



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:14 PM UTC

PDB ID : 8WKI / pdb\_00008wki  
EMDB ID : EMD-37600  
Title : Cryo-EM structure of the distal rod-hook within the flagellar motor-hook complex in the CW state.  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-09-27  
Resolution : 3.30 Å(reported)  
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

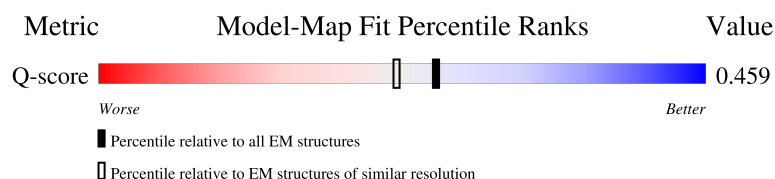
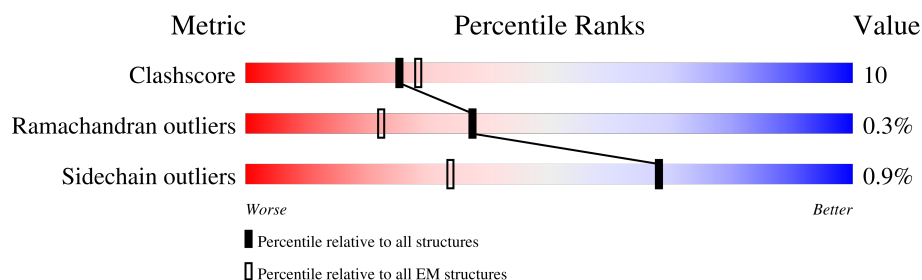
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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                       | 15087 ( 2.80 - 3.80 )                                    |

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   | ZF    | 403    | <div> <div>42%</div> <div>81%</div> <div>18%</div> <div>.</div> </div> |
| 1   | ZG    | 403    | <div> <div>16%</div> <div>75%</div> <div>23%</div> <div>.</div> </div> |
| 1   | ZH    | 403    | <div> <div>11%</div> <div>78%</div> <div>20%</div> <div>.</div> </div> |
| 1   | ZI    | 403    | <div> <div>9%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | ZJ    | 403    | <div> <div>11%</div> <div>77%</div> <div>23%</div> </div> |
| 1   | ZK    | 403    | <div> <div>17%</div> <div>79%</div> <div>20%</div> </div> |
| 1   | ZL    | 403    | <div> <div>15%</div> <div>79%</div> <div>20%</div> </div> |
| 1   | ZM    | 403    | <div> <div>12%</div> <div>75%</div> <div>24%</div> </div> |
| 1   | ZN    | 403    | <div> <div>13%</div> <div>79%</div> <div>20%</div> </div> |
| 1   | ZO    | 403    | <div> <div>16%</div> <div>78%</div> <div>20%</div> </div> |
| 1   | ZP    | 403    | <div> <div>16%</div> <div>74%</div> <div>25%</div> </div> |
| 1   | ZQ    | 403    | <div> <div>19%</div> <div>77%</div> <div>22%</div> </div> |
| 1   | ZR    | 403    | <div> <div>22%</div> <div>77%</div> <div>21%</div> </div> |
| 1   | ZS    | 403    | <div> <div>22%</div> <div>70%</div> <div>29%</div> </div> |
| 1   | ZT    | 403    | <div> <div>29%</div> <div>77%</div> <div>23%</div> </div> |
| 1   | ZU    | 403    | <div> <div>33%</div> <div>75%</div> <div>24%</div> </div> |
| 1   | ZV    | 403    | <div> <div>35%</div> <div>75%</div> <div>25%</div> </div> |
| 1   | ZW    | 403    | <div> <div>34%</div> <div>77%</div> <div>23%</div> </div> |
| 1   | ZX    | 403    | <div> <div>38%</div> <div>80%</div> <div>20%</div> </div> |
| 1   | ZY    | 403    | <div> <div>40%</div> <div>75%</div> <div>24%</div> </div> |
| 1   | ZZ    | 403    | <div> <div>41%</div> <div>79%</div> <div>20%</div> </div> |
| 1   | Za    | 403    | <div> <div>46%</div> <div>84%</div> <div>16%</div> </div> |
| 1   | Zb    | 403    | <div> <div>47%</div> <div>78%</div> <div>21%</div> </div> |
| 1   | Zc    | 403    | <div> <div>49%</div> <div>80%</div> <div>19%</div> </div> |
| 1   | Zd    | 403    | <div> <div>54%</div> <div>82%</div> <div>17%</div> </div> |
| 1   | Ze    | 403    | <div> <div>60%</div> <div>79%</div> <div>19%</div> </div> |
| 1   | Zf    | 403    | <div> <div>64%</div> <div>80%</div> <div>19%</div> </div> |
| 1   | Zg    | 403    | <div> <div>67%</div> <div>83%</div> <div>16%</div> </div> |
| 1   | Zh    | 403    | <div> <div>68%</div> <div>86%</div> <div>14%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | 0     | 260    |                  |
| 2   | 1     | 260    |                  |
| 2   | 2     | 260    |                  |
| 2   | 3     | 260    |                  |
| 2   | 4     | 260    |                  |
| 2   | 5     | 260    |                  |
| 2   | 6     | 260    |                  |
| 2   | 7     | 260    |                  |
| 2   | 8     | 260    |                  |
| 2   | 9     | 260    |                  |
| 2   | ZA    | 260    |                  |
| 2   | ZB    | 260    |                  |
| 2   | ZC    | 260    |                  |
| 2   | ZD    | 260    |                  |
| 2   | ZE    | 260    |                  |
| 2   | r     | 260    |                  |
| 2   | s     | 260    |                  |
| 2   | t     | 260    |                  |
| 2   | u     | 260    |                  |
| 2   | v     | 260    |                  |
| 2   | w     | 260    |                  |
| 2   | x     | 260    |                  |
| 2   | y     | 260    |                  |
| 2   | z     | 260    |                  |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 131528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar hook protein FlgE.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | ZF    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZG    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZH    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZI    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZJ    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZK    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZL    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZM    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZN    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZO    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZP    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZQ    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZR    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZS    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZT    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZU    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZV    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | ZW    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZX    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZY    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | ZZ    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Za    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Zb    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Zc    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Zd    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Ze    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Zf    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Zg    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |
| 1   | Zh    | 401      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2947  | 1814 | 507 | 618 | 8 |         |       |

- Molecule 2 is a protein called Flagellar basal-body rod protein FlgG.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 2     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |
| 2   | 3     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |
| 2   | 4     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |
| 2   | 5     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |
| 2   | 6     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |
| 2   | 7     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |
| 2   | 8     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |

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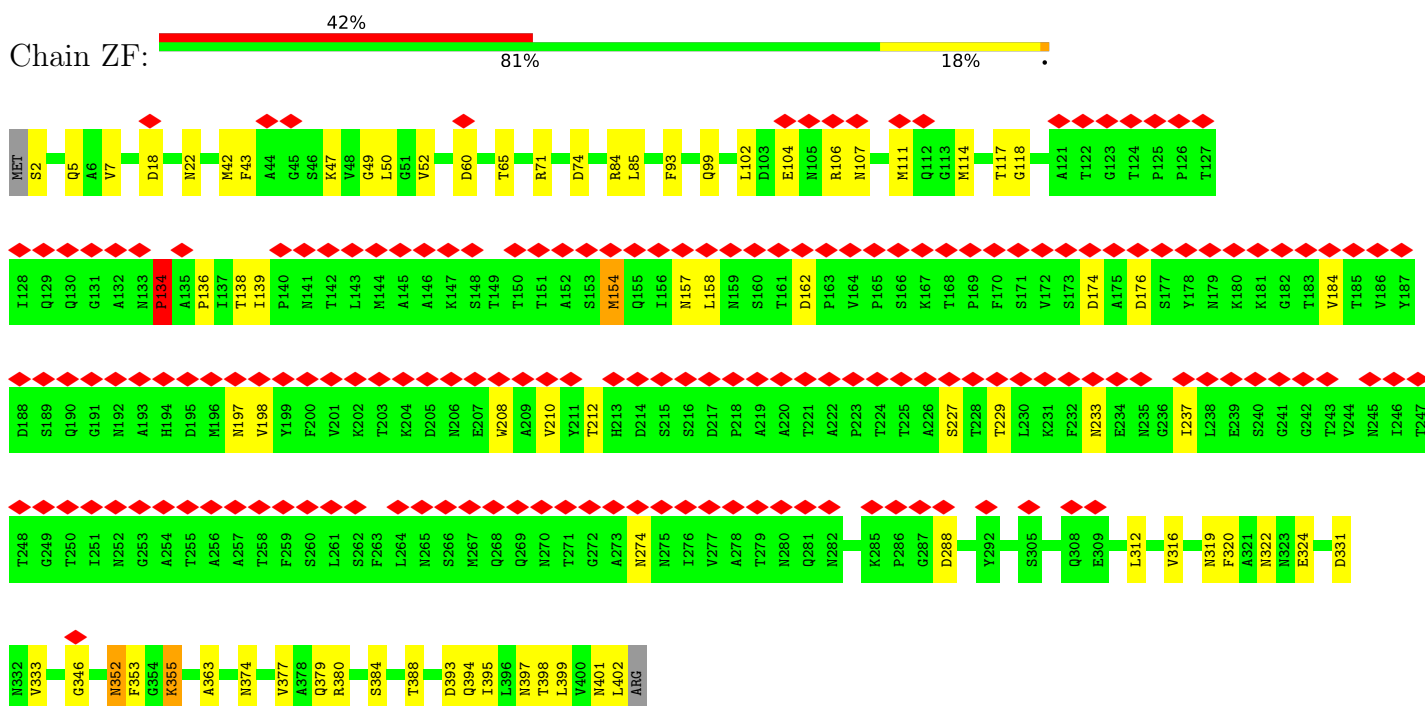
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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2   | 9     | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 2   | ZA    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 2   | ZB    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 2   | ZC    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 2   | ZD    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 2   | ZE    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 2   | 0     | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |
| 2   | 1     | 252      | Total<br>1894 | C<br>1172 | N<br>331 | O<br>385 | S<br>6 | 0       | 0     |
| 2   | r     | 254      | Total<br>1903 | C<br>1175 | N<br>334 | O<br>389 | S<br>5 | 0       | 0     |
| 2   | s     | 255      | Total<br>1911 | C<br>1181 | N<br>335 | O<br>390 | S<br>5 | 0       | 0     |
| 2   | t     | 256      | Total<br>1919 | C<br>1186 | N<br>336 | O<br>391 | S<br>6 | 0       | 0     |
| 2   | u     | 254      | Total<br>1903 | C<br>1175 | N<br>334 | O<br>389 | S<br>5 | 0       | 0     |
| 2   | v     | 255      | Total<br>1911 | C<br>1181 | N<br>335 | O<br>390 | S<br>5 | 0       | 0     |
| 2   | w     | 243      | Total<br>1823 | C<br>1127 | N<br>318 | O<br>373 | S<br>5 | 0       | 0     |
| 2   | x     | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |
| 2   | y     | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |
| 2   | z     | 248      | Total<br>1866 | C<br>1154 | N<br>327 | O<br>379 | S<br>6 | 0       | 0     |

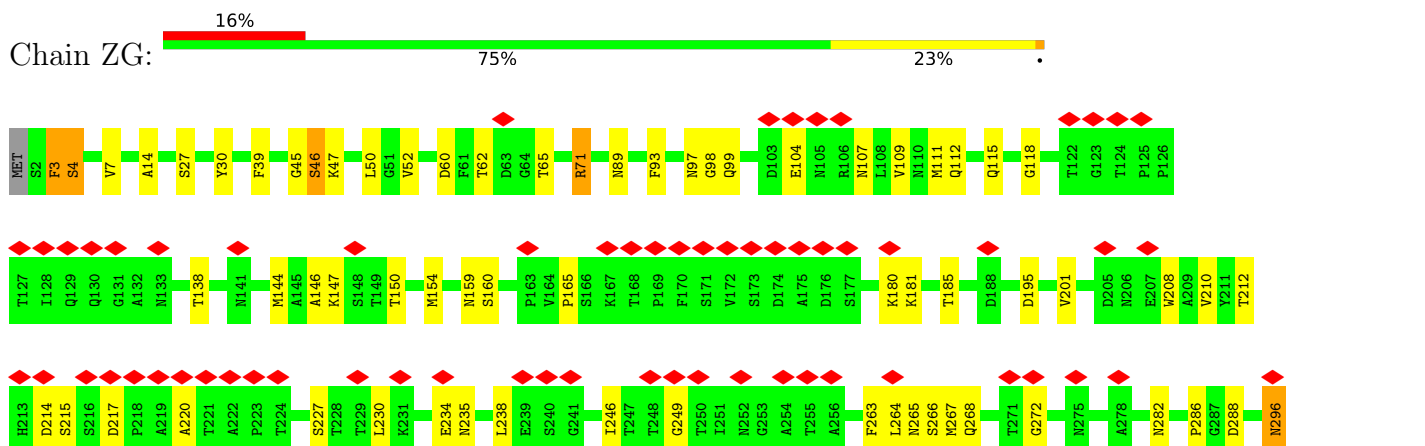
### 3 Residue-property plots

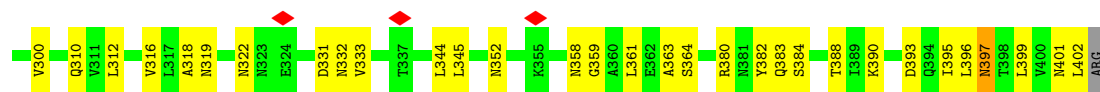
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Flagellar hook protein FlgE

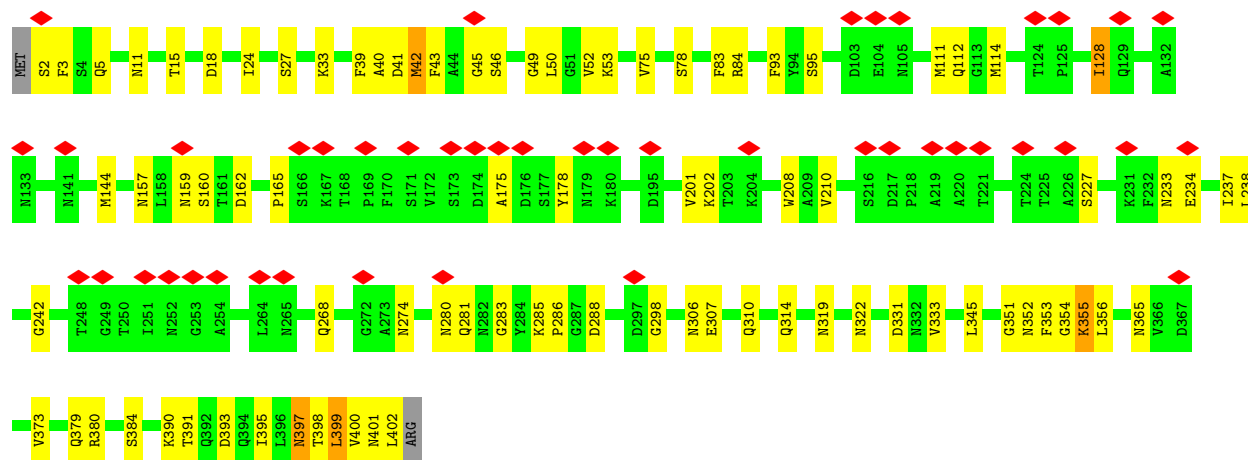
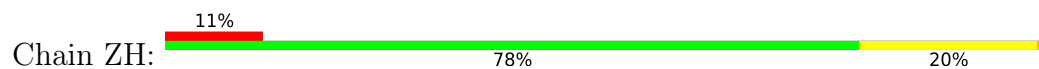


#### • Molecule 1: Flagellar hook protein FlgE

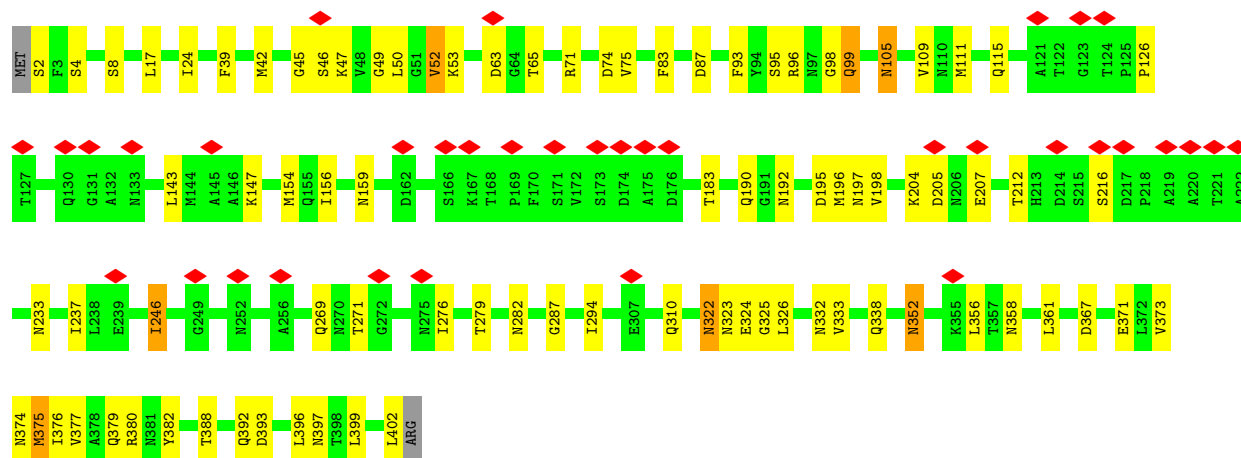
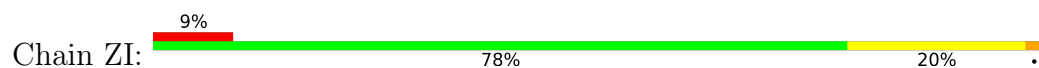




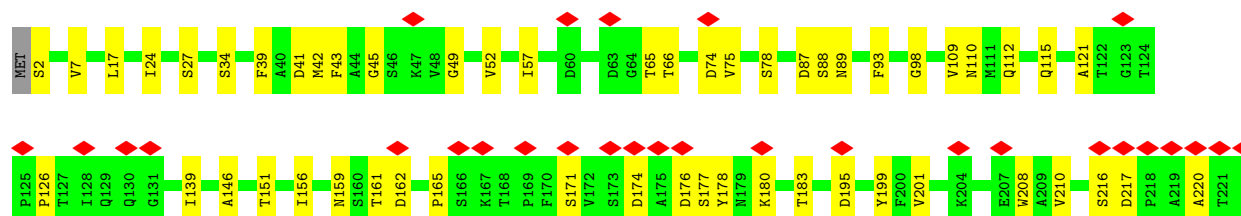
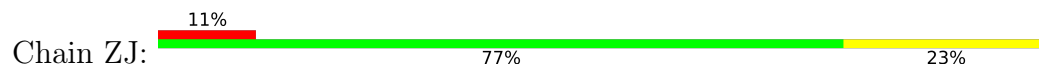
• Molecule 1: Flagellar hook protein FlgE

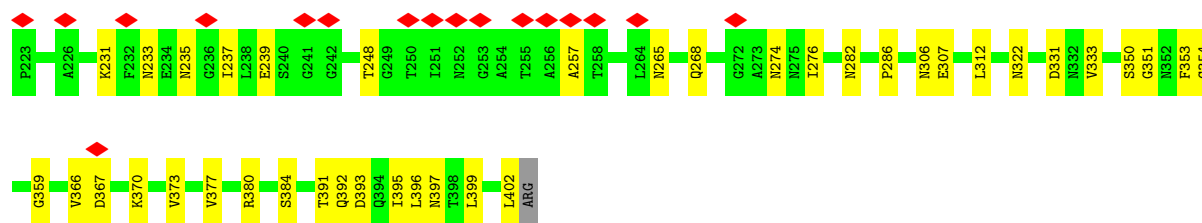


• Molecule 1: Flagellar hook protein FlgE

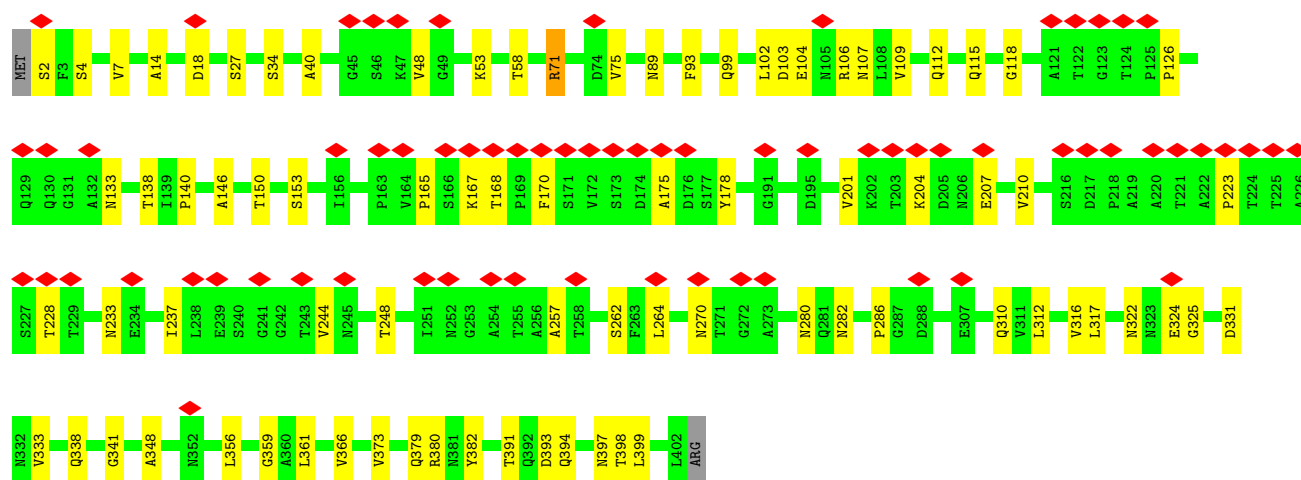
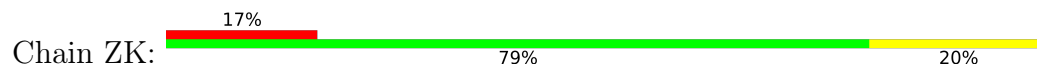


