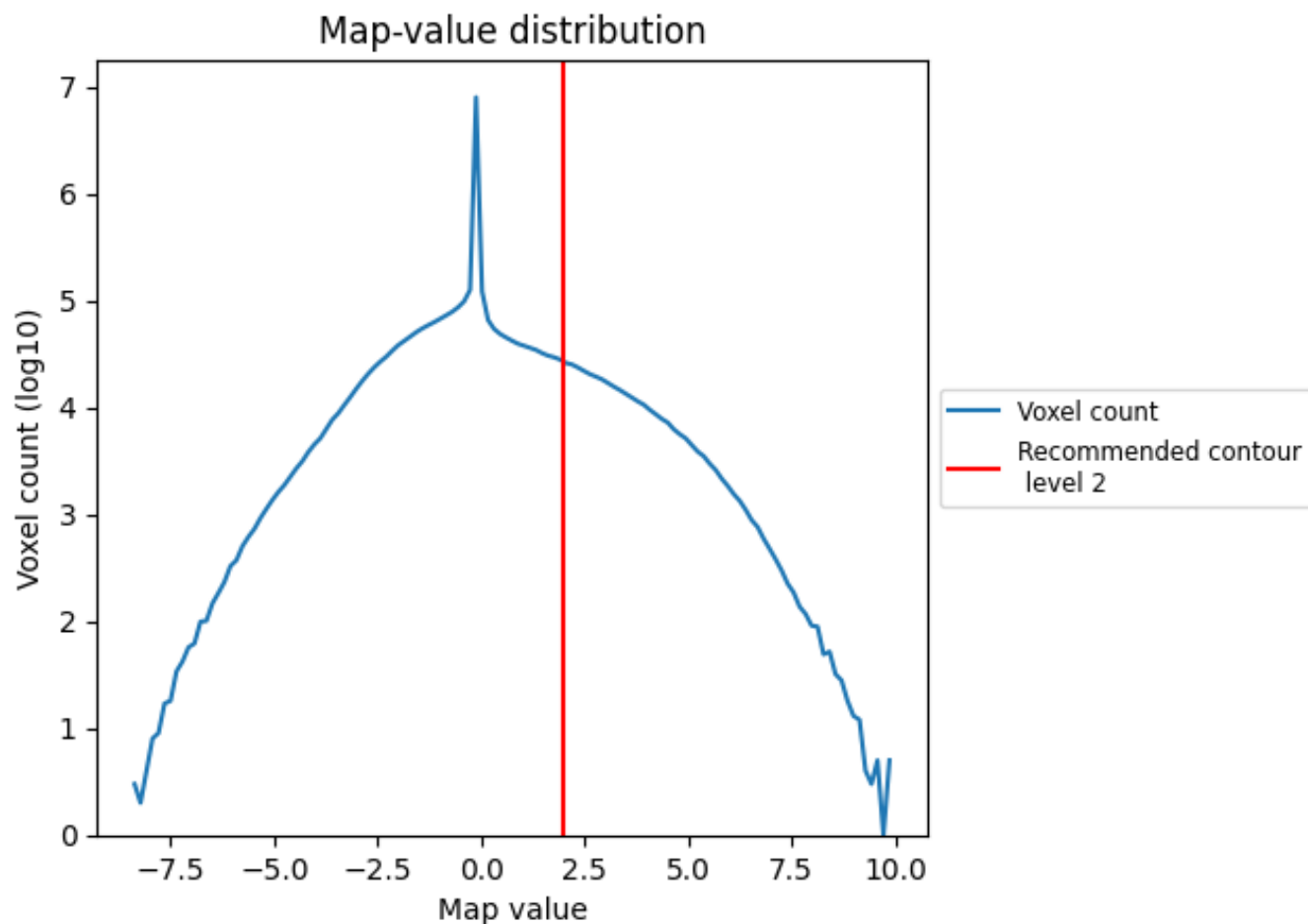
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