• Molecule 1: Flagellar hook protein FlgE

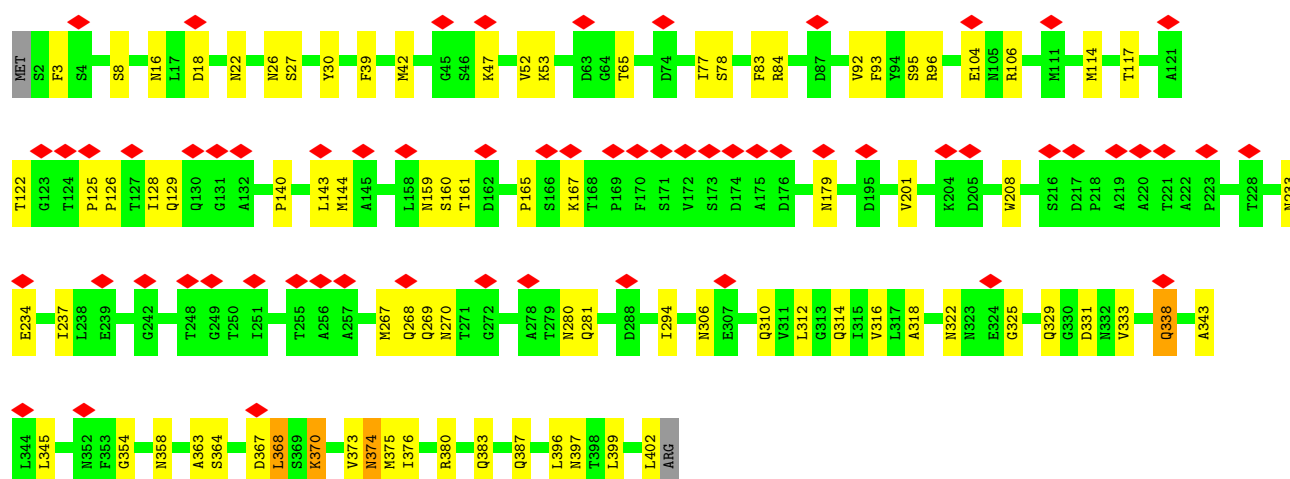
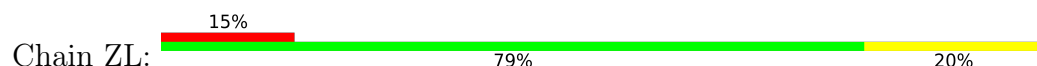




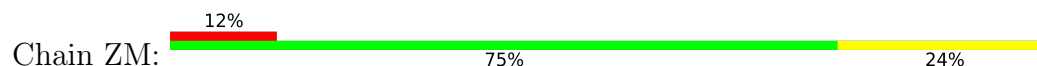
• Molecule 1: Flagellar hook protein FlgE

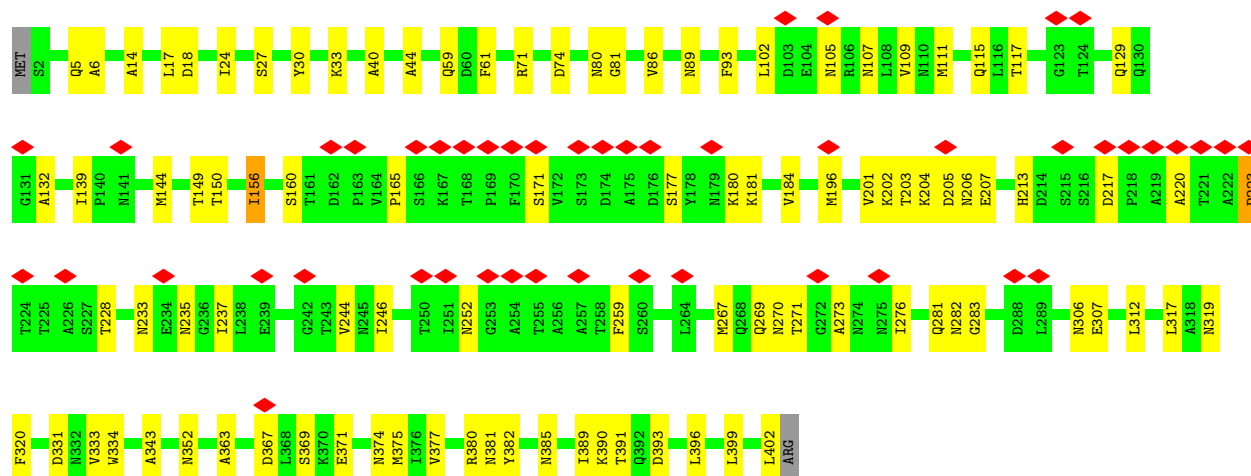


• Molecule 1: Flagellar hook protein FlgE

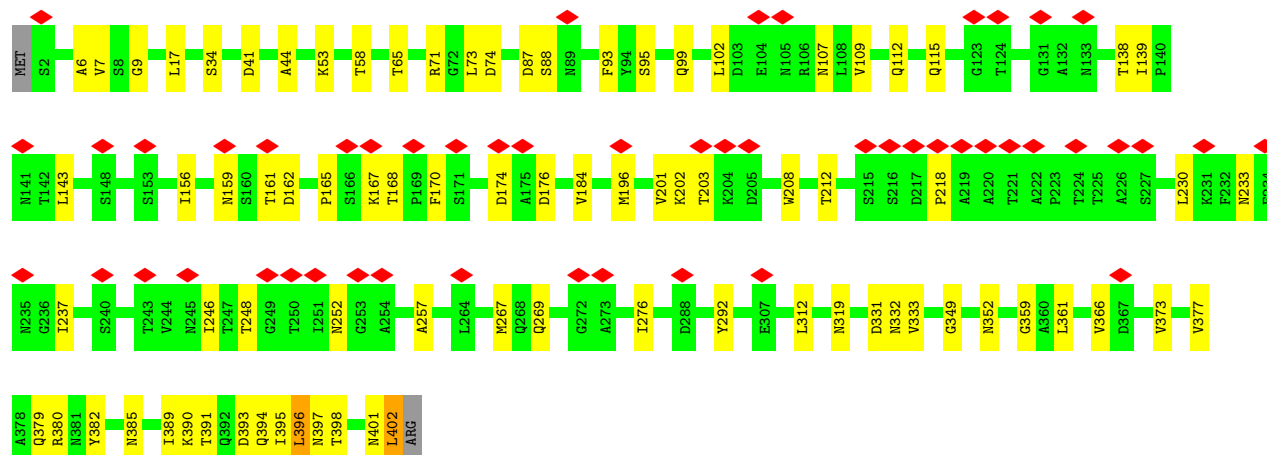
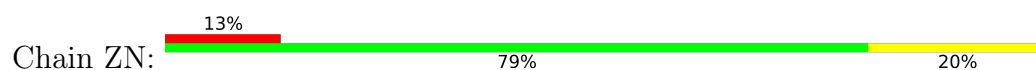


• Molecule 1: Flagellar hook protein FlgE

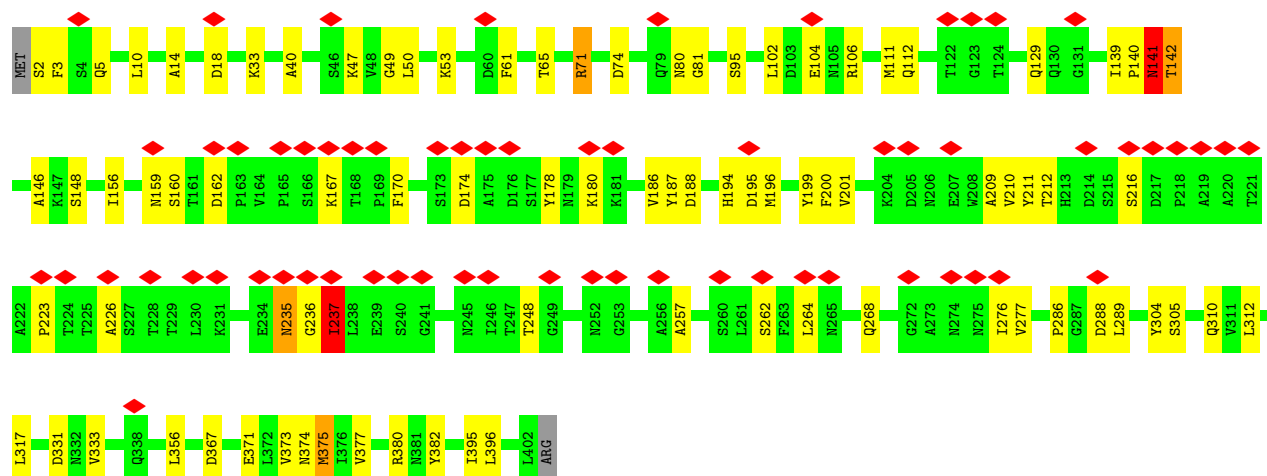
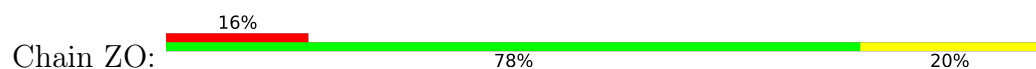




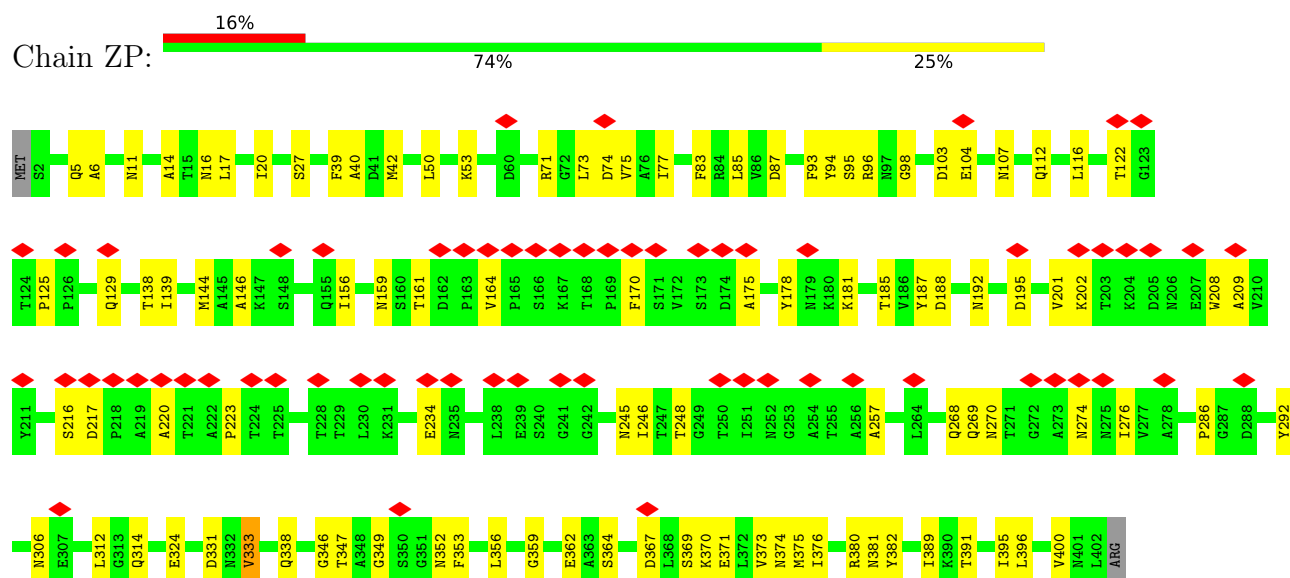
• Molecule 1: Flagellar hook protein FlgE



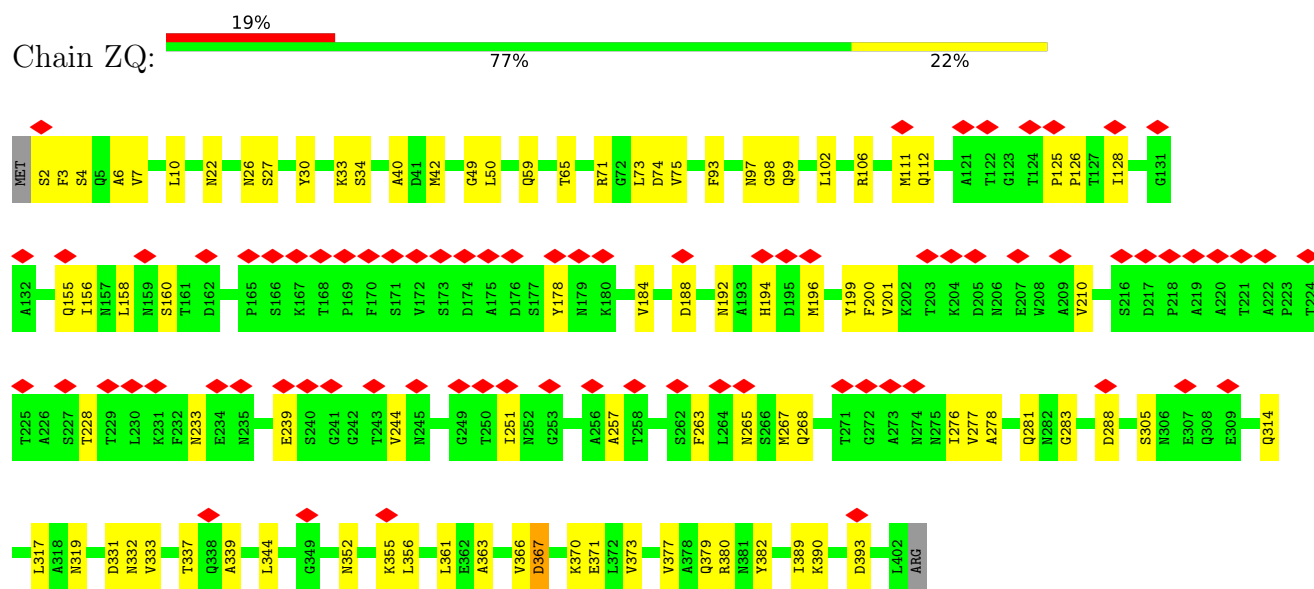
• Molecule 1: Flagellar hook protein FlgE



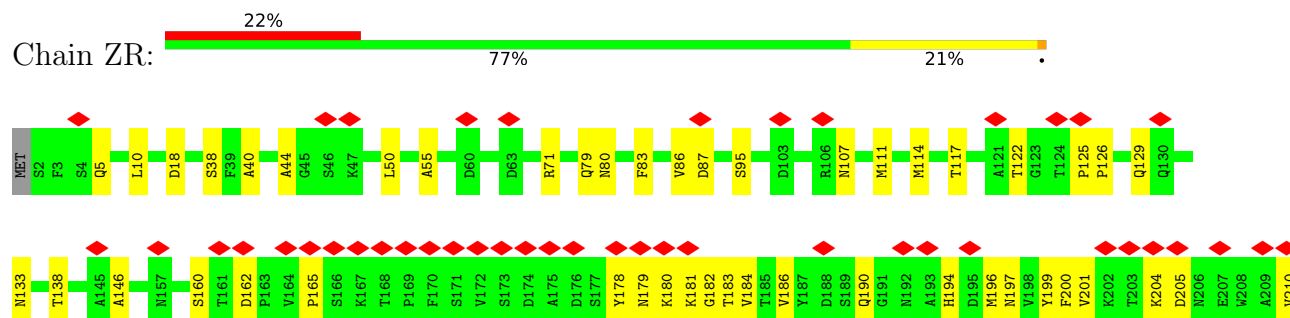
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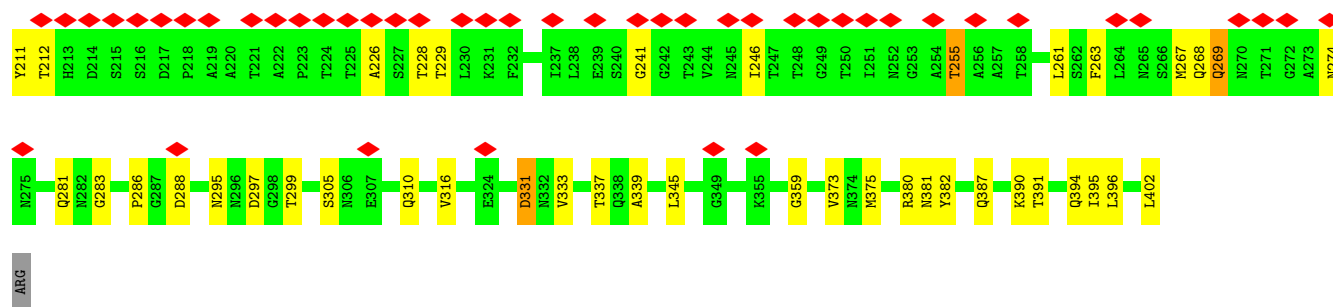


- Molecule 1: Flagellar hook protein FlgE

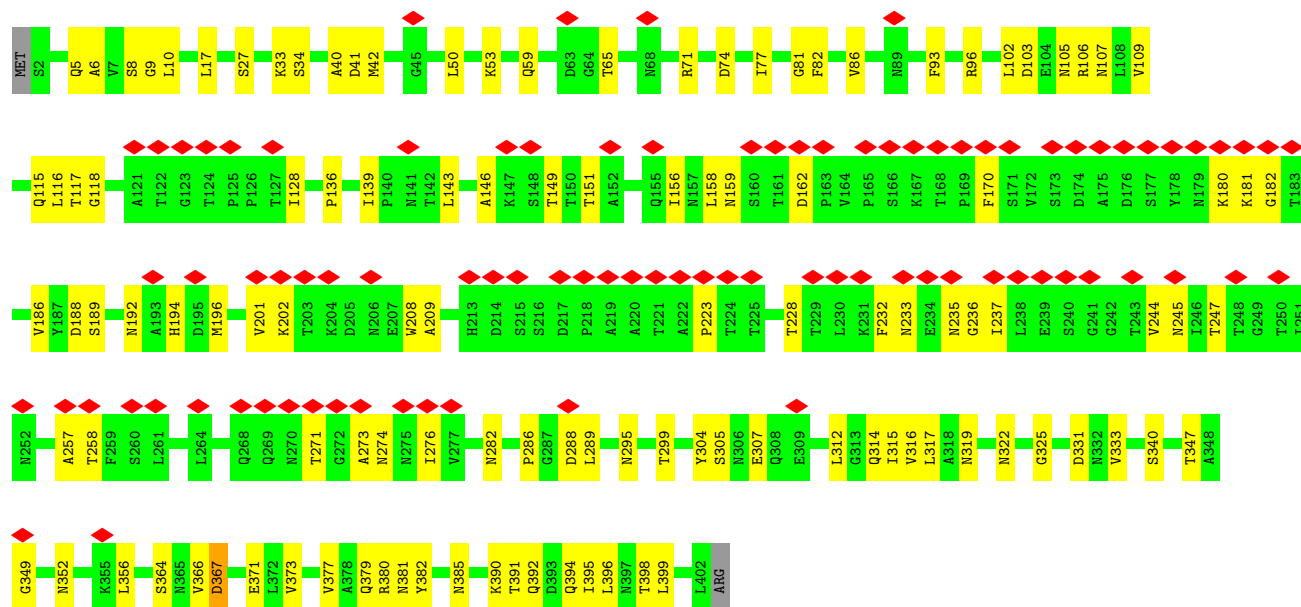
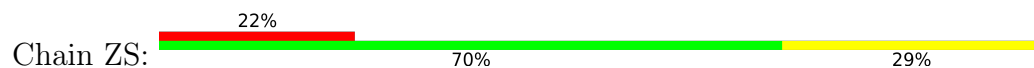


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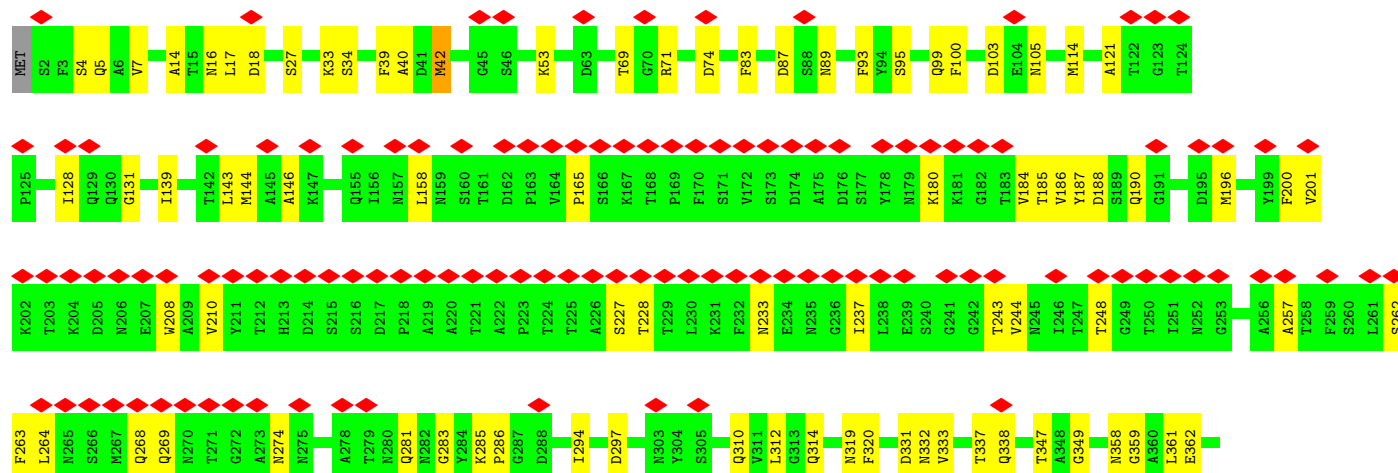
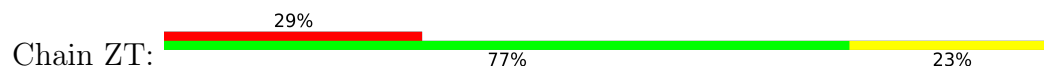




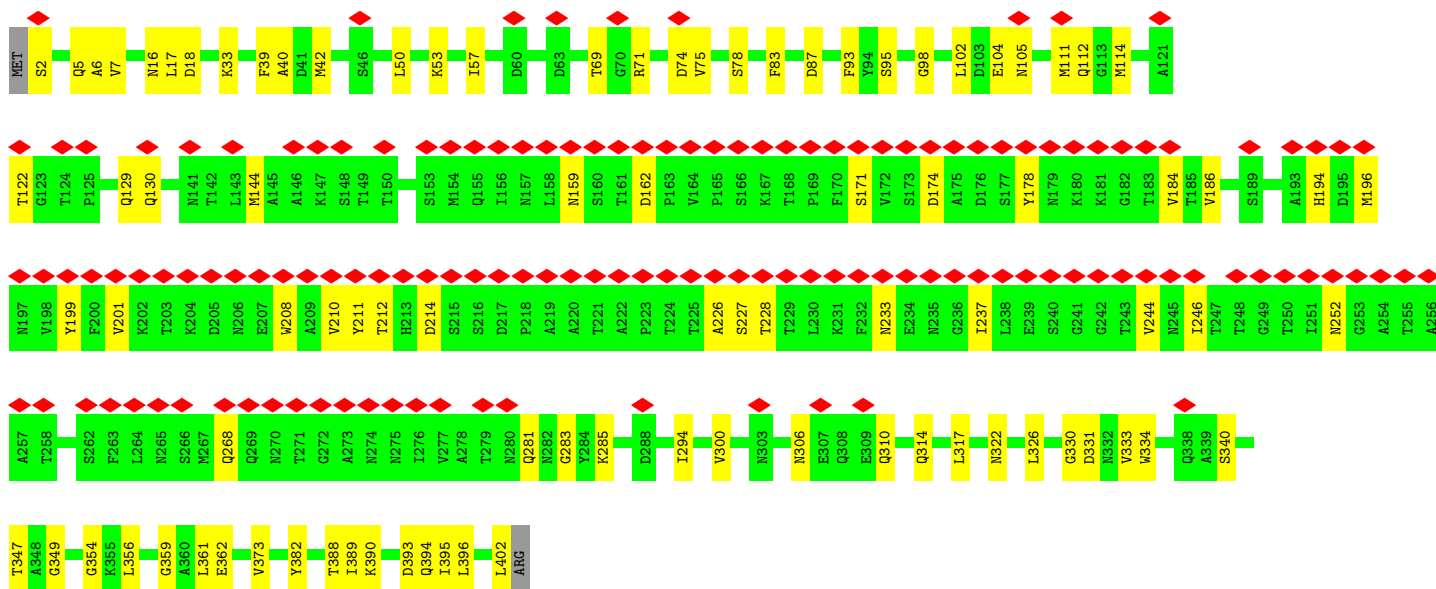
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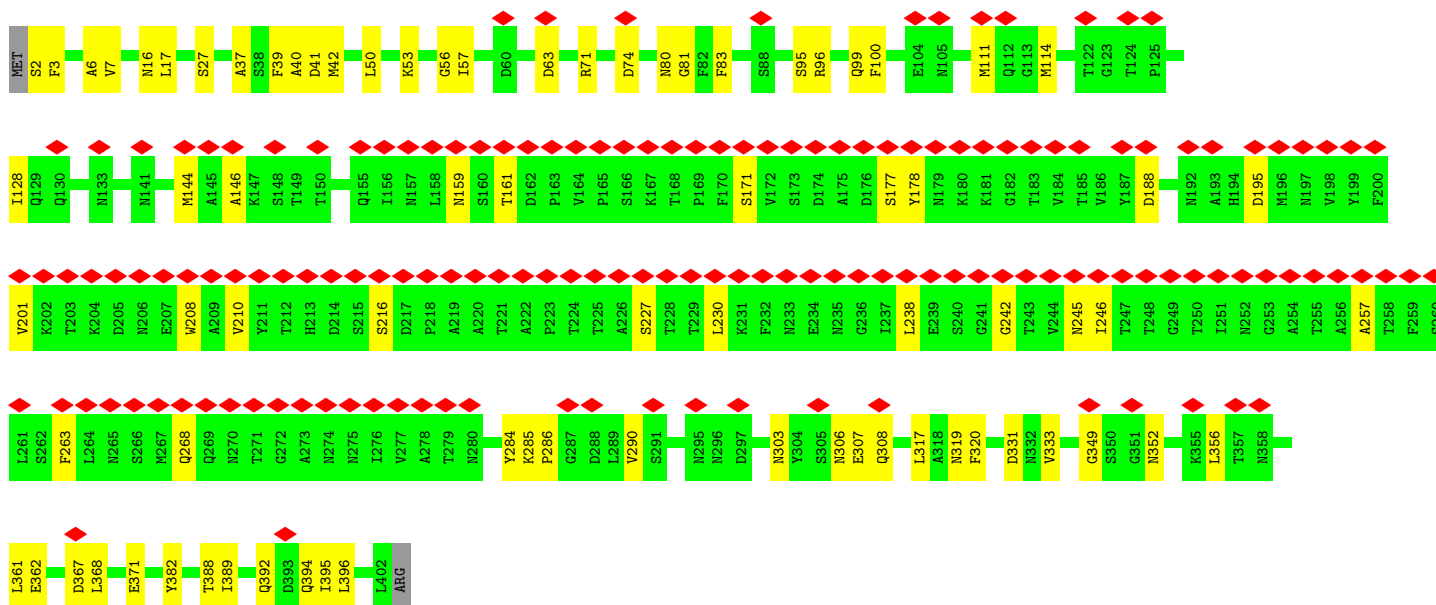
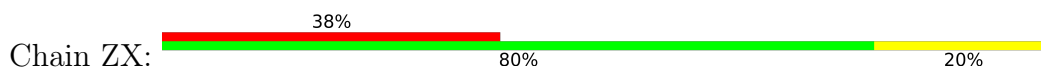
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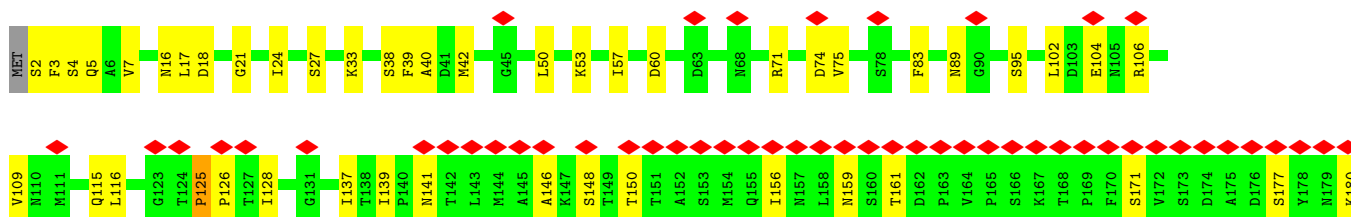
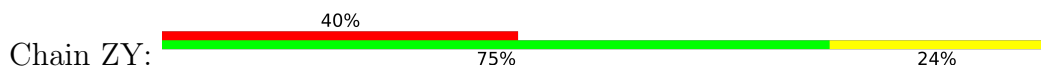


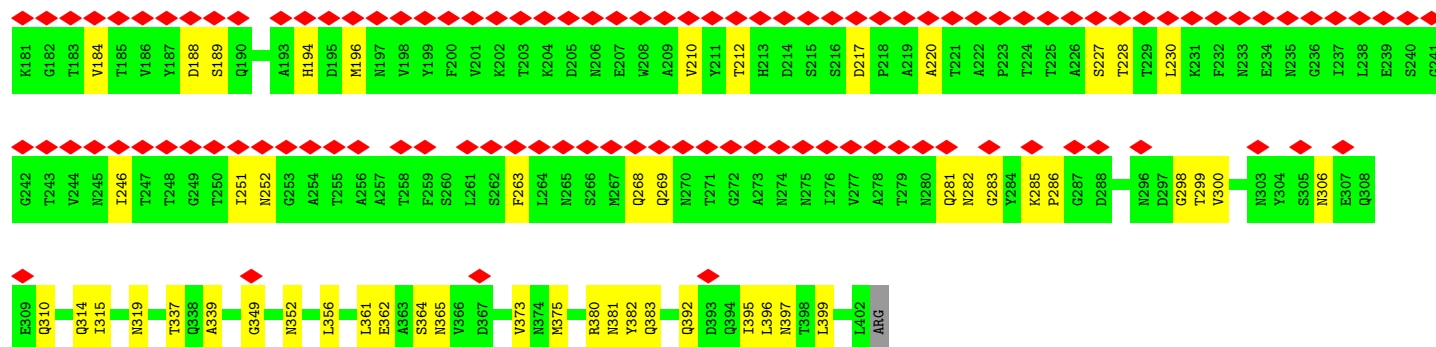


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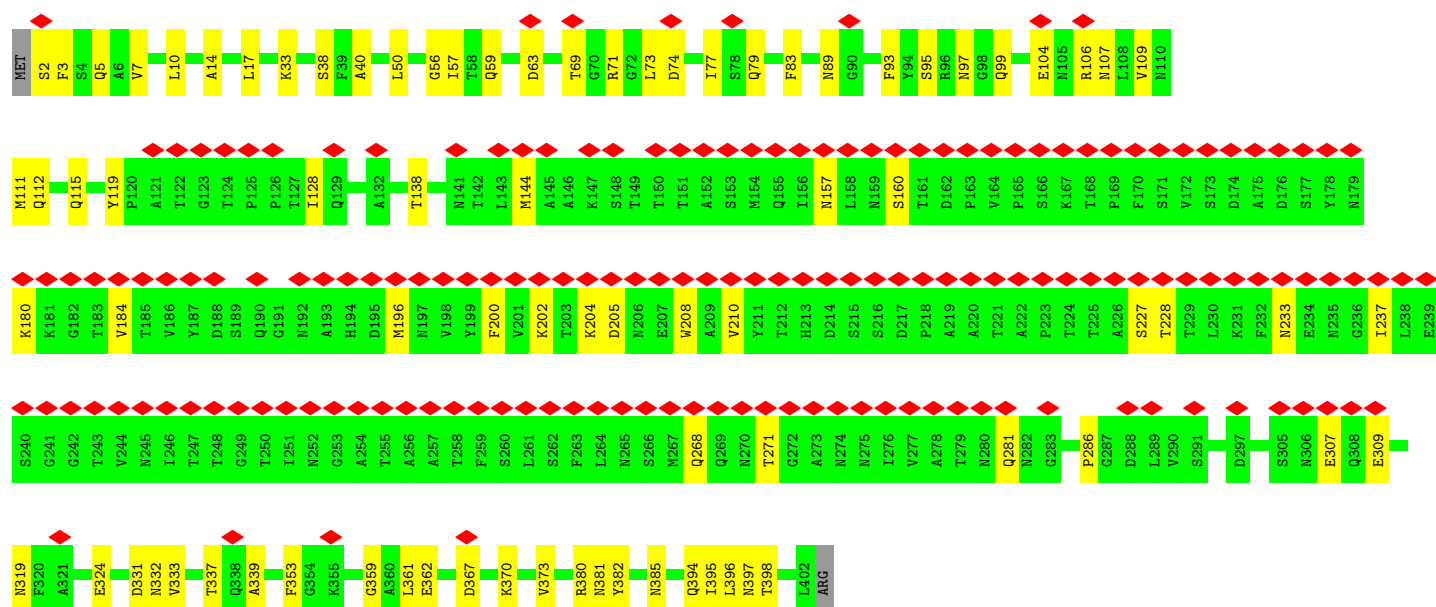
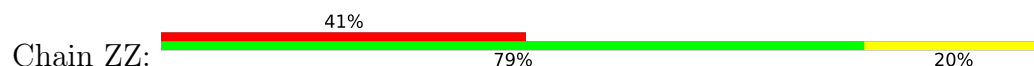


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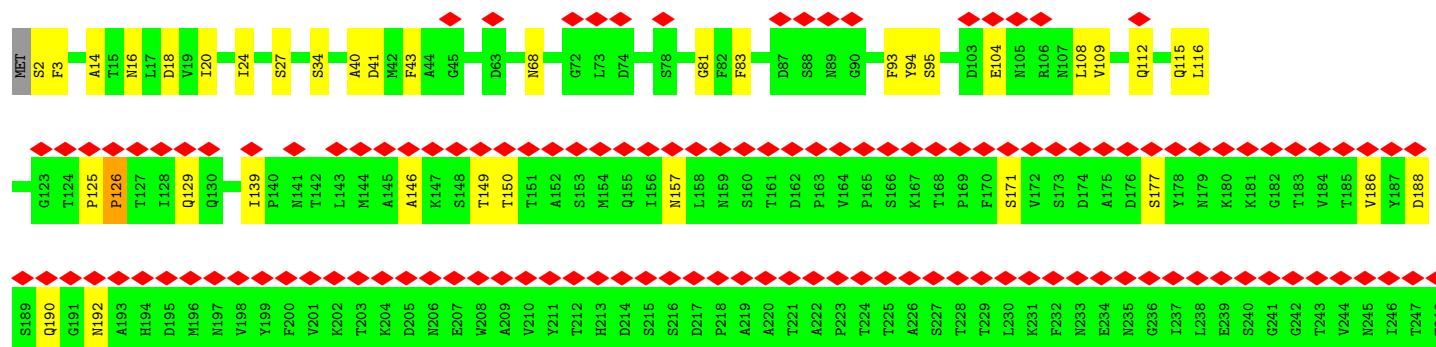
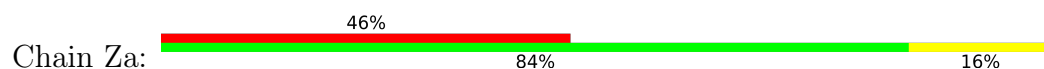


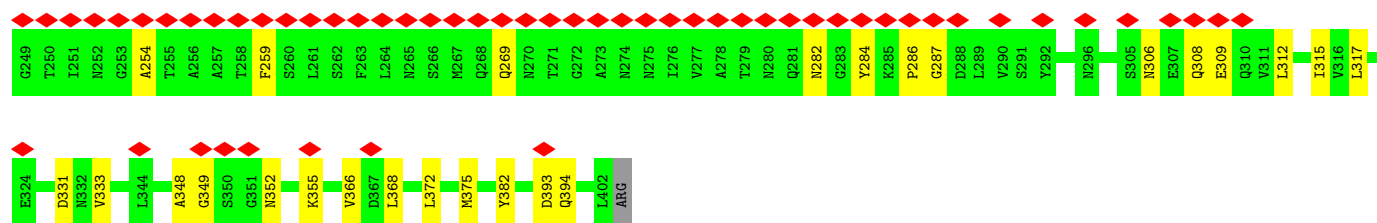


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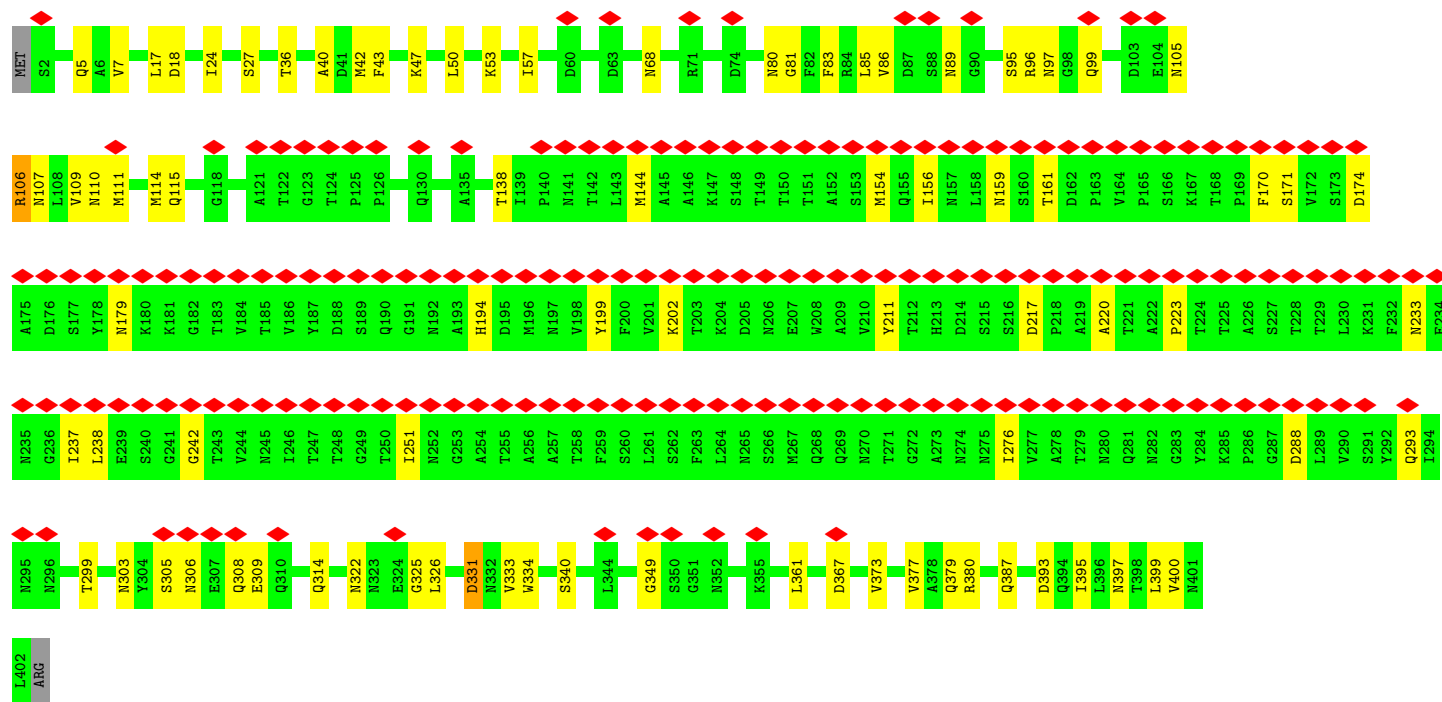
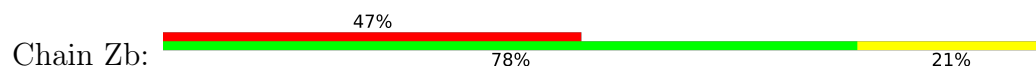


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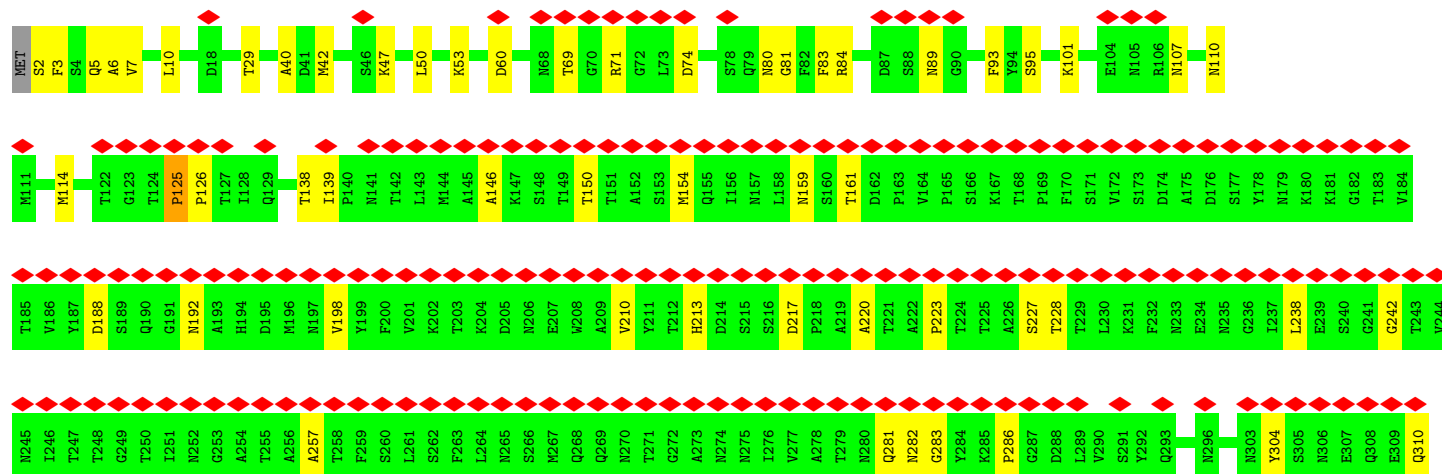
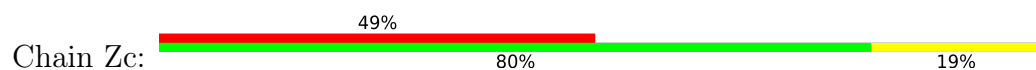