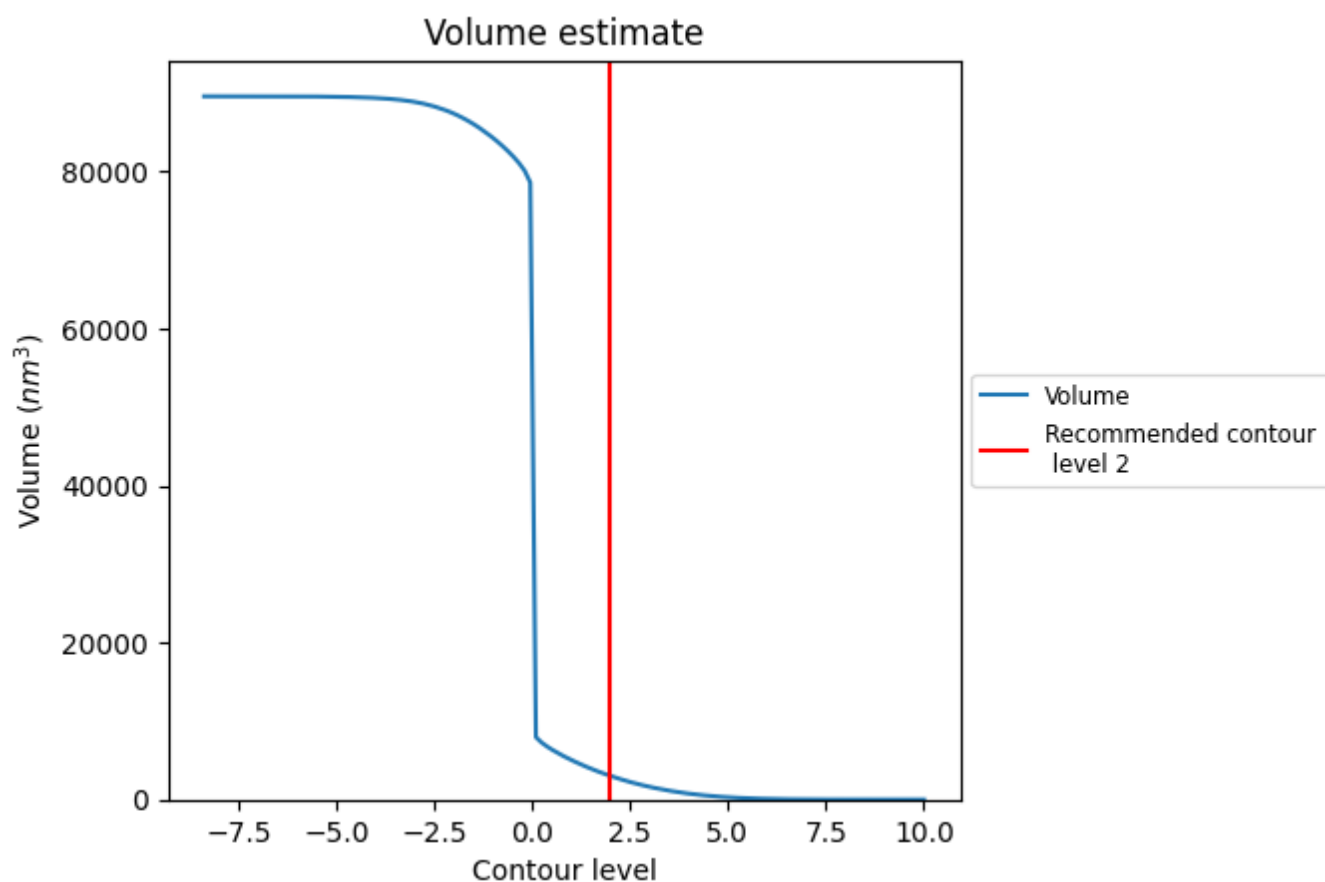
This section contains the results of statistical analysis of the map.