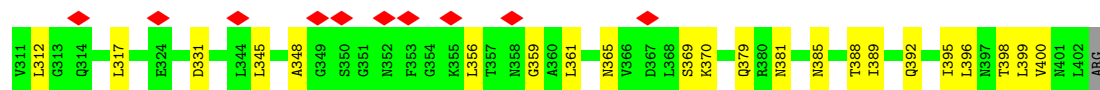


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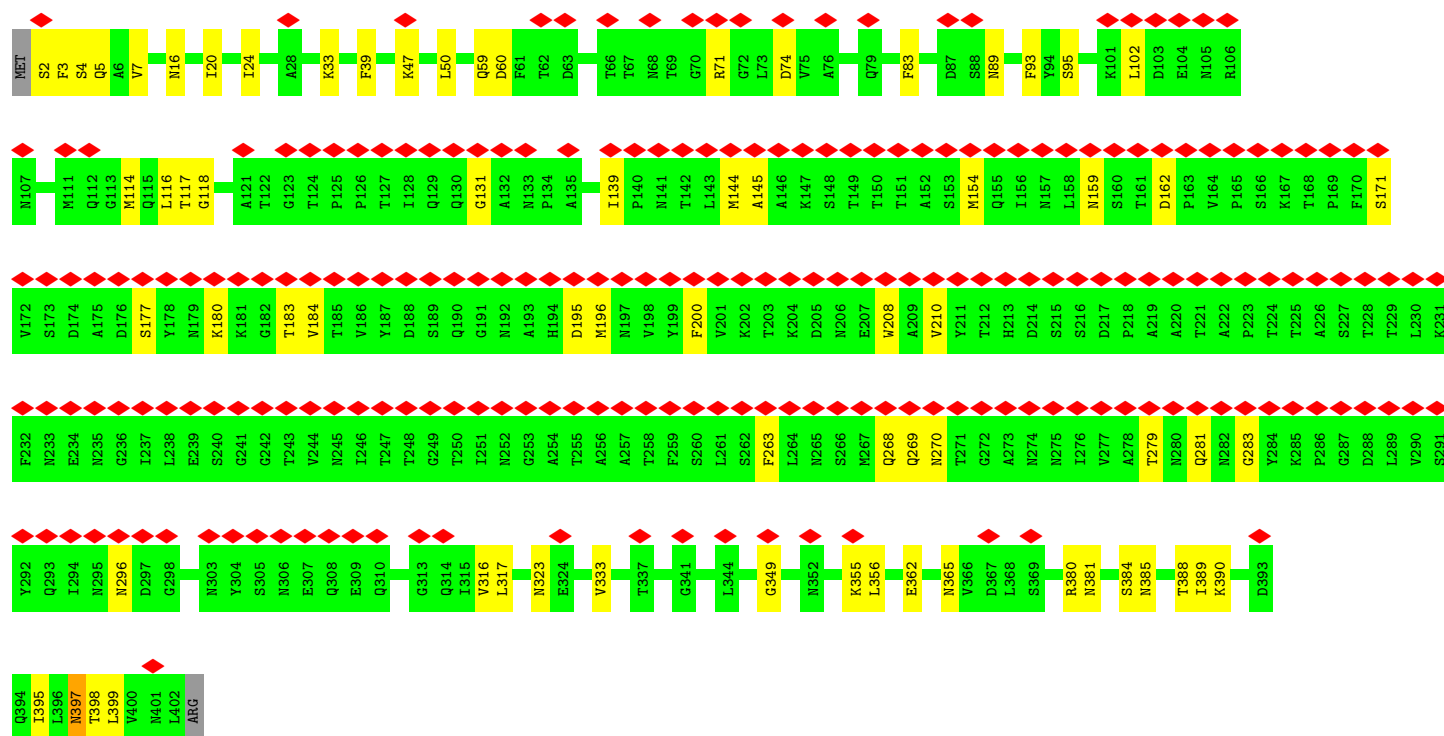
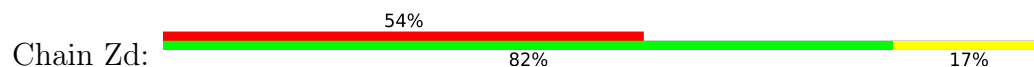


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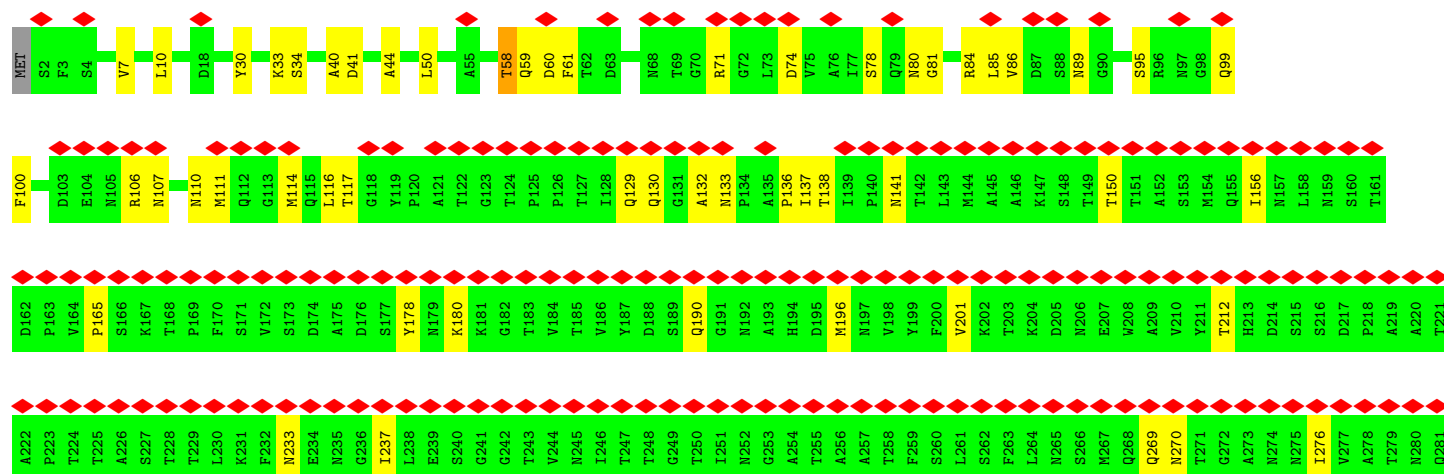
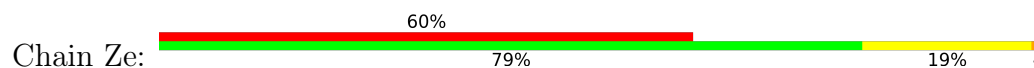


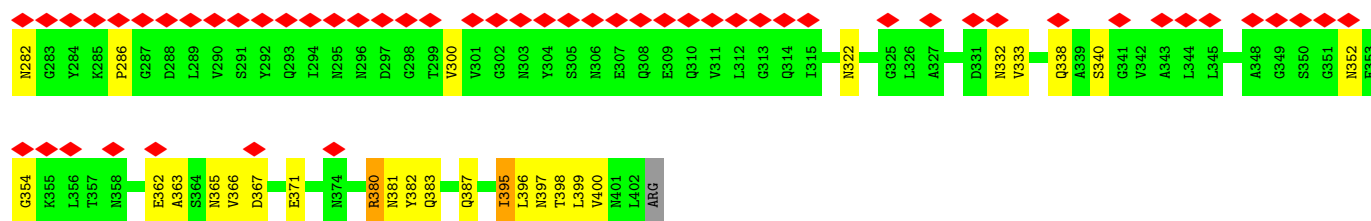


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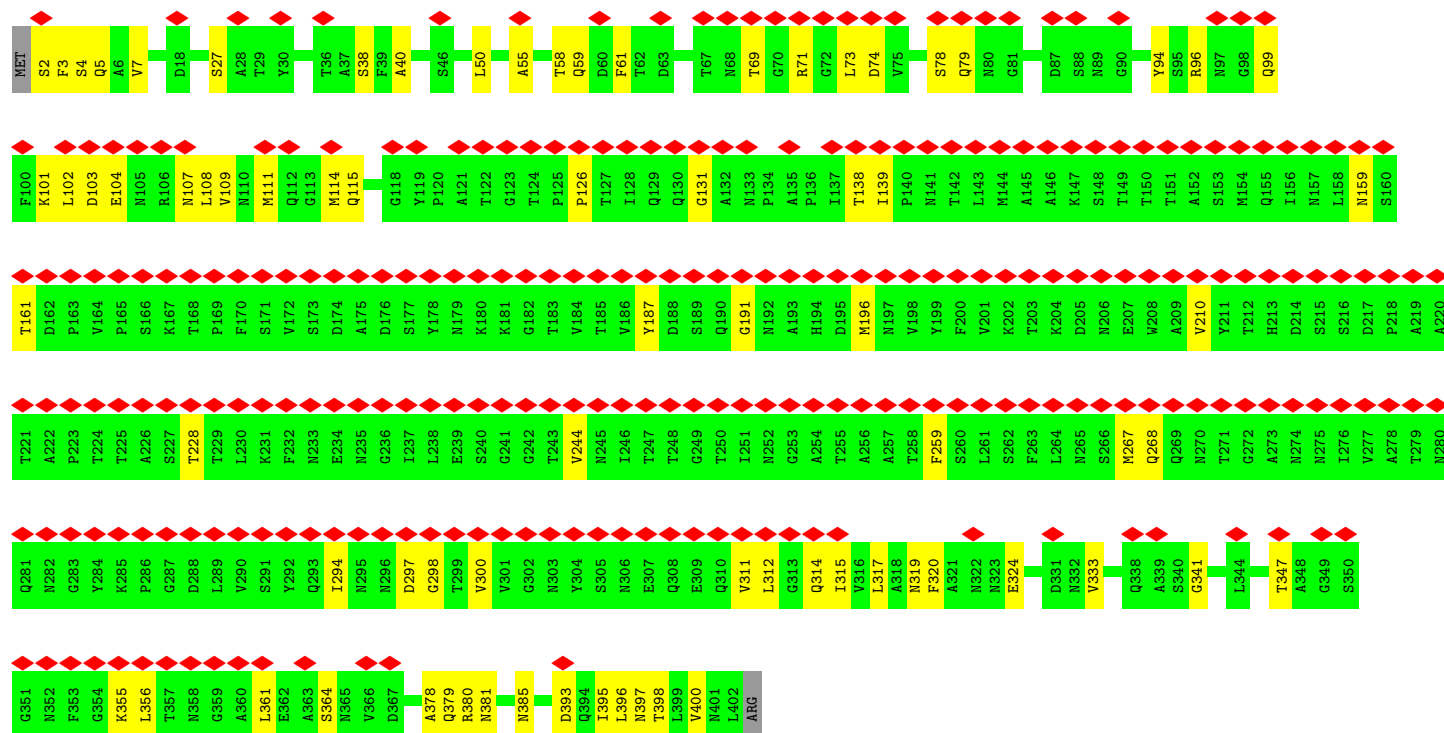
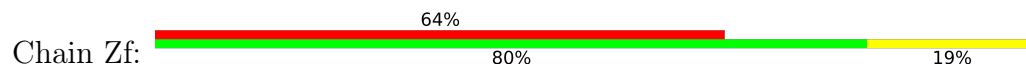


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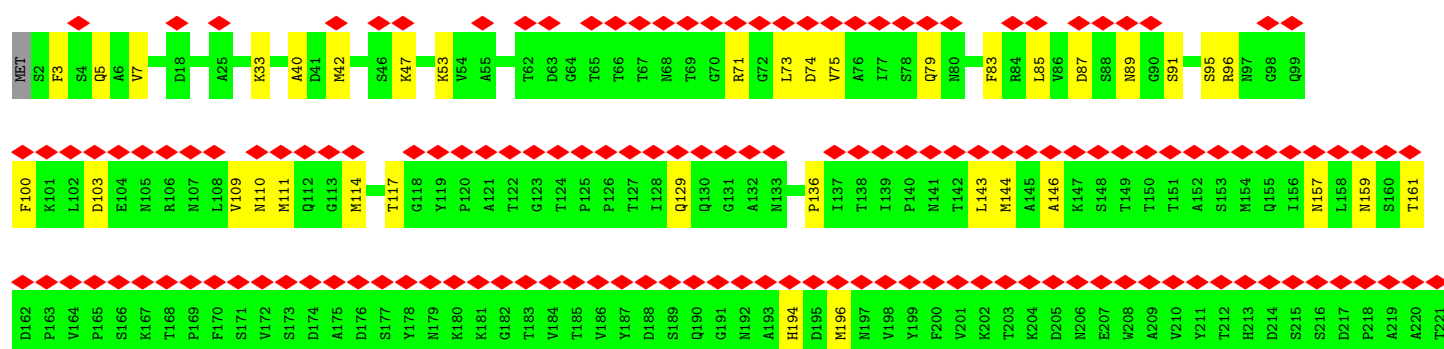
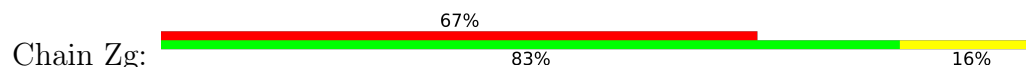


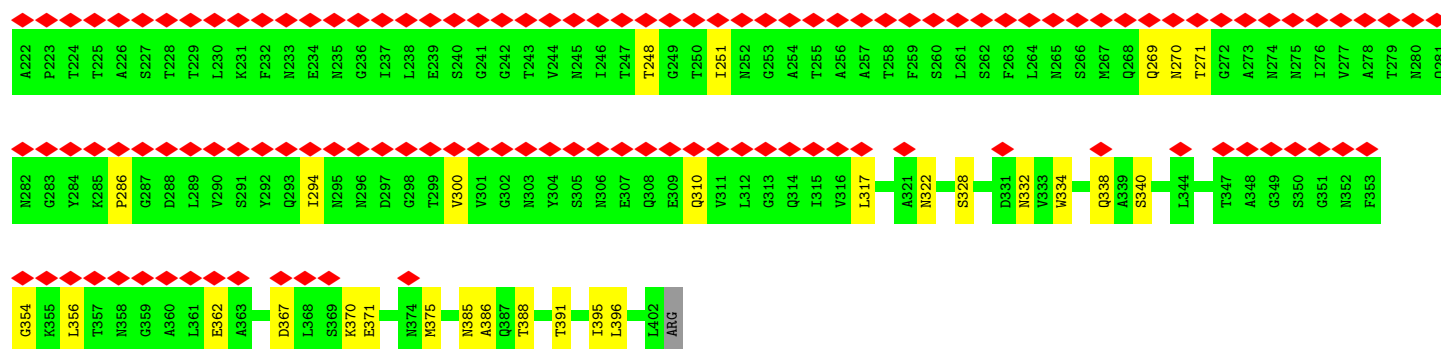


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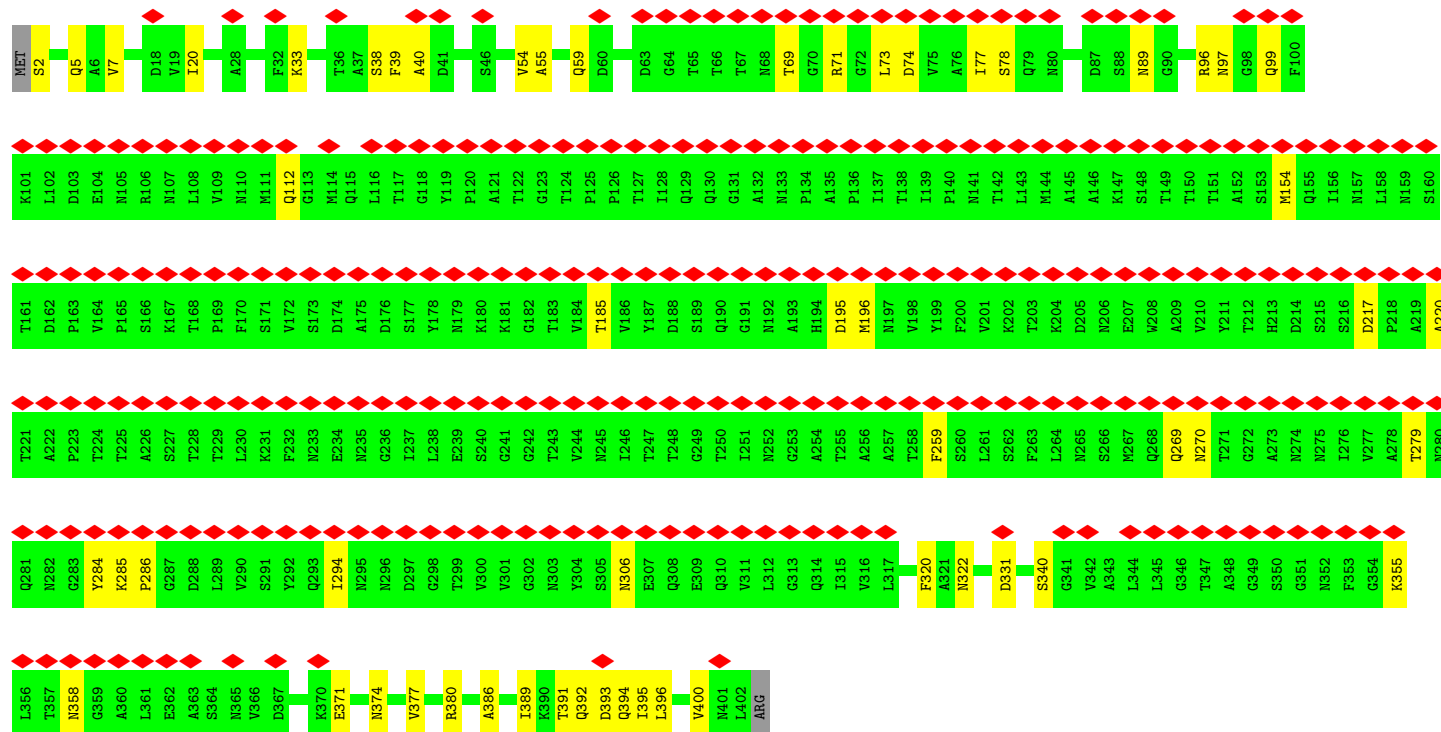
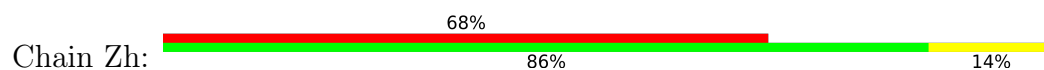


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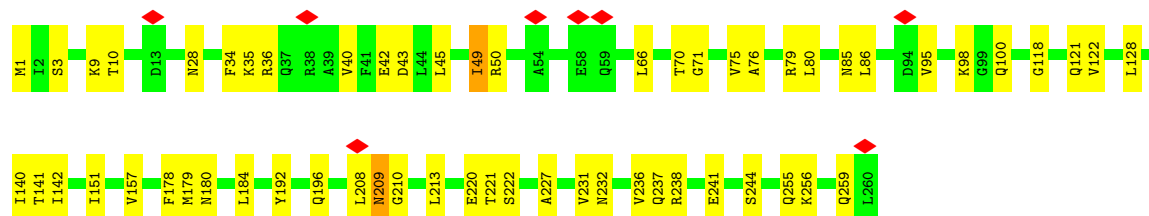
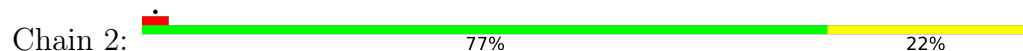




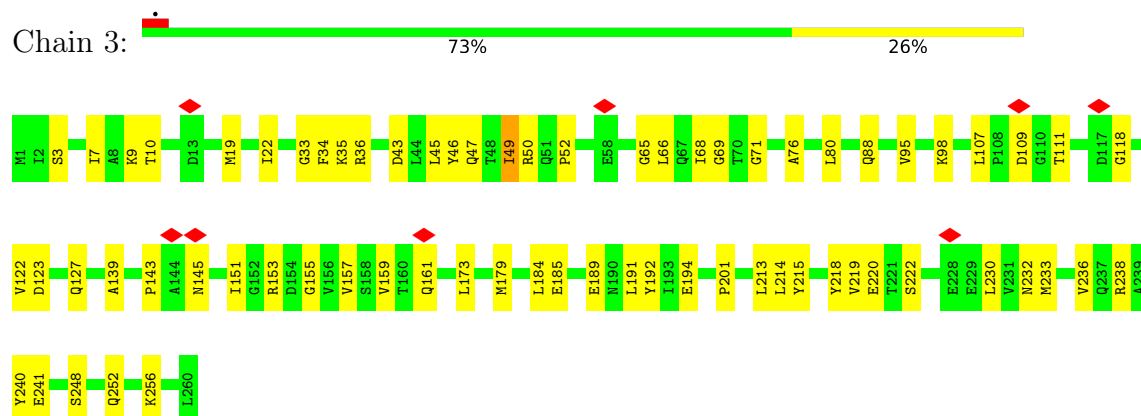
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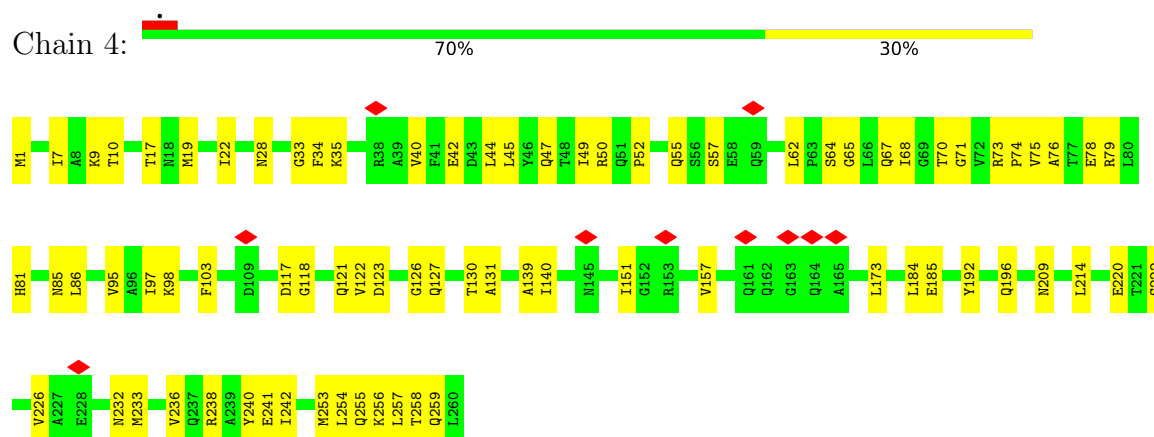
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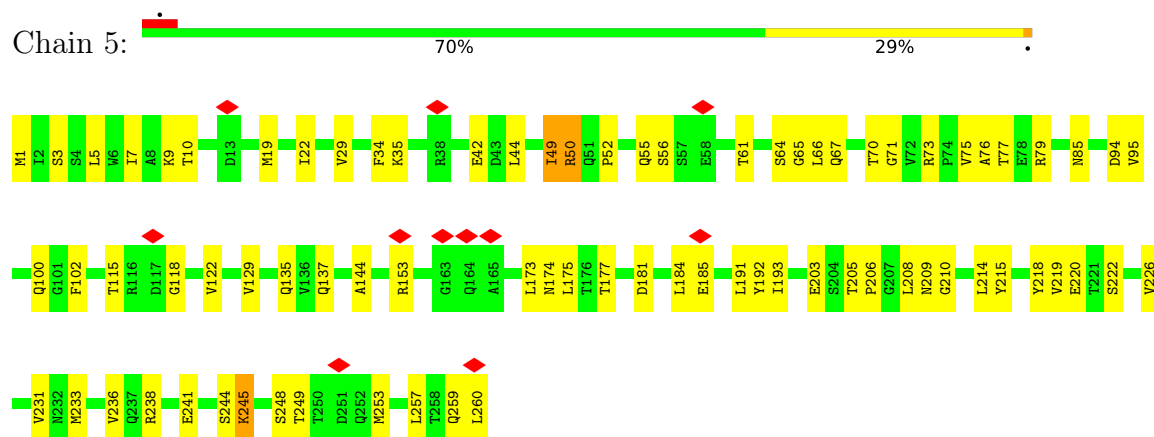
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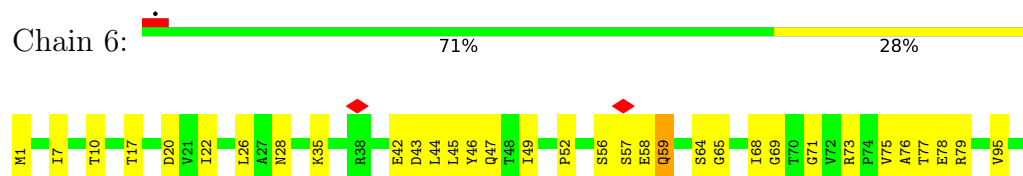
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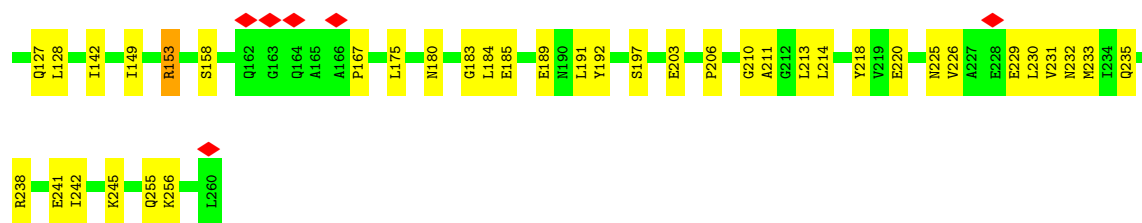


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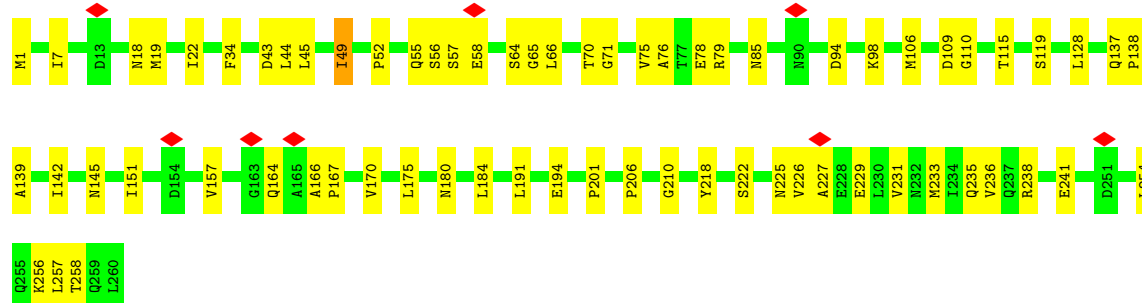
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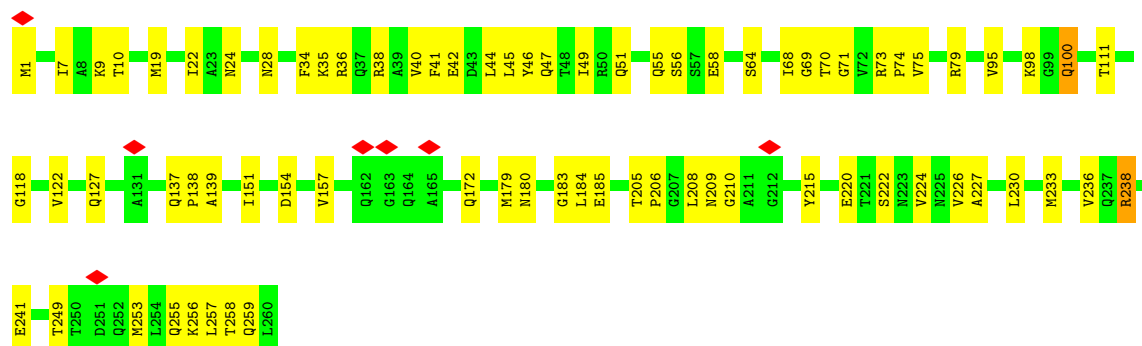
• Molecule 2: Flagellar basal-body rod protein FlgG

Chain 7: 74% 26%



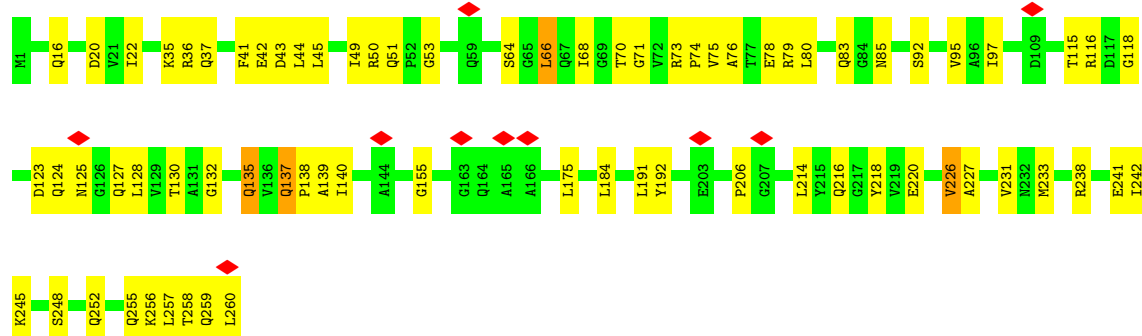
• Molecule 2: Flagellar basal-body rod protein FlgG

Chain 8: 71% 28%

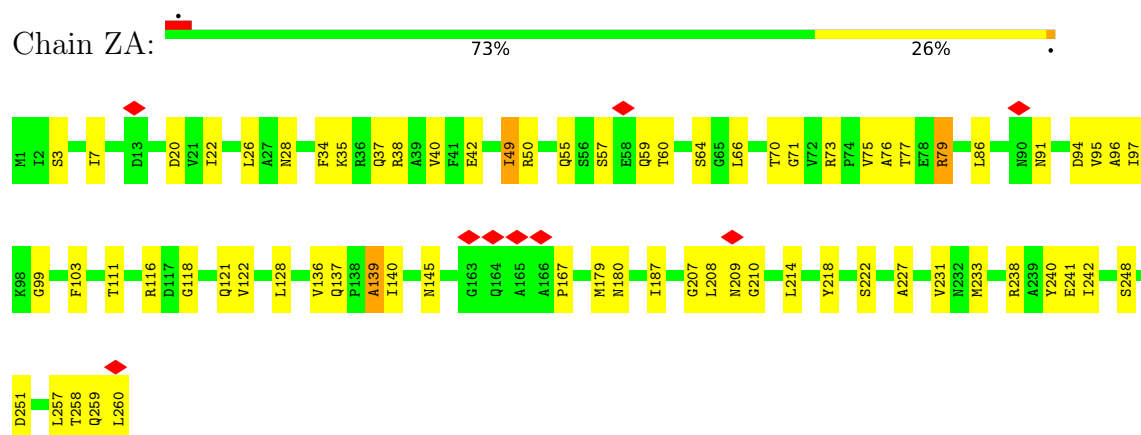


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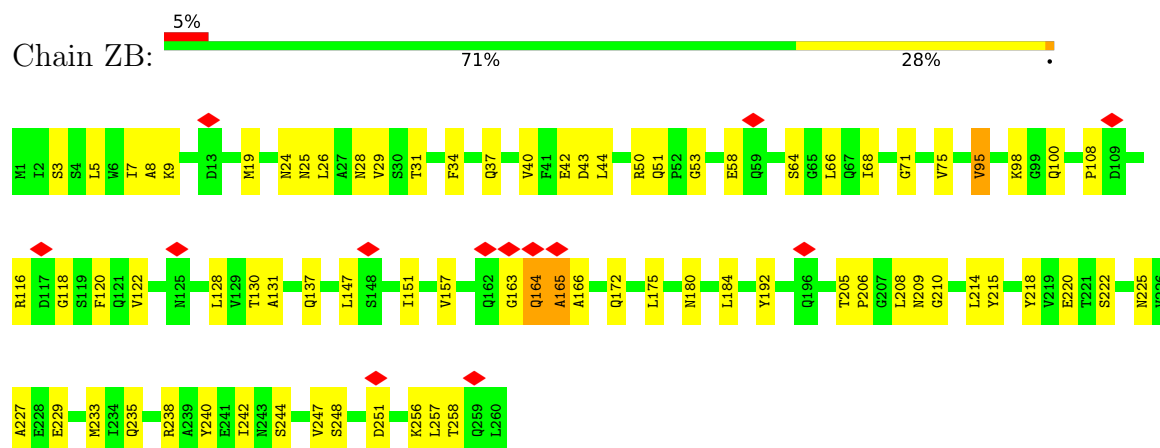
Chain 9: 72% 27%



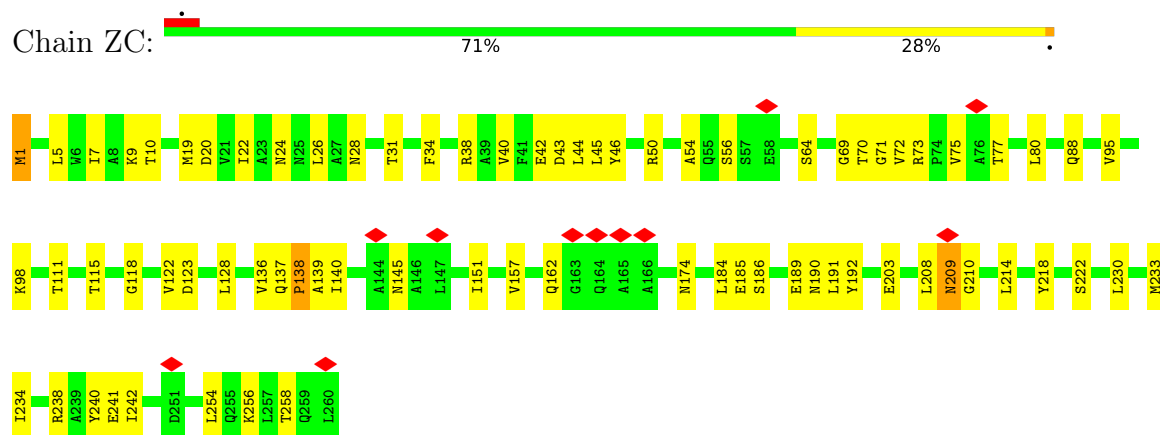
- Molecule 2: Flagellar basal-body rod protein FlgG



- Molecule 2: Flagellar basal-body rod protein FlgG

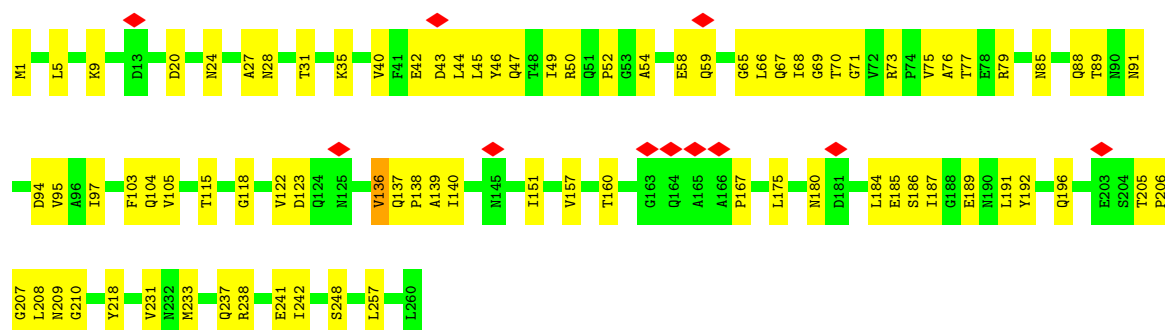


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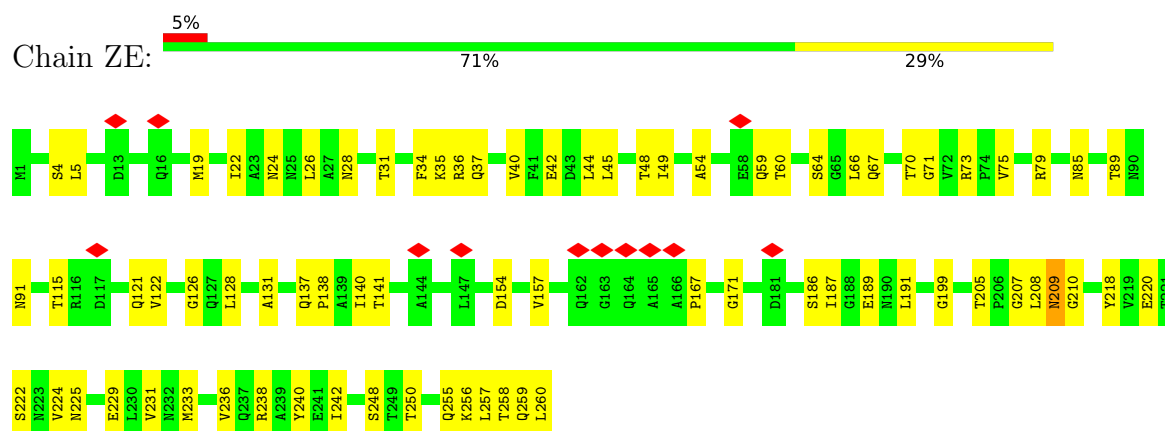


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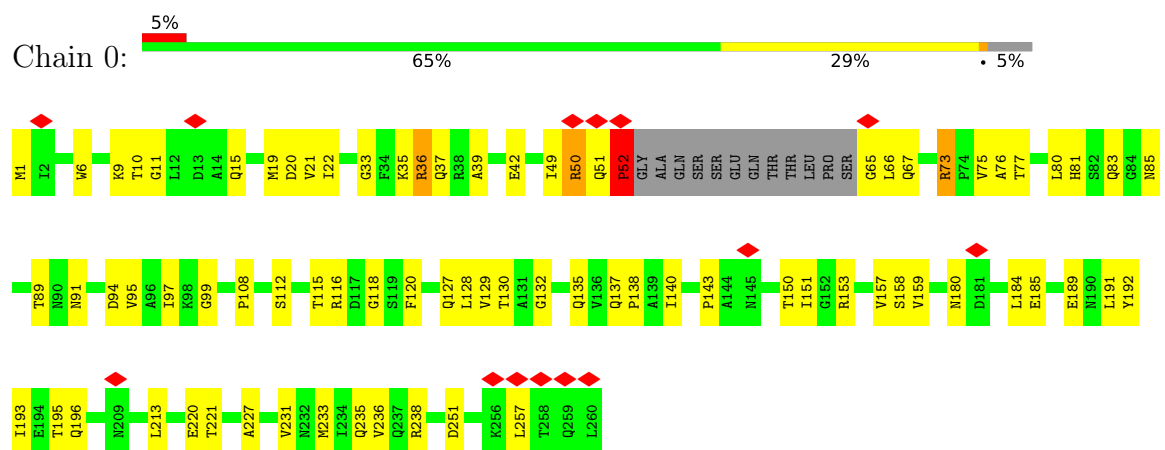




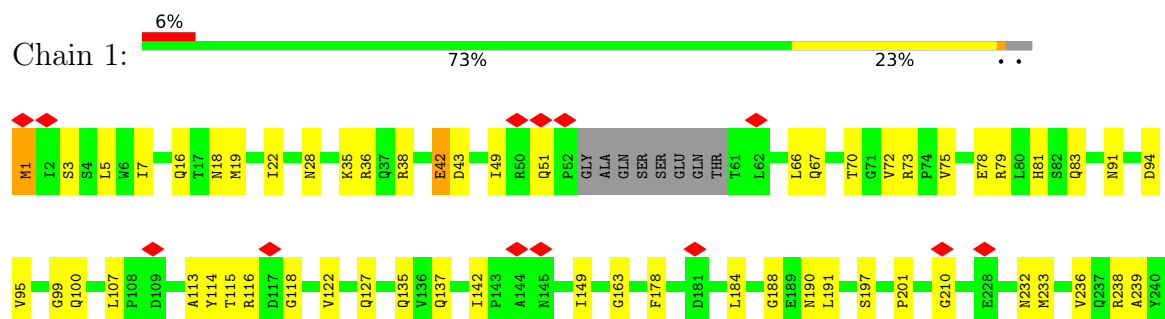
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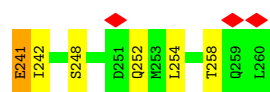


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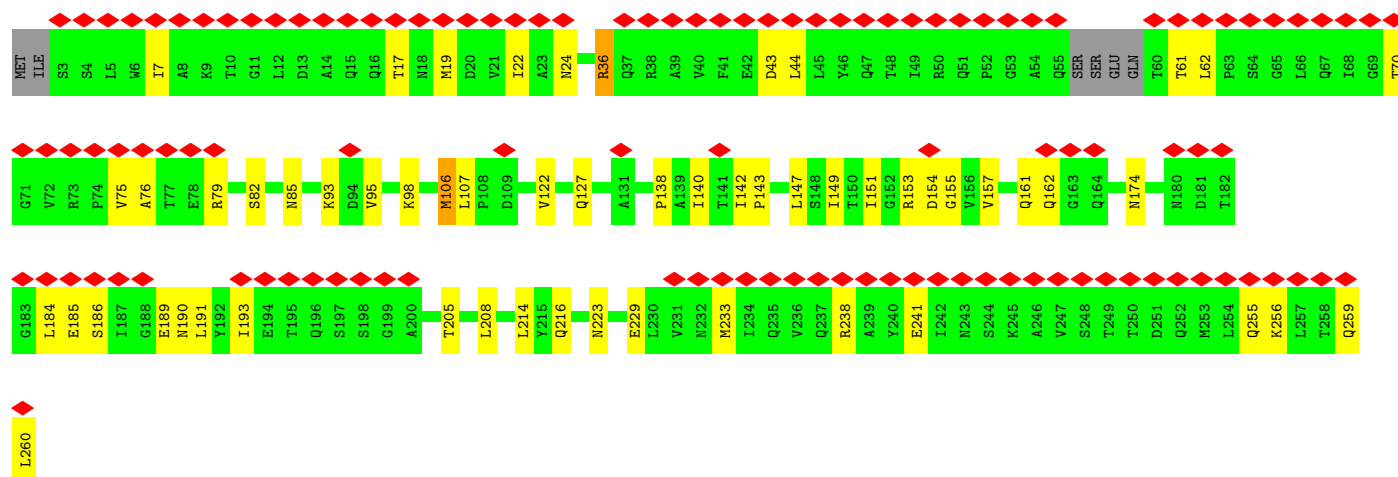
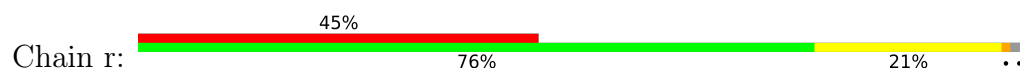


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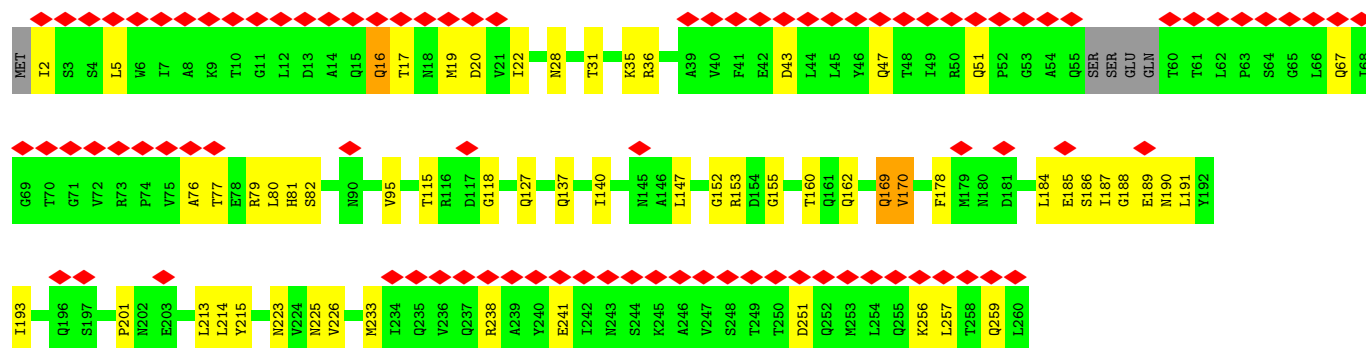
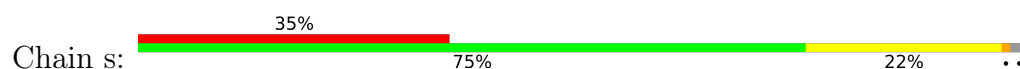