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



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

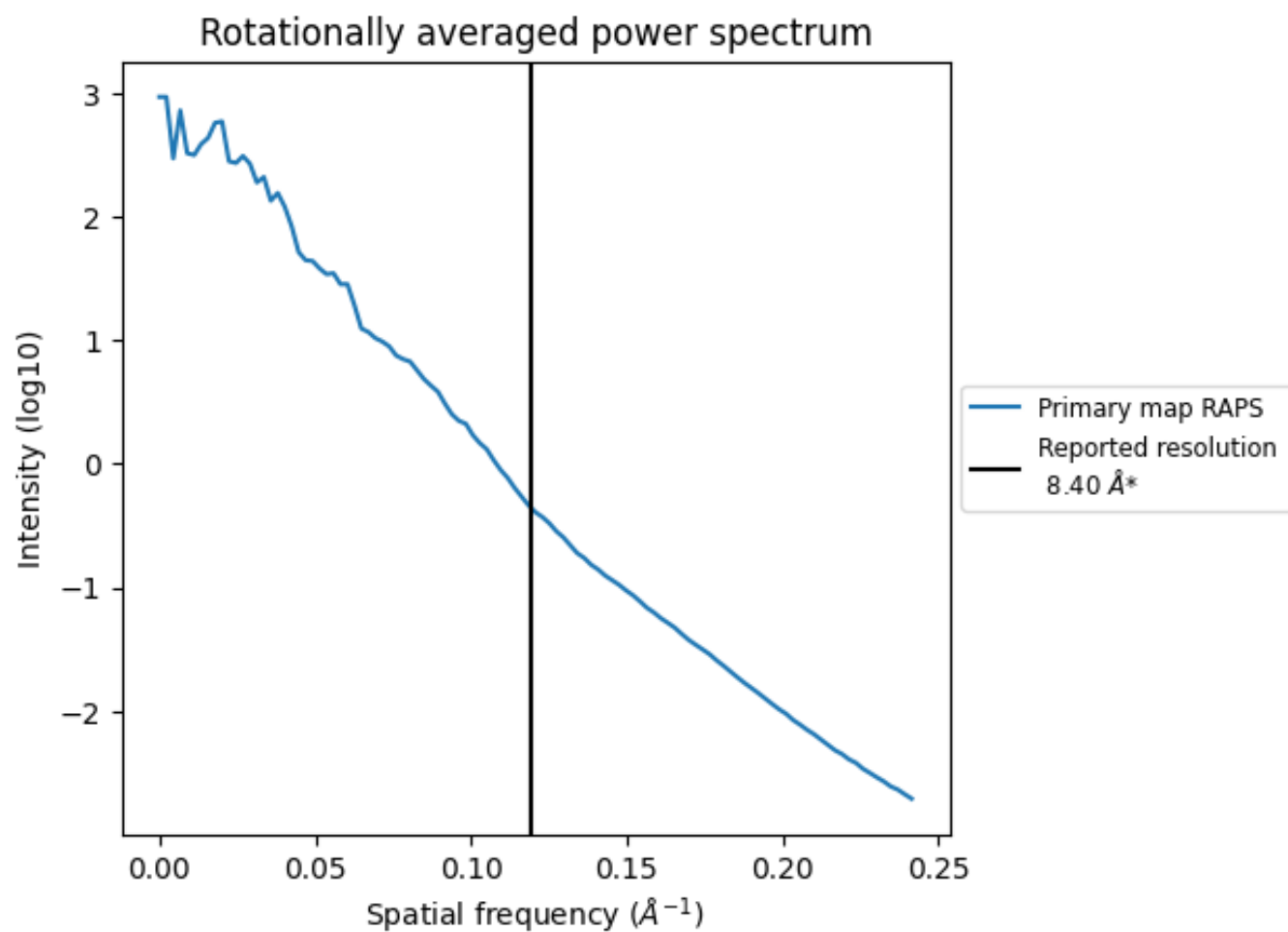
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3015 nm<sup>3</sup>; this corresponds to an approximate mass of 2724 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 0.119 Å<sup>-1</sup>