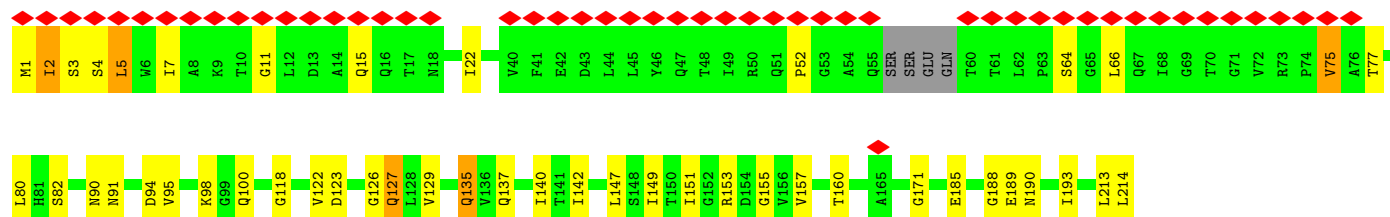
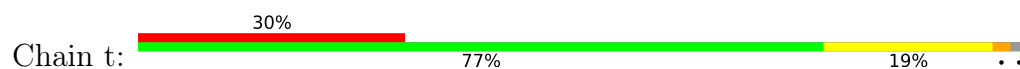
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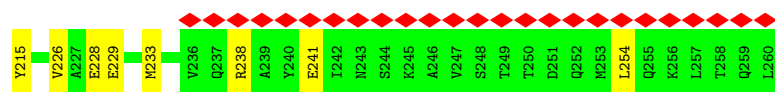


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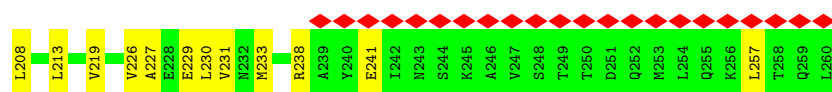
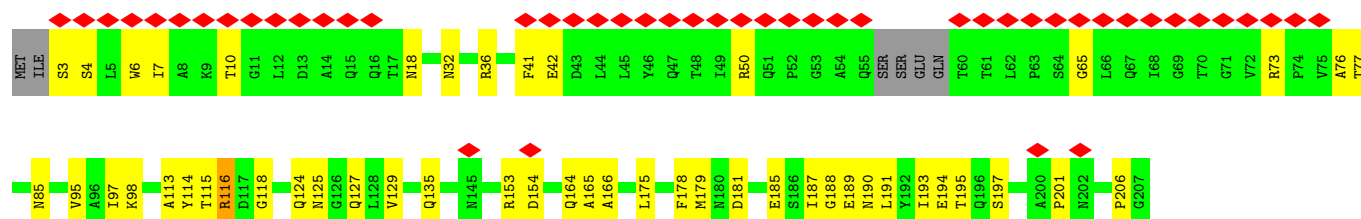
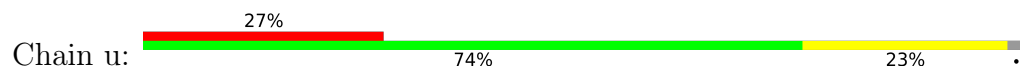


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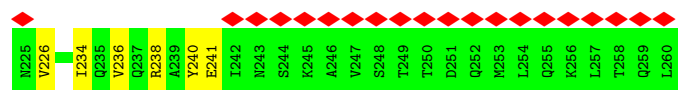
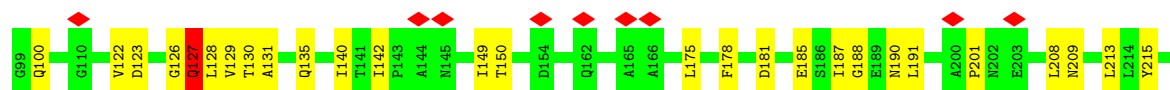
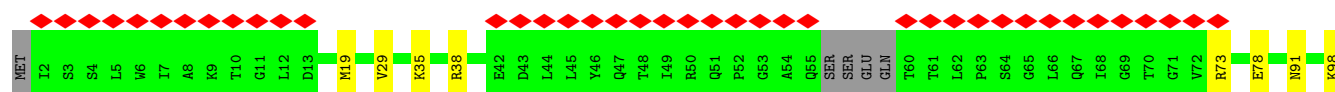
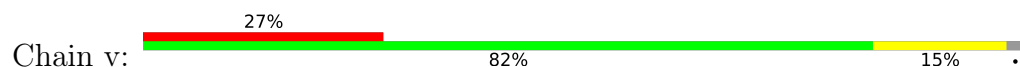




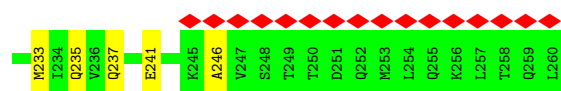
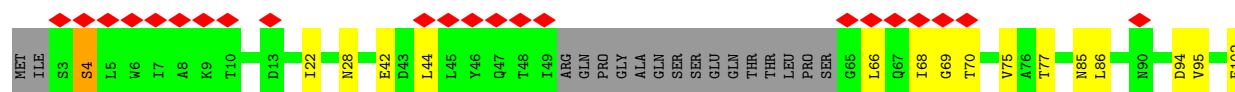
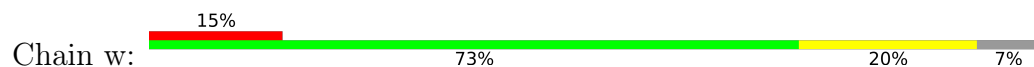
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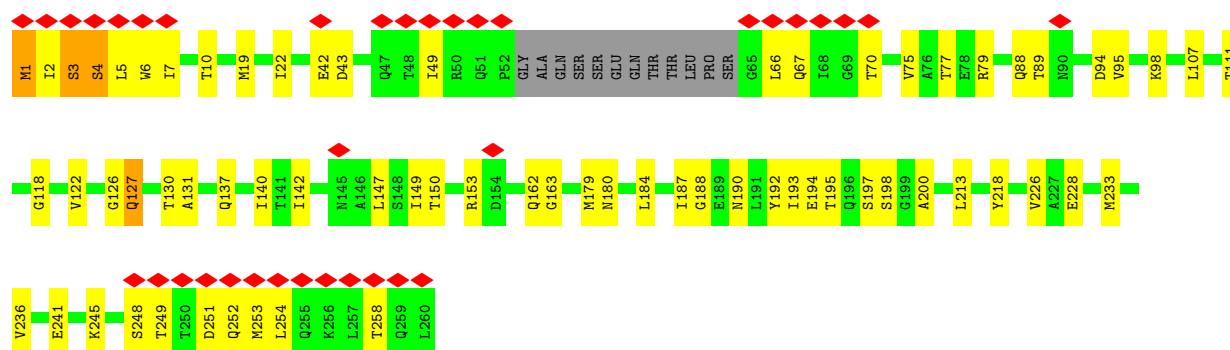
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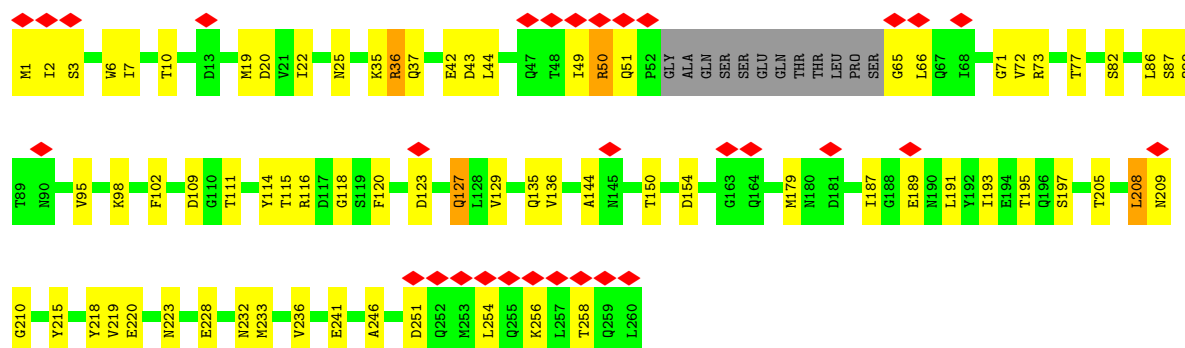
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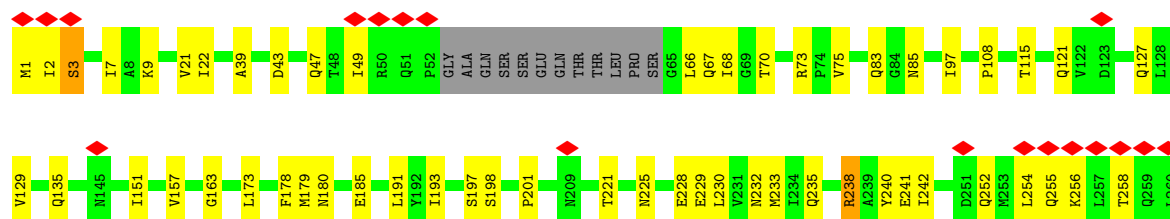
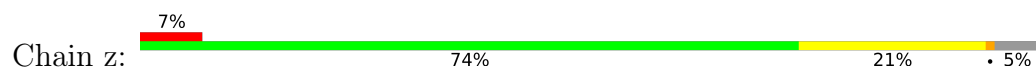
• Molecule 2: Flagellar basal-body rod protein FlgG



• Molecule 2: Flagellar basal-body rod protein FlgG



• Molecule 2: Flagellar basal-body rod protein FlgG



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 24190                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.771                                   | Depositor |
| Minimum map value                    | -1.263                                  | Depositor |
| Average map value                    | -0.002                                  | Depositor |
| Map value standard deviation         | 0.083                                   | Depositor |
| Recommended contour level            | 0.35                                    | Depositor |
| Map size (Å)                         | 614.4, 614.4, 614.4                     | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.2, 1.2, 1.2                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | ZF    | 0.23         | 0/2991        | 0.48        | 2/4076 (0.0%) |
| 1   | ZG    | 0.29         | 1/2991 (0.0%) | 0.53        | 4/4076 (0.1%) |
| 1   | ZH    | 0.24         | 0/2991        | 0.48        | 1/4076 (0.0%) |
| 1   | ZI    | 0.27         | 0/2991        | 0.50        | 1/4076 (0.0%) |
| 1   | ZJ    | 0.28         | 0/2991        | 0.51        | 0/4076        |
| 1   | ZK    | 0.17         | 0/2991        | 0.39        | 0/4076        |
| 1   | ZL    | 0.23         | 0/2991        | 0.44        | 0/4076        |
| 1   | ZM    | 0.22         | 0/2991        | 0.49        | 1/4076 (0.0%) |
| 1   | ZN    | 0.21         | 0/2991        | 0.46        | 1/4076 (0.0%) |
| 1   | ZO    | 0.26         | 0/2991        | 0.49        | 1/4076 (0.0%) |
| 1   | ZP    | 0.20         | 0/2991        | 0.43        | 1/4076 (0.0%) |
| 1   | ZQ    | 0.22         | 0/2991        | 0.48        | 0/4076        |
| 1   | ZR    | 0.24         | 1/2991 (0.0%) | 0.50        | 2/4076 (0.0%) |
| 1   | ZS    | 0.21         | 0/2991        | 0.44        | 0/4076        |
| 1   | ZT    | 0.13         | 0/2991        | 0.35        | 0/4076        |
| 1   | ZU    | 0.21         | 0/2991        | 0.43        | 0/4076        |
| 1   | ZV    | 0.48         | 4/2991 (0.1%) | 0.65        | 7/4076 (0.2%) |
| 1   | ZW    | 0.14         | 0/2991        | 0.37        | 0/4076        |
| 1   | ZX    | 0.18         | 0/2991        | 0.41        | 0/4076        |
| 1   | ZY    | 0.22         | 1/2991 (0.0%) | 0.45        | 2/4076 (0.0%) |
| 1   | ZZ    | 0.13         | 0/2991        | 0.35        | 0/4076        |
| 1   | Za    | 0.18         | 0/2991        | 0.41        | 1/4076 (0.0%) |
| 1   | Zb    | 0.25         | 0/2991        | 0.48        | 1/4076 (0.0%) |
| 1   | Zc    | 0.23         | 0/2991        | 0.49        | 3/4076 (0.1%) |
| 1   | Zd    | 0.25         | 0/2991        | 0.50        | 1/4076 (0.0%) |
| 1   | Ze    | 0.21         | 0/2991        | 0.48        | 0/4076        |
| 1   | Zf    | 0.21         | 0/2991        | 0.45        | 0/4076        |
| 1   | Zg    | 0.18         | 0/2991        | 0.42        | 0/4076        |
| 1   | Zh    | 0.16         | 0/2991        | 0.38        | 0/4076        |
| 2   | 0     | 0.28         | 0/1888        | 0.51        | 1/2564 (0.0%) |
| 2   | 1     | 0.27         | 0/1917        | 0.52        | 0/2605        |
| 2   | 2     | 0.21         | 0/1973        | 0.46        | 0/2682        |
| 2   | 3     | 0.23         | 0/1973        | 0.47        | 0/2682        |
| 2   | 4     | 0.20         | 0/1973        | 0.46        | 0/2682        |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 2   | 5     | 0.32         | 0/1973          | 0.58        | 0/2682           |
| 2   | 6     | 0.30         | 0/1973          | 0.57        | 0/2682           |
| 2   | 7     | 0.22         | 0/1973          | 0.45        | 0/2682           |
| 2   | 8     | 0.26         | 0/1973          | 0.52        | 0/2682           |
| 2   | 9     | 0.23         | 0/1973          | 0.54        | 2/2682 (0.1%)    |
| 2   | ZA    | 0.27         | 0/1973          | 0.51        | 0/2682           |
| 2   | ZB    | 0.26         | 0/1973          | 0.50        | 0/2682           |
| 2   | ZC    | 0.23         | 0/1973          | 0.51        | 0/2682           |
| 2   | ZD    | 0.25         | 0/1973          | 0.53        | 0/2682           |
| 2   | ZE    | 0.23         | 0/1973          | 0.46        | 0/2682           |
| 2   | r     | 0.35         | 0/1926          | 0.60        | 0/2618           |
| 2   | s     | 0.40         | 0/1934          | 0.69        | 0/2629           |
| 2   | t     | 0.35         | 0/1942          | 0.64        | 3/2639 (0.1%)    |
| 2   | u     | 0.33         | 0/1926          | 0.60        | 2/2618 (0.1%)    |
| 2   | v     | 0.31         | 0/1934          | 0.55        | 0/2629           |
| 2   | w     | 0.32         | 0/1844          | 0.58        | 1/2505 (0.0%)    |
| 2   | x     | 0.30         | 0/1888          | 0.53        | 0/2564           |
| 2   | y     | 0.30         | 0/1888          | 0.57        | 0/2564           |
| 2   | z     | 0.28         | 0/1888          | 0.50        | 0/2564           |
| All | All   | 0.25         | 7/133363 (0.0%) | 0.49        | 38/181569 (0.0%) |

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   | ZG    | 0                   | 1                   |
| 1   | ZI    | 0                   | 1                   |
| 1   | ZK    | 0                   | 1                   |
| 1   | ZO    | 0                   | 1                   |
| 1   | ZW    | 0                   | 1                   |
| 1   | Zb    | 0                   | 1                   |
| 1   | Zd    | 0                   | 1                   |
| 1   | Ze    | 0                   | 1                   |
| 2   | 0     | 0                   | 2                   |
| 2   | 1     | 0                   | 1                   |
| 2   | 5     | 0                   | 1                   |
| 2   | 6     | 0                   | 1                   |
| 2   | 8     | 0                   | 1                   |
| 2   | ZA    | 0                   | 1                   |
| 2   | r     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | u     | 0                   | 1                   |
| 2   | y     | 0                   | 2                   |
| 2   | z     | 0                   | 1                   |
| All | All   | 0                   | 20                  |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | ZV    | 140 | PRO  | CG-CD | -15.65 | 0.97        | 1.50     |
| 1   | ZV    | 125 | PRO  | CG-CD | -12.77 | 1.17        | 1.51     |
| 1   | ZV    | 140 | PRO  | N-CD  | 8.38   | 1.59        | 1.47     |
| 1   | ZY    | 125 | PRO  | CG-CD | -7.01  | 1.32        | 1.51     |
| 1   | ZV    | 125 | PRO  | N-CD  | 6.64   | 1.57        | 1.47     |
| 1   | ZR    | 125 | PRO  | CG-CD | -6.60  | 1.33        | 1.51     |
| 1   | ZG    | 4   | SER  | CA-CB | -5.78  | 1.46        | 1.54     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | ZV    | 140 | PRO  | N-CD-CG  | -17.34 | 77.19       | 103.20   |
| 1   | ZV    | 125 | PRO  | N-CD-CG  | -14.54 | 86.35       | 103.80   |
| 1   | ZR    | 125 | PRO  | CA-N-CD  | -13.96 | 91.96       | 111.50   |
| 1   | ZY    | 125 | PRO  | CA-N-CD  | -13.35 | 92.81       | 111.50   |
| 1   | ZV    | 125 | PRO  | CA-N-CD  | -13.26 | 92.94       | 111.50   |
| 1   | Zc    | 125 | PRO  | CA-N-CD  | -11.21 | 95.80       | 111.50   |
| 1   | ZV    | 140 | PRO  | CA-N-CD  | -10.60 | 97.16       | 112.00   |
| 1   | ZR    | 125 | PRO  | N-CD-CG  | -9.98  | 91.83       | 103.80   |
| 1   | ZY    | 125 | PRO  | N-CD-CG  | -9.84  | 92.00       | 103.80   |
| 1   | ZV    | 140 | PRO  | CA-CB-CG | -9.55  | 86.35       | 104.50   |
| 2   | t     | 2   | ILE  | N-CA-C   | -8.97  | 103.65      | 112.17   |
| 1   | ZM    | 223 | PRO  | CA-N-CD  | -8.79  | 99.70       | 112.00   |
| 1   | Zc    | 125 | PRO  | N-CD-CG  | -7.82  | 94.42       | 103.80   |
| 1   | ZG    | 235 | ASN  | N-CA-C   | -7.33  | 104.86      | 114.31   |
| 1   | Zb    | 397 | ASN  | N-CA-C   | -6.25  | 104.39      | 111.14   |
| 2   | 0     | 52  | PRO  | N-CA-CB  | -6.08  | 96.31       | 103.00   |
| 2   | t     | 5   | LEU  | N-CA-C   | -5.78  | 106.07      | 113.23   |
| 2   | 9     | 135 | GLN  | CA-C-N   | 5.77   | 128.86      | 122.22   |
| 2   | 9     | 135 | GLN  | C-N-CA   | 5.77   | 128.86      | 122.22   |
| 1   | ZI    | 322 | ASN  | CB-CA-C  | -5.75  | 103.03      | 111.77   |
| 2   | t     | 4   | SER  | N-CA-C   | -5.66  | 107.37      | 114.56   |
| 1   | ZV    | 125 | PRO  | CA-CB-CG | -5.66  | 93.25       | 104.00   |
| 1   | ZG    | 4   | SER  | N-CA-C   | -5.63  | 107.05      | 114.31   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | ZF    | 134 | PRO  | N-CA-CB  | -5.61 | 98.31       | 103.25   |
| 1   | Zc    | 125 | PRO  | CB-CG-CD | -5.58 | 92.58       | 105.40   |
| 1   | ZP    | 125 | PRO  | CA-N-CD  | -5.57 | 103.70      | 111.50   |
| 1   | ZH    | 397 | ASN  | N-CA-C   | -5.56 | 105.12      | 111.07   |
| 1   | ZV    | 140 | PRO  | N-CA-CB  | -5.50 | 98.41       | 103.31   |
| 2   | w     | 4   | SER  | N-CA-C   | -5.48 | 106.37      | 113.16   |
| 1   | ZG    | 47  | LYS  | N-CA-C   | -5.38 | 106.64      | 114.12   |
| 1   | ZF    | 394 | GLN  | N-CA-C   | -5.36 | 105.84      | 112.38   |
| 1   | ZO    | 141 | ASN  | N-CA-C   | -5.36 | 106.74      | 113.28   |
| 2   | u     | 257 | LEU  | CA-C-N   | -5.26 | 112.31      | 120.31   |
| 2   | u     | 257 | LEU  | C-N-CA   | -5.26 | 112.31      | 120.31   |
| 1   | ZN    | 218 | PRO  | CA-N-CD  | -5.15 | 104.79      | 112.00   |
| 1   | ZG    | 3   | PHE  | N-CA-C   | -5.14 | 106.41      | 113.30   |
| 1   | Za    | 126 | PRO  | CA-N-CD  | -5.11 | 104.85      | 112.00   |
| 1   | Zd    | 323 | ASN  | N-CA-C   | -5.07 | 105.94      | 111.82   |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 0     | 36  | ARG  | Sidechain |
| 2   | 0     | 50  | ARG  | Sidechain |
| 2   | 1     | 36  | ARG  | Sidechain |
| 2   | 5     | 50  | ARG  | Sidechain |
| 2   | 6     | 153 | ARG  | Sidechain |
| 2   | 8     | 238 | ARG  | Sidechain |
| 2   | ZA    | 79  | ARG  | Sidechain |
| 1   | ZG    | 71  | ARG  | Sidechain |
| 1   | ZI    | 380 | ARG  | Sidechain |
| 1   | ZK    | 71  | ARG  | Sidechain |
| 1   | ZO    | 71  | ARG  | Sidechain |
| 1   | ZW    | 71  | ARG  | Sidechain |
| 1   | Zb    | 106 | ARG  | Sidechain |
| 1   | Zd    | 380 | ARG  | Sidechain |
| 1   | Ze    | 380 | ARG  | Sidechain |
| 2   | r     | 36  | ARG  | Sidechain |
| 2   | u     | 116 | ARG  | Sidechain |
| 2   | y     | 36  | ARG  | Sidechain |
| 2   | y     | 50  | ARG  | Sidechain |
| 2   | z     | 238 | ARG  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | ZF    | 2947  | 0        | 2839     | 75      | 0            |
| 1   | ZG    | 2947  | 0        | 2839     | 86      | 0            |
| 1   | ZH    | 2947  | 0        | 2839     | 94      | 0            |
| 1   | ZI    | 2947  | 0        | 2839     | 103     | 0            |
| 1   | ZJ    | 2947  | 0        | 2839     | 87      | 0            |
| 1   | ZK    | 2947  | 0        | 2839     | 68      | 0            |
| 1   | ZL    | 2947  | 0        | 2839     | 64      | 0            |
| 1   | ZM    | 2947  | 0        | 2839     | 70      | 0            |
| 1   | ZN    | 2947  | 0        | 2839     | 71      | 0            |
| 1   | ZO    | 2947  | 0        | 2839     | 72      | 0            |
| 1   | ZP    | 2947  | 0        | 2839     | 79      | 0            |
| 1   | ZQ    | 2947  | 0        | 2839     | 66      | 0            |
| 1   | ZR    | 2947  | 0        | 2839     | 70      | 0            |
| 1   | ZS    | 2947  | 0        | 2839     | 92      | 0            |
| 1   | ZT    | 2947  | 0        | 2839     | 70      | 0            |
| 1   | ZU    | 2947  | 0        | 2839     | 69      | 0            |
| 1   | ZV    | 2947  | 0        | 2839     | 71      | 0            |
| 1   | ZW    | 2947  | 0        | 2839     | 64      | 0            |
| 1   | ZX    | 2947  | 0        | 2839     | 60      | 0            |
| 1   | ZY    | 2947  | 0        | 2839     | 74      | 0            |
| 1   | ZZ    | 2947  | 0        | 2839     | 61      | 0            |
| 1   | Za    | 2947  | 0        | 2839     | 44      | 0            |
| 1   | Zb    | 2947  | 0        | 2839     | 63      | 0            |
| 1   | Zc    | 2947  | 0        | 2839     | 51      | 0            |
| 1   | Zd    | 2947  | 0        | 2839     | 53      | 0            |
| 1   | Ze    | 2947  | 0        | 2839     | 52      | 0            |
| 1   | Zf    | 2947  | 0        | 2839     | 47      | 0            |
| 1   | Zg    | 2947  | 0        | 2839     | 44      | 0            |
| 1   | Zh    | 2947  | 0        | 2839     | 39      | 0            |
| 2   | 0     | 1866  | 0        | 1848     | 53      | 0            |
| 2   | 1     | 1894  | 0        | 1878     | 47      | 0            |
| 2   | 2     | 1949  | 0        | 1926     | 48      | 0            |
| 2   | 3     | 1949  | 0        | 1926     | 48      | 0            |
| 2   | 4     | 1949  | 0        | 1926     | 61      | 0            |
| 2   | 5     | 1949  | 0        | 1926     | 68      | 0            |
| 2   | 6     | 1949  | 0        | 1926     | 62      | 0            |
| 2   | 7     | 1949  | 0        | 1926     | 57      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | 8     | 1949   | 0        | 1926     | 65      | 0            |
| 2   | 9     | 1949   | 0        | 1926     | 60      | 0            |
| 2   | ZA    | 1949   | 0        | 1926     | 78      | 0            |
| 2   | ZB    | 1949   | 0        | 1926     | 85      | 0            |
| 2   | ZC    | 1949   | 0        | 1926     | 90      | 0            |
| 2   | ZD    | 1949   | 0        | 1926     | 102     | 0            |
| 2   | ZE    | 1949   | 0        | 1926     | 88      | 0            |
| 2   | r     | 1903   | 0        | 1878     | 44      | 0            |
| 2   | s     | 1911   | 0        | 1889     | 38      | 0            |
| 2   | t     | 1919   | 0        | 1901     | 46      | 0            |
| 2   | u     | 1903   | 0        | 1878     | 39      | 0            |
| 2   | v     | 1911   | 0        | 1889     | 29      | 0            |
| 2   | w     | 1823   | 0        | 1797     | 46      | 0            |
| 2   | x     | 1866   | 0        | 1848     | 64      | 0            |
| 2   | y     | 1866   | 0        | 1848     | 53      | 0            |
| 2   | z     | 1866   | 0        | 1848     | 45      | 0            |
| All | All   | 131528 | 0        | 127871   | 2686    | 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 10.

All (2686) 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:ZI:388:THR:HA   | 2:ZD:233:MET:CE   | 1.40                     | 1.48              |
| 1:ZI:388:THR:CA   | 2:ZD:233:MET:HE1  | 1.55                     | 1.36              |
| 1:ZJ:322:ASN:HB2  | 2:ZE:122:VAL:O    | 1.33                     | 1.25              |
| 1:ZG:395:ILE:CG2  | 2:ZB:240:TYR:CD2  | 2.18                     | 1.25              |
| 1:ZH:3:PHE:CD2    | 2:ZB:235:GLN:NE2  | 2.06                     | 1.22              |
| 1:ZF:2:SER:HB2    | 2:ZA:20:ASP:OD1   | 1.38                     | 1.21              |
| 1:ZI:388:THR:HA   | 2:ZD:233:MET:HE2  | 1.21                     | 1.19              |
| 1:ZI:388:THR:CB   | 2:ZD:233:MET:HE1  | 1.73                     | 1.16              |
| 1:ZF:43:PHE:CZ    | 2:ZA:37:GLN:NE2   | 2.16                     | 1.14              |
| 1:ZI:46:SER:HB2   | 2:ZD:185:GLU:OE2  | 1.48                     | 1.14              |
| 1:ZK:4:SER:CB     | 2:9:85:ASN:HD22   | 1.58                     | 1.14              |
| 1:ZK:4:SER:HB2    | 2:9:85:ASN:ND2    | 1.61                     | 1.13              |
| 1:ZI:46:SER:HB2   | 2:ZD:185:GLU:CD   | 1.74                     | 1.10              |
| 1:ZI:393:ASP:OD2  | 2:ZC:234:ILE:HG21 | 1.50                     | 1.10              |
| 1:ZJ:395:ILE:HG23 | 2:ZE:240:TYR:CE2  | 1.86                     | 1.09              |
| 1:ZH:399:LEU:HD11 | 2:ZC:240:TYR:CE2  | 1.90                     | 1.06              |
| 1:ZF:43:PHE:HZ    | 2:ZA:37:GLN:NE2   | 1.50                     | 1.05              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:ZG:395:ILE:HG21 | 2:ZB:240:TYR:CD2 | 1.90                     | 1.02              |
| 1:ZJ:393:ASP:OD1  | 2:ZD:238:ARG:NE  | 1.93                     | 1.02              |
| 1:ZI:388:THR:CA   | 2:ZD:233:MET:CE  | 2.21                     | 1.01              |
| 1:ZH:399:LEU:CD1  | 2:ZC:240:TYR:HE2 | 1.74                     | 1.01              |
| 1:ZJ:395:ILE:HG23 | 2:ZE:240:TYR:CD2 | 1.94                     | 1.01              |
| 1:ZG:395:ILE:HG23 | 2:ZB:240:TYR:HD2 | 1.27                     | 0.99              |
| 1:ZK:393:ASP:OD1  | 2:ZE:238:ARG:NH2 | 1.96                     | 0.99              |
| 1:ZI:388:THR:OG1  | 2:ZD:233:MET:HE1 | 1.63                     | 0.97              |
| 1:ZJ:395:ILE:HD11 | 2:ZE:19:MET:HE3  | 1.45                     | 0.97              |
| 1:ZO:53:LYS:HD2   | 2:ZD:218:TYR:OH  | 1.65                     | 0.97              |
| 1:ZH:395:ILE:CG2  | 2:ZC:240:TYR:CD2 | 2.48                     | 0.97              |
| 1:ZI:47:LYS:HE3   | 2:ZD:76:ALA:HB1  | 1.45                     | 0.97              |
| 1:ZI:393:ASP:OD2  | 2:ZC:234:ILE:CG2 | 2.13                     | 0.95              |
| 2:9:45:LEU:HD22   | 2:y:98:LYS:HG3   | 1.47                     | 0.95              |
| 1:ZG:395:ILE:CG2  | 2:ZB:240:TYR:CE2 | 2.49                     | 0.95              |
| 1:ZG:395:ILE:HG23 | 2:ZB:240:TYR:CD2 | 2.00                     | 0.95              |
| 1:ZH:399:LEU:HD11 | 2:ZC:240:TYR:HE2 | 1.25                     | 0.94              |
| 1:ZI:52:VAL:HG21  | 2:ZD:27:ALA:O    | 1.67                     | 0.94              |
| 1:ZK:4:SER:HB2    | 2:9:85:ASN:HD22  | 0.78                     | 0.94              |
| 1:ZI:388:THR:HA   | 2:ZD:233:MET:HE1 | 1.11                     | 0.93              |
| 1:ZJ:395:ILE:CG2  | 2:ZE:240:TYR:CE2 | 2.51                     | 0.93              |
| 1:ZH:46:SER:HB2   | 2:ZC:185:GLU:OE1 | 1.69                     | 0.93              |
| 1:ZG:89:ASN:ND2   | 2:ZA:207:GLY:O   | 2.01                     | 0.92              |
| 1:ZP:53:LYS:HD2   | 2:ZE:218:TYR:OH  | 1.70                     | 0.92              |
| 1:ZF:395:ILE:HG23 | 2:ZA:240:TYR:CE2 | 2.04                     | 0.92              |
| 1:ZH:395:ILE:HG23 | 2:ZC:240:TYR:CD2 | 2.05                     | 0.90              |
| 2:5:257:LEU:HG    | 2:u:230:LEU:HD12 | 1.53                     | 0.89              |
| 1:ZO:50:LEU:HD13  | 2:ZD:85:ASN:OD1  | 1.72                     | 0.89              |
| 1:ZJ:322:ASN:CB   | 2:ZE:122:VAL:O   | 2.20                     | 0.89              |
| 2:7:235:GLN:NE2   | 2:ZD:9:LYS:HD2   | 1.88                     | 0.88              |
| 2:7:235:GLN:HE22  | 2:ZD:9:LYS:HD2   | 1.39                     | 0.88              |
| 1:ZG:4:SER:OG     | 2:5:85:ASN:ND2   | 2.06                     | 0.87              |
| 1:ZG:395:ILE:HG22 | 2:ZB:240:TYR:CE2 | 2.08                     | 0.87              |
| 2:2:244:SER:OG    | 2:7:256:LYS:NZ   | 2.10                     | 0.85              |
| 2:6:255:GLN:HB2   | 2:0:238:ARG:HH21 | 1.42                     | 0.84              |
| 1:ZI:4:SER:OG     | 2:7:85:ASN:ND2   | 2.11                     | 0.84              |
| 1:ZI:388:THR:CB   | 2:ZD:233:MET:CE  | 2.55                     | 0.84              |
| 2:5:231:VAL:HG11  | 2:ZB:9:LYS:HG2   | 1.60                     | 0.84              |
| 1:ZH:52:VAL:HG23  | 2:ZC:28:ASN:OD1  | 1.77                     | 0.83              |
| 1:ZI:49:GLY:HA3   | 2:ZD:24:ASN:ND2  | 1.93                     | 0.83              |
| 2:y:3:SER:O       | 2:y:7:ILE:HG13   | 1.79                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:9:42:GLU:HG2    | 2:9:75:VAL:HG23   | 1.62                     | 0.82              |
| 1:ZF:47:LYS:HD2   | 2:ZA:77:THR:H     | 1.45                     | 0.82              |
| 2:t:2:ILE:HG13    | 2:t:254:LEU:HD11  | 1.62                     | 0.82              |
| 1:ZG:399:LEU:HD11 | 2:ZB:240:TYR:OH   | 1.79                     | 0.81              |
| 1:ZG:322:ASN:CG   | 2:ZB:122:VAL:O    | 2.23                     | 0.81              |
| 2:u:185:GLU:HG3   | 2:z:67:GLN:HE22   | 1.46                     | 0.81              |
| 1:ZO:236:GLY:HA2  | 1:ZO:268:GLN:H    | 1.46                     | 0.80              |
| 2:0:51:GLN:HB3    | 2:0:52:PRO:HD2    | 1.62                     | 0.80              |
| 2:0:153:ARG:HD2   | 2:0:213:LEU:HD13  | 1.63                     | 0.80              |
| 2:6:231:VAL:HG11  | 2:ZC:9:LYS:HG2    | 1.63                     | 0.80              |
| 2:s:28:ASN:HD21   | 2:x:43:ASP:HB3    | 1.45                     | 0.80              |
| 1:ZI:47:LYS:HE3   | 2:ZD:76:ALA:CB    | 2.12                     | 0.79              |
| 2:2:179:MET:HE2   | 2:x:126:GLY:HA2   | 1.65                     | 0.78              |
| 2:9:241:GLU:HG2   | 2:ZE:256:LYS:HG3  | 1.64                     | 0.78              |
| 1:ZQ:160:SER:HA   | 1:ZQ:268:GLN:HE21 | 1.48                     | 0.78              |
| 2:5:52:PRO:HB3    | 2:5:65:GLY:H      | 1.48                     | 0.78              |
| 1:ZF:352:ASN:ND2  | 2:ZA:145:ASN:OD1  | 2.15                     | 0.78              |
| 1:ZJ:399:LEU:HD11 | 2:ZE:240:TYR:CE2  | 2.18                     | 0.78              |
| 1:ZQ:2:SER:OG     | 1:ZQ:3:PHE:N      | 2.17                     | 0.78              |
| 2:6:226:VAL:HG11  | 2:ZB:242:ILE:HD13 | 1.65                     | 0.78              |
| 2:t:157:VAL:HB    | 2:t:171:GLY:HA3   | 1.66                     | 0.77              |
| 1:ZI:126:PRO:HG2  | 1:ZI:310:GLN:HG2  | 1.64                     | 0.77              |
| 2:5:226:VAL:HG11  | 2:ZA:242:ILE:HD13 | 1.65                     | 0.77              |
| 1:ZG:388:THR:OG1  | 2:ZB:233:MET:HE1  | 1.84                     | 0.77              |
| 1:ZJ:395:ILE:CD1  | 2:ZE:19:MET:HE3   | 2.14                     | 0.77              |
| 1:ZI:46:SER:CB    | 2:ZD:185:GLU:OE2  | 2.33                     | 0.76              |
| 1:ZM:319:ASN:ND2  | 1:ZM:352:ASN:OD1  | 2.18                     | 0.76              |
| 1:ZF:43:PHE:CE1   | 2:ZA:37:GLN:NE2   | 2.52                     | 0.76              |
| 1:ZU:380:ARG:NH1  | 1:Za:393:ASP:OD1  | 2.18                     | 0.76              |
| 1:ZF:118:GLY:HA2  | 1:ZF:316:VAL:HG12 | 1.68                     | 0.76              |
| 1:Zh:196:MET:HE3  | 1:Zh:259:PHE:HZ   | 1.51                     | 0.75              |
| 1:ZH:41:ASP:OD2   | 2:ZC:190:ASN:OD1  | 2.05                     | 0.75              |
| 1:ZI:2:SER:HB3    | 1:ZI:392:GLN:HE21 | 1.51                     | 0.75              |
| 2:ZC:10:THR:CG2   | 2:ZC:71:GLY:HA3   | 2.17                     | 0.75              |
| 2:s:147:LEU:HD11  | 2:s:162:GLN:HG2   | 1.68                     | 0.75              |
| 1:ZH:391:THR:HG21 | 2:ZC:19:MET:HE1   | 1.68                     | 0.75              |
| 1:ZH:395:ILE:HG23 | 2:ZC:240:TYR:HD2  | 1.52                     | 0.75              |
| 1:ZI:46:SER:HB2   | 2:ZD:185:GLU:OE1  | 1.85                     | 0.74              |
| 2:6:57:SER:HB3    | 2:w:108:PRO:HB3   | 1.68                     | 0.74              |
| 1:ZH:322:ASN:HB2  | 2:ZC:122:VAL:O    | 1.88                     | 0.74              |
| 1:Zh:112:GLN:HE21 | 1:Zh:331:ASP:HB2  | 1.51                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZN:401:ASN:O    | 1:ZN:402:LEU:C    | 2.31                     | 0.74              |
| 1:Za:18:ASP:OD2   | 1:Zf:2:SER:N      | 2.21                     | 0.74              |
| 2:9:37:GLN:HE21   | 2:9:79:ARG:HH12   | 1.34                     | 0.74              |
| 1:ZJ:402:LEU:CD2  | 2:ZE:248:SER:HB2  | 2.18                     | 0.74              |
| 1:ZP:270:ASN:HD22 | 1:ZV:192:ASN:HA   | 1.51                     | 0.73              |
| 1:ZW:130:GLN:OE1  | 1:ZW:130:GLN:N    | 2.21                     | 0.73              |
| 1:ZY:71:ARG:NH1   | 1:ZY:74:ASP:OD1   | 2.20                     | 0.73              |
| 1:ZI:388:THR:HG23 | 2:ZD:233:MET:HE3  | 1.70                     | 0.73              |
| 1:ZO:235:ASN:HD22 | 1:ZU:189:SER:HB2  | 1.53                     | 0.73              |
| 2:v:100:GLN:NE2   | 2:v:181:ASP:OD2   | 2.21                     | 0.73              |
| 1:ZN:44:ALA:HB2   | 2:ZC:98:LYS:HE3   | 1.70                     | 0.73              |
| 2:7:226:VAL:HG11  | 2:ZC:242:ILE:HD13 | 1.70                     | 0.73              |
| 1:ZS:77:ILE:HG22  | 1:ZS:356:LEU:HD22 | 1.71                     | 0.73              |
| 2:5:122:VAL:O     | 2:ZA:180:ASN:ND2  | 2.20                     | 0.73              |
| 2:t:98:LYS:HD2    | 2:t:215:TYR:CE2   | 2.23                     | 0.73              |
| 1:ZM:44:ALA:HB2   | 2:ZB:98:LYS:HE3   | 1.69                     | 0.73              |
| 1:ZN:53:LYS:HD2   | 2:ZC:218:TYR:OH   | 1.87                     | 0.73              |
| 2:0:180:ASN:HD22  | 2:v:122:VAL:HG23  | 1.54                     | 0.73              |
| 1:ZH:322:ASN:ND2  | 2:ZC:122:VAL:O    | 2.22                     | 0.72              |
| 1:ZS:77:ILE:HD11  | 1:ZS:96:ARG:HD3   | 1.70                     | 0.72              |
| 1:ZN:53:LYS:CD    | 2:ZC:218:TYR:OH   | 2.36                     | 0.72              |
| 1:ZY:285:LYS:O    | 1:ZY:306:ASN:ND2  | 2.20                     | 0.72              |
| 1:ZI:52:VAL:CG2   | 2:ZD:27:ALA:O     | 2.37                     | 0.72              |
| 2:x:98:LYS:HD2    | 2:x:213:LEU:HD12  | 1.69                     | 0.72              |
| 1:Zd:118:GLY:HA2  | 1:Zd:316:VAL:HG12 | 1.71                     | 0.72              |
| 1:ZH:45:GLY:O     | 2:ZC:186:SER:O    | 2.07                     | 0.72              |
| 1:ZH:52:VAL:CG2   | 2:ZC:28:ASN:OD1   | 2.36                     | 0.72              |
| 1:ZH:53:LYS:HG3   | 2:6:218:TYR:OH    | 1.90                     | 0.71              |
| 2:6:235:GLN:HG2   | 2:ZC:5:LEU:HD21   | 1.71                     | 0.71              |
| 2:8:42:GLU:HB2    | 2:8:75:VAL:HG23   | 1.72                     | 0.71              |
| 1:ZP:324:GLU:OE1  | 1:ZP:324:GLU:N    | 2.23                     | 0.71              |
| 2:9:226:VAL:HG11  | 2:ZE:242:ILE:HD13 | 1.72                     | 0.71              |
| 1:ZJ:402:LEU:HD22 | 2:ZE:248:SER:HB2  | 1.73                     | 0.71              |
| 1:Zc:2:SER:OG     | 1:Zc:3:PHE:N      | 2.21                     | 0.71              |
| 1:ZH:399:LEU:CD1  | 2:ZC:240:TYR:CE2  | 2.61                     | 0.71              |
| 2:8:208:LEU:O     | 2:8:210:GLY:N     | 2.23                     | 0.71              |
| 1:ZH:165:PRO:HG2  | 1:ZH:201:VAL:HG13 | 1.71                     | 0.71              |
| 1:ZH:391:THR:CG2  | 2:ZC:19:MET:HE1   | 2.21                     | 0.71              |
| 2:7:79:ARG:NH2    | 2:7:184:LEU:O     | 2.23                     | 0.71              |
| 1:ZZ:157:ASN:HB3  | 1:ZZ:271:THR:HG21 | 1.72                     | 0.70              |
| 1:ZG:322:ASN:ND2  | 2:ZB:122:VAL:O    | 2.23                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zg:110:ASN:HB2  | 1:Zg:114:MET:HB2  | 1.73                     | 0.70              |
| 1:ZG:45:GLY:O     | 1:ZG:46:SER:HB3   | 1.90                     | 0.70              |
| 1:ZF:397:ASN:HB2  | 2:9:238:ARG:NH2   | 2.05                     | 0.70              |
| 2:v:128:LEU:HD12  | 2:v:140:ILE:HD13  | 1.72                     | 0.70              |
| 1:ZY:42:MET:HG2   | 1:ZY:53:LYS:HG2   | 1.73                     | 0.70              |
| 1:ZR:160:SER:HA   | 1:ZR:268:GLN:HE21 | 1.55                     | 0.70              |
| 1:Zc:159:ASN:ND2  | 1:Zc:161:THR:OG1  | 2.24                     | 0.70              |
| 2:9:70:THR:HG22   | 2:9:71:GLY:H      | 1.57                     | 0.70              |
| 2:u:77:THR:HG23   | 2:z:66:LEU:HB2    | 1.74                     | 0.70              |
| 1:ZG:45:GLY:O     | 1:ZG:46:SER:CB    | 2.38                     | 0.70              |
| 1:ZJ:391:THR:OG1  | 2:ZE:233:MET:HE3  | 1.91                     | 0.70              |
| 2:0:51:GLN:O      | 2:0:52:PRO:C      | 2.35                     | 0.70              |
| 2:ZA:42:GLU:HG2   | 2:ZA:75:VAL:HG23  | 1.73                     | 0.70              |
| 2:ZE:42:GLU:OE2   | 2:ZE:73:ARG:NH1   | 2.24                     | 0.70              |
| 1:ZK:397:ASN:HB2  | 2:ZE:238:ARG:NH2  | 2.07                     | 0.70              |
| 1:ZS:390:LYS:HE2  | 1:ZS:394:GLN:HE22 | 1.57                     | 0.70              |
| 1:ZF:42:MET:HE2   | 2:4:86:LEU:HD12   | 1.75                     | 0.69              |
| 1:ZH:3:PHE:HD2    | 2:ZB:235:GLN:NE2  | 1.82                     | 0.69              |
| 1:ZH:46:SER:CB    | 2:ZC:185:GLU:OE1  | 2.40                     | 0.69              |
| 1:ZO:111:MET:HA   | 1:ZO:111:MET:HE3  | 1.75                     | 0.69              |
| 2:2:208:LEU:O     | 2:x:162:GLN:NE2   | 2.26                     | 0.69              |
| 1:ZJ:399:LEU:CD2  | 2:8:227:ALA:HB1   | 2.22                     | 0.69              |
| 1:ZM:156:ILE:HD12 | 1:ZM:276:ILE:HG12 | 1.75                     | 0.69              |
| 1:Zb:387:GLN:NE2  | 1:Zh:400:VAL:O    | 2.26                     | 0.69              |
| 1:ZF:352:ASN:HD22 | 2:ZA:145:ASN:HA   | 1.58                     | 0.69              |
| 1:ZJ:180:LYS:HD3  | 1:ZJ:274:ASN:HD22 | 1.57                     | 0.69              |
| 1:ZK:107:ASN:ND2  | 1:ZK:138:THR:OG1  | 2.26                     | 0.69              |