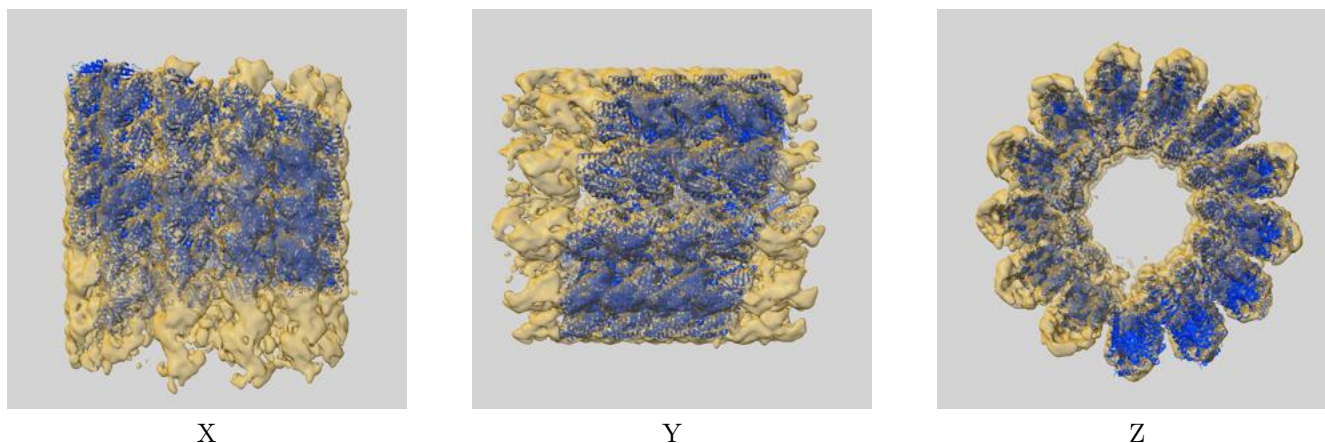
## 8 Fourier-Shell correlation

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

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

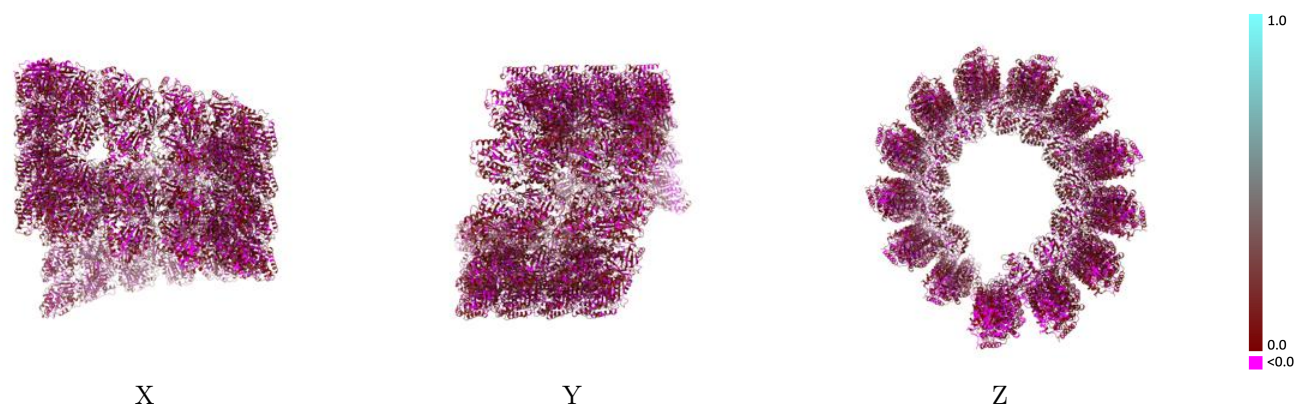
This section contains information regarding the fit between EMDB map EMD-26018 and PDB model 7TNQ. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

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



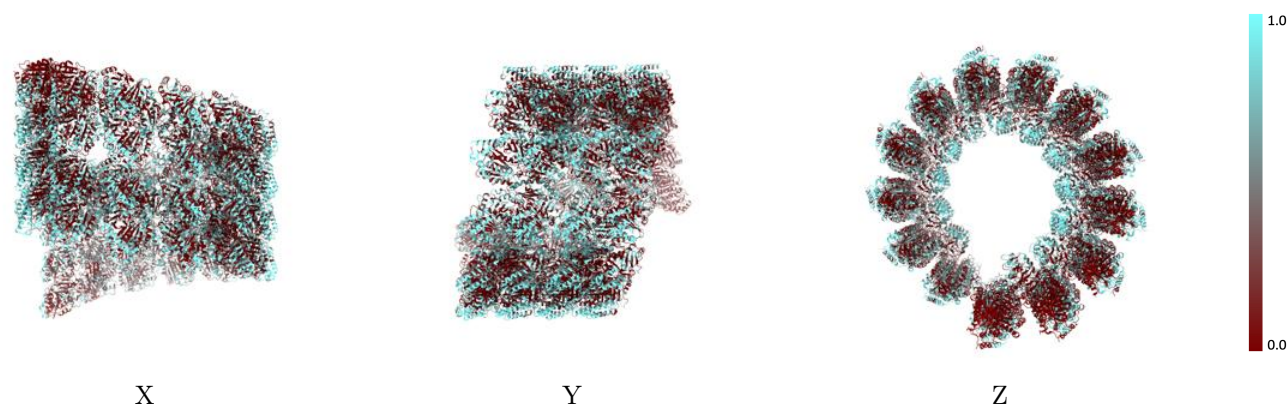
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



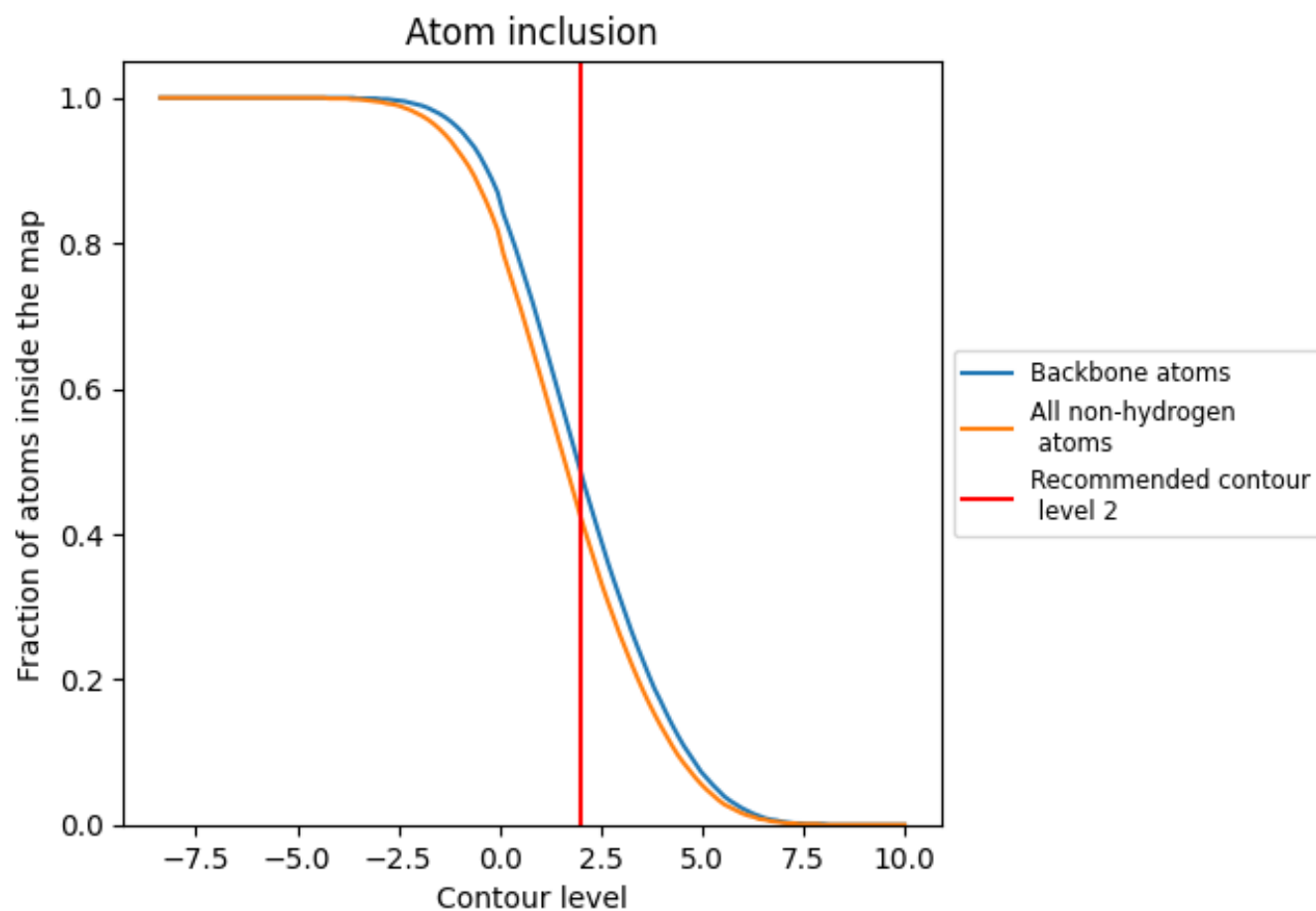
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4240   |  0.0760   |
| 0     |  0.1290   |  0.1680   |
| 1     |  0.0000   |  0.0940   |
| 10    |  0.0820   |  0.0720   |
| 11    |  0.0470   |  0.1110   |
| 12    |  0.1710   |  0.1250   |
| 13    |  0.1470   |  0.1000   |
| 14    |  0.0180   |  0.0900   |
| 15    |  0.0940   |  0.1000   |
| 16    |  0.1350   |  0.1160   |
| 17    |  0.2590   |  0.1140   |
| 18    |  0.1820   |  0.0380   |
| 19    |  0.2410   |  0.0440   |
| 2     |  0.1120   |  0.1250   |
| 20    |  0.1410  |  0.0080  |
| 21    |  0.4230 |  0.0670 |
| 22    |  0.0190 |  0.0960 |
| 23    |  0.0130 |  0.1160 |
| 3     |  0.0650 |  0.1040 |
| 4     |  0.1290 |  0.1020 |
| 5     |  0.1180 |  0.1400 |
| 6     |  0.1290 |  0.0710 |
| 7     |  0.1470 |  0.1150 |
| 8     |  0.0760 |  0.0500 |
| 9     |  0.0290 |  0.0540 |
| A0    |  0.4570 |  0.0780 |
| A1    |  0.4220 |  0.0750 |
| A2    |  0.4210 |  0.0760 |
| A3    |  0.2960 |  0.0730 |
| A4    |  0.4700 |  0.0730 |
| A5    |  0.4630 |  0.0750 |
| A6    |  0.4380 |  0.0780 |
| A7    |  0.3430 |  0.0670 |
| A8    |  0.4370 |  0.0720 |
| A9    |  0.4450 |  0.0830 |



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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| B0    | 0.4220         | 0.0810  |
| B1    | 0.3690         | 0.0780  |
| B2    | 0.4200         | 0.0800  |
| B3    | 0.4480         | 0.0790  |
| B4    | 0.4340         | 0.0810  |
| B5    | 0.3970         | 0.0760  |
| B6    | 0.4140         | 0.0790  |
| B7    | 0.5220         | 0.0920  |
| B8    | 0.4770         | 0.0920  |
| B9    | 0.4330         | 0.0850  |
| C0    | 0.4230         | 0.0770  |
| C1    | 0.5340         | 0.0910  |
| C2    | 0.4690         | 0.0920  |
| C3    | 0.4730         | 0.0890  |
| C4    | 0.4010         | 0.0880  |
| C5    | 0.4720         | 0.0910  |
| C6    | 0.4550         | 0.0830  |
| C7    | 0.4460         | 0.0890  |
| C8    | 0.3750         | 0.0630  |
| C9    | 0.4450         | 0.0740  |
| D0    | 0.4290         | 0.0600  |
| D1    | 0.3940         | 0.0560  |
| D2    | 0.3460         | 0.0480  |
| D3    | 0.4020         | 0.0600  |
| D4    | 0.4090         | 0.0630  |
| D5    | 0.3920         | 0.0520  |
| D6    | 0.3360         | 0.0680  |
| D7    | 0.4160         | 0.0710  |
| D8    | 0.4200         | 0.0730  |
| D9    | 0.4310         | 0.0690  |
| E0    | 0.2840         | 0.0700  |
| E1    | 0.4700         | 0.0890  |
| E2    | 0.4410         | 0.0810  |
| E3    | 0.4960         | 0.0820  |
| E4    | 0.1810         | 0.0390  |
| E5    | 0.4740         | 0.0670  |
| E6    | 0.4780         | 0.0800  |
| E7    | 0.5310         | 0.0850  |
| E8    | 0.1180         | -0.0050 |
| E9    | 0.4120         | 0.0750  |
| F0    | 0.4420         | 0.0840  |
| F1    | 0.5000         | 0.0860  |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.3480   |  0.1010   |
| b     |  0.2640   |  0.0810   |
| c     |  0.4900   |  0.1010   |
| d     |  0.3900   |  0.0780   |
| e     |  0.5520   |  0.0950   |
| f     |  0.4870   |  0.0930   |
| g     |  0.5360   |  0.0850   |
| h     |  0.5170   |  0.0850   |
| i     |  0.4540   |  0.0550   |
| j     |  0.4620   |  0.0640   |
| k     |  0.4650   |  0.0850   |
| l     |  0.4770   |  0.0960   |
| m     |  0.4800   |  0.0800   |
| n     |  0.5180   |  0.1010   |
| o     |  0.5300   |  0.0910   |
| p     |  0.5650   |  0.1010   |
| q     |  0.5510   |  0.0870   |
| r     |  0.5860   |  0.1040   |
| s     |  0.5570   |  0.0850   |
| t     |  0.6030  |  0.0800  |
| u     |  0.4430 |  0.0570 |
| v     |  0.5680 |  0.0740 |
| w     |  0.1920 |  0.0270 |
| x     |  0.2870 |  0.0190 |