| 1:ZQ:380:ARG:NH2  | 1:ZW:393:ASP:OD1  | 2.26                     | 0.69              |
| 1:Zc:238:LEU:HD21 | 1:Zc:242:GLY:HA3  | 1.73                     | 0.69              |
| 1:ZF:5:GLN:NE2    | 1:ZF:49:GLY:O     | 2.26                     | 0.68              |
| 1:ZJ:399:LEU:CD1  | 2:ZE:240:TYR:HE2  | 2.06                     | 0.68              |
| 1:ZR:165:PRO:HG2  | 1:ZR:201:VAL:HG13 | 1.73                     | 0.68              |
| 1:ZY:27:SER:OG    | 1:Zd:381:ASN:ND2  | 2.26                     | 0.68              |
| 2:9:42:GLU:OE2    | 2:9:73:ARG:NE     | 2.27                     | 0.68              |
| 1:Zb:238:LEU:HD21 | 1:Zb:242:GLY:HA3  | 1.75                     | 0.68              |
| 1:Ze:60:ASP:O     | 1:Ze:365:ASN:ND2  | 2.26                     | 0.68              |
| 1:ZI:52:VAL:HG22  | 2:ZD:28:ASN:OD1   | 1.93                     | 0.68              |
| 1:ZI:388:THR:OG1  | 2:ZD:233:MET:CE   | 2.41                     | 0.68              |
| 1:ZH:208:TRP:NE1  | 1:ZH:268:GLN:OE1  | 2.25                     | 0.68              |
| 1:Zd:2:SER:OG     | 1:Zd:3:PHE:N      | 2.25                     | 0.68              |
| 2:ZB:205:THR:HB   | 2:ZB:208:LEU:HG   | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:x:195:THR:HG22  | 2:x:197:SER:H     | 1.59                     | 0.68              |
| 1:ZH:395:ILE:CG2  | 2:ZC:240:TYR:CE2  | 2.76                     | 0.68              |
| 2:0:42:GLU:HG3    | 2:v:190:ASN:HB2   | 1.76                     | 0.68              |
| 1:ZM:204:LYS:HD2  | 1:ZM:205:ASP:H    | 1.59                     | 0.68              |
| 1:ZU:159:ASN:ND2  | 1:ZU:161:THR:OG1  | 2.26                     | 0.68              |
| 1:ZV:102:LEU:HD21 | 1:ZV:106:ARG:HD3  | 1.74                     | 0.68              |
| 1:ZY:18:ASP:HB3   | 1:Zd:5:GLN:HE22   | 1.56                     | 0.68              |
| 1:ZF:65:THR:HB    | 1:ZF:363:ALA:HB3  | 1.75                     | 0.68              |
| 1:ZI:111:MET:HE1  | 1:ZN:58:THR:HB    | 1.76                     | 0.68              |
| 1:ZT:210:VAL:O    | 1:ZT:227:SER:N    | 2.28                     | 0.68              |
| 2:4:121:GLN:NE2   | 2:9:78:GLU:OE1    | 2.27                     | 0.68              |
| 1:ZT:208:TRP:NE1  | 1:ZT:268:GLN:OE1  | 2.26                     | 0.67              |
| 2:ZA:22:ILE:HG21  | 2:ZA:233:MET:HG3  | 1.76                     | 0.67              |
| 2:1:22:ILE:HG21   | 2:1:233:MET:HG3   | 1.77                     | 0.67              |
| 2:2:45:LEU:HD22   | 2:r:98:LYS:HD2    | 1.75                     | 0.67              |
| 2:3:241:GLU:HG2   | 2:8:256:LYS:HG2   | 1.75                     | 0.67              |
| 2:5:238:ARG:NE    | 2:ZB:251:ASP:OD1  | 2.27                     | 0.67              |
| 2:ZA:137:GLN:HA   | 2:ZA:139:ALA:H    | 1.58                     | 0.67              |
| 1:ZI:397:ASN:HB2  | 2:ZC:238:ARG:NH2  | 2.10                     | 0.67              |
| 1:ZL:373:VAL:O    | 1:ZL:376:ILE:N    | 2.27                     | 0.67              |
| 1:ZN:349:GLY:O    | 1:ZT:89:ASN:ND2   | 2.28                     | 0.67              |
| 1:Zc:210:VAL:O    | 1:Zc:227:SER:N    | 2.26                     | 0.67              |
| 1:ZN:17:LEU:HD13  | 1:ZS:395:ILE:HD11 | 1.77                     | 0.67              |
| 1:ZP:349:GLY:O    | 1:ZV:89:ASN:ND2   | 2.27                     | 0.67              |
| 1:ZF:52:VAL:HB    | 2:ZA:28:ASN:OD1   | 1.93                     | 0.67              |
| 1:ZX:285:LYS:O    | 1:ZX:306:ASN:ND2  | 2.23                     | 0.67              |
| 1:ZG:89:ASN:HD21  | 2:ZA:207:GLY:C    | 2.01                     | 0.67              |
| 2:0:99:GLY:O      | 2:0:116:ARG:NH2   | 2.28                     | 0.67              |
| 1:ZH:285:LYS:HG2  | 1:ZH:286:PRO:HD2  | 1.76                     | 0.67              |
| 1:ZQ:178:TYR:HA   | 1:ZQ:201:VAL:HG12 | 1.74                     | 0.67              |
| 1:Za:309:GLU:OE1  | 1:Za:309:GLU:N    | 2.27                     | 0.67              |
| 1:ZZ:380:ARG:NH1  | 1:Zf:393:ASP:OD1  | 2.27                     | 0.67              |
| 2:r:229:GLU:O     | 2:r:233:MET:HG3   | 1.95                     | 0.67              |
| 1:ZO:50:LEU:CD1   | 2:ZD:85:ASN:OD1   | 2.42                     | 0.66              |
| 1:Zd:154:MET:HE2  | 1:Zd:263:PHE:HE1  | 1.60                     | 0.66              |
| 2:5:259:GLN:O     | 2:5:260:LEU:C     | 2.37                     | 0.66              |
| 2:7:238:ARG:HB3   | 2:ZD:1:MET:HE1    | 1.77                     | 0.66              |
| 2:0:112:SER:HB3   | 2:0:137:GLN:HE22  | 1.61                     | 0.66              |
| 2:y:22:ILE:HD11   | 2:y:232:ASN:HB3   | 1.76                     | 0.66              |
| 1:ZF:65:THR:HG23  | 1:ZQ:50:LEU:HD21  | 1.78                     | 0.66              |
| 1:ZG:50:LEU:HD22  | 2:5:85:ASN:HA     | 1.76                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZL:294:ILE:O    | 1:ZL:358:ASN:ND2  | 2.27                     | 0.66              |
| 1:ZO:317:LEU:HD11 | 1:ZO:356:LEU:HD21 | 1.76                     | 0.66              |
| 1:ZT:349:GLY:O    | 1:ZZ:89:ASN:ND2   | 2.28                     | 0.66              |
| 1:ZR:375:MET:HE1  | 1:ZW:388:THR:HG23 | 1.76                     | 0.66              |
| 1:ZW:42:MET:HE3   | 1:ZW:53:LYS:HB3   | 1.76                     | 0.66              |
| 1:ZZ:210:VAL:O    | 1:ZZ:227:SER:N    | 2.28                     | 0.66              |
| 2:9:175:LEU:HD11  | 2:9:214:LEU:HD21  | 1.77                     | 0.66              |
| 1:ZF:42:MET:CE    | 2:4:86:LEU:HD12   | 2.25                     | 0.66              |
| 1:ZH:379:GLN:HE21 | 1:ZM:391:THR:HG23 | 1.59                     | 0.66              |
| 2:ZD:205:THR:HB   | 2:ZD:208:LEU:HD23 | 1.77                     | 0.66              |
| 2:ZC:115:THR:HB   | 2:ZC:191:LEU:HD23 | 1.77                     | 0.66              |
| 1:Zb:18:ASP:CG    | 1:Zg:5:GLN:HE22   | 2.02                     | 0.66              |
| 2:t:98:LYS:HD2    | 2:t:215:TYR:HE2   | 1.58                     | 0.66              |
| 1:ZG:118:GLY:HA2  | 1:ZG:316:VAL:HG12 | 1.77                     | 0.66              |
| 1:ZI:65:THR:HG21  | 1:ZT:4:SER:HB3    | 1.77                     | 0.66              |
| 1:ZI:156:ILE:HG13 | 1:ZI:276:ILE:HA   | 1.76                     | 0.66              |
| 1:ZP:338:GLN:NE2  | 2:ZE:167:PRO:HG2  | 2.10                     | 0.66              |
| 2:4:70:THR:HG22   | 2:4:71:GLY:H      | 1.60                     | 0.66              |
| 2:1:51:GLN:NE2    | 2:w:75:VAL:O      | 2.29                     | 0.66              |
| 2:t:229:GLU:O     | 2:t:233:MET:HG3   | 1.96                     | 0.66              |
| 1:ZR:337:THR:HG22 | 1:ZR:339:ALA:H    | 1.61                     | 0.66              |
| 1:ZW:57:ILE:HD12  | 1:Zb:47:LYS:HB2   | 1.78                     | 0.66              |
| 1:Za:331:ASP:HA   | 1:Zf:40:ALA:HB1   | 1.78                     | 0.66              |
| 2:1:43:ASP:HA     | 2:1:72:VAL:HA     | 1.78                     | 0.65              |
| 2:w:130:THR:HG23  | 2:w:132:GLY:H     | 1.60                     | 0.65              |
| 1:ZK:112:GLN:HE21 | 1:ZK:331:ASP:HB3  | 1.61                     | 0.65              |
| 1:ZL:165:PRO:HG3  | 1:ZL:179:ASN:HD21 | 1.60                     | 0.65              |
| 1:ZM:33:LYS:HD2   | 1:ZM:61:PHE:HA    | 1.77                     | 0.65              |
| 2:ZA:208:LEU:O    | 2:ZA:210:GLY:N    | 2.30                     | 0.65              |
| 2:u:124:GLN:NE2   | 2:u:125:ASN:OD1   | 2.30                     | 0.65              |
| 1:ZJ:384:SER:OG   | 2:ZE:26:LEU:HD22  | 1.96                     | 0.65              |
| 2:ZE:54:ALA:HB1   | 2:y:150:THR:HG21  | 1.77                     | 0.65              |
| 1:ZQ:288:ASP:H    | 1:ZQ:305:SER:HB3  | 1.61                     | 0.65              |
| 1:ZS:196:MET:HA   | 1:ZS:196:MET:HE3  | 1.78                     | 0.65              |
| 1:ZV:77:ILE:HD12  | 1:ZV:96:ARG:HD3   | 1.78                     | 0.65              |
| 2:2:122:VAL:O     | 2:7:180:ASN:ND2   | 2.29                     | 0.65              |
| 2:8:46:TYR:HA     | 2:8:69:GLY:HA2    | 1.79                     | 0.65              |
| 1:ZL:269:GLN:HG3  | 1:ZL:270:ASN:H    | 1.61                     | 0.65              |
| 1:ZI:46:SER:CB    | 2:ZD:185:GLU:OE1  | 2.44                     | 0.65              |
| 1:ZL:144:MET:HE3  | 1:ZL:306:ASN:HD21 | 1.61                     | 0.65              |
| 1:ZP:50:LEU:HD21  | 2:ZE:85:ASN:CG    | 2.21                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZY:2:SER:OG     | 1:ZY:3:PHE:N      | 2.24                     | 0.65              |
| 1:ZV:267:MET:HE3  | 1:ZV:269:GLN:HE21 | 1.61                     | 0.65              |
| 2:6:241:GLU:HG2   | 2:ZB:256:LYS:HG3  | 1.78                     | 0.65              |
| 2:7:254:LEU:O     | 2:7:258:THR:HG23  | 1.97                     | 0.65              |
| 2:ZB:28:ASN:HD22  | 2:ZB:31:THR:HG21  | 1.62                     | 0.65              |
| 1:ZI:379:GLN:HG3  | 1:ZN:391:THR:HG23 | 1.77                     | 0.65              |
| 2:4:79:ARG:NH2    | 2:4:184:LEU:O     | 2.30                     | 0.65              |
| 2:1:79:ARG:HH12   | 2:1:184:LEU:HB2   | 1.62                     | 0.65              |
| 1:ZJ:2:SER:HB3    | 1:ZJ:392:GLN:HG3  | 1.78                     | 0.65              |
| 1:ZX:2:SER:OG     | 1:ZX:3:PHE:N      | 2.27                     | 0.65              |
| 2:2:140:ILE:HD13  | 2:2:157:VAL:HG21  | 1.78                     | 0.65              |
| 2:u:241:GLU:HG2   | 2:z:256:LYS:HG2   | 1.78                     | 0.65              |
| 2:w:153:ARG:HG2   | 2:w:213:LEU:HD12  | 1.78                     | 0.65              |
| 1:ZK:53:LYS:HB2   | 2:9:218:TYR:OH    | 1.97                     | 0.64              |
| 1:ZK:380:ARG:NH2  | 1:ZQ:393:ASP:OD1  | 2.30                     | 0.64              |
| 2:6:28:ASN:ND2    | 2:ZB:43:ASP:OD1   | 2.29                     | 0.64              |
| 2:ZE:205:THR:HB   | 2:ZE:208:LEU:HD22 | 1.77                     | 0.64              |
| 1:ZX:27:SER:HB3   | 1:ZX:368:LEU:HD21 | 1.78                     | 0.64              |
| 1:ZY:128:ILE:HD13 | 1:ZY:314:GLN:HB2  | 1.78                     | 0.64              |
| 1:ZI:294:ILE:O    | 1:ZI:358:ASN:ND2  | 2.29                     | 0.64              |
| 1:ZP:338:GLN:NE2  | 2:ZE:167:PRO:CG   | 2.61                     | 0.64              |
| 2:ZE:259:GLN:O    | 2:ZE:260:LEU:C    | 2.40                     | 0.64              |
| 1:ZJ:52:VAL:HB    | 2:ZE:28:ASN:OD1   | 1.96                     | 0.64              |
| 1:Za:349:GLY:O    | 1:Zg:89:ASN:ND2   | 2.31                     | 0.64              |
| 2:ZC:70:THR:HG22  | 2:ZC:71:GLY:H     | 1.63                     | 0.64              |
| 2:r:259:GLN:O     | 2:r:260:LEU:C     | 2.39                     | 0.64              |
| 1:ZH:322:ASN:CG   | 2:ZC:122:VAL:O    | 2.41                     | 0.64              |
| 1:ZI:2:SER:HB2    | 2:ZD:20:ASP:OD1   | 1.97                     | 0.64              |
| 1:ZR:269:GLN:HB3  | 1:ZX:286:PRO:HG3  | 1.79                     | 0.64              |
| 1:Zc:379:GLN:HE22 | 1:Zh:394:GLN:HE21 | 1.46                     | 0.64              |
| 2:7:70:THR:HG22   | 2:7:71:GLY:H      | 1.62                     | 0.64              |
| 2:7:231:VAL:HG11  | 2:ZD:9:LYS:HG2    | 1.78                     | 0.64              |
| 2:ZA:42:GLU:OE2   | 2:ZA:73:ARG:NH1   | 2.28                     | 0.64              |
| 2:ZA:91:ASN:ND2   | 2:ZA:94:ASP:OD2   | 2.30                     | 0.64              |
| 1:ZV:379:GLN:NE2  | 1:Za:394:GLN:OE1  | 2.31                     | 0.64              |
| 2:y:187:ILE:HD12  | 2:y:193:ILE:HD11  | 1.79                     | 0.64              |
| 2:0:115:THR:HB    | 2:0:191:LEU:HD23  | 1.79                     | 0.64              |
| 2:ZD:52:PRO:HA    | 2:ZD:65:GLY:H     | 1.63                     | 0.64              |
| 1:ZF:47:LYS:NZ    | 2:ZA:76:ALA:HA    | 2.13                     | 0.64              |
| 1:ZH:331:ASP:HA   | 1:ZM:40:ALA:HB1   | 1.78                     | 0.64              |
| 1:ZN:44:ALA:HB2   | 2:ZC:98:LYS:CE    | 2.28                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:0:130:THR:HG23  | 2:0:132:GLY:H     | 1.63                     | 0.64              |
| 1:ZQ:22:ASN:ND2   | 1:ZV:49:GLY:O     | 2.32                     | 0.64              |
| 1:ZX:71:ARG:HD3   | 1:ZX:74:ASP:OD1   | 1.98                     | 0.64              |
| 1:Zc:154:MET:HE1  | 1:Zc:198:VAL:HG21 | 1.79                     | 0.64              |
| 1:ZI:159:ASN:ND2  | 1:ZI:271:THR:O    | 2.31                     | 0.63              |
| 1:ZU:65:THR:HG21  | 1:Zf:4:SER:HB3    | 1.80                     | 0.63              |
| 2:8:151:ILE:HG23  | 2:8:157:VAL:HG22  | 1.79                     | 0.63              |
| 1:ZK:248:THR:OG1  | 1:ZK:257:ALA:N    | 2.31                     | 0.63              |
| 1:ZY:159:ASN:ND2  | 1:ZY:161:THR:OG1  | 2.30                     | 0.63              |
| 1:ZU:155:GLN:HG3  | 1:ZU:277:VAL:HB   | 1.79                     | 0.63              |
| 1:ZY:281:GLN:NE2  | 1:ZY:283:GLY:O    | 2.32                     | 0.63              |
| 1:Za:146:ALA:HB2  | 1:Za:286:PRO:HD3  | 1.80                     | 0.63              |
| 2:ZD:238:ARG:O    | 2:ZD:242:ILE:HG13 | 1.98                     | 0.63              |
| 1:ZP:373:VAL:O    | 1:ZP:376:ILE:N    | 2.30                     | 0.63              |
| 2:3:179:MET:HE1   | 2:y:144:ALA:HB2   | 1.80                     | 0.63              |
| 1:ZI:374:ASN:O    | 1:ZI:377:VAL:N    | 2.31                     | 0.63              |
| 1:ZW:281:GLN:NE2  | 1:ZW:283:GLY:O    | 2.29                     | 0.63              |
| 2:4:98:LYS:NZ     | 2:ZA:187:ILE:O    | 2.31                     | 0.63              |
| 2:y:37:GLN:NE2    | 2:y:77:THR:OG1    | 2.32                     | 0.63              |
| 1:ZH:162:ASP:OD1  | 1:ZH:274:ASN:ND2  | 2.30                     | 0.63              |
| 2:3:256:LYS:HG2   | 2:y:241:GLU:HG2   | 1.81                     | 0.63              |
| 2:9:16:GLN:NE2    | 2:9:20:ASP:OD1    | 2.32                     | 0.63              |
| 1:ZW:17:LEU:HD13  | 1:Zb:395:ILE:HD11 | 1.81                     | 0.63              |
| 1:ZF:395:ILE:HG23 | 2:ZA:240:TYR:CD2  | 2.34                     | 0.63              |
| 1:ZI:373:VAL:HG21 | 1:ZO:10:LEU:CD2   | 2.28                     | 0.63              |
| 1:ZP:217:ASP:HB3  | 1:ZP:220:ALA:HB2  | 1.80                     | 0.63              |
| 1:ZT:87:ASP:HB3   | 1:ZT:114:MET:HE2  | 1.80                     | 0.63              |
| 1:Zb:199:TYR:HB2  | 1:Zb:211:TYR:HB2  | 1.80                     | 0.63              |
| 1:Zh:112:GLN:OE1  | 1:Zh:112:GLN:N    | 2.32                     | 0.63              |
| 1:ZQ:112:GLN:OE1  | 1:ZQ:112:GLN:N    | 2.31                     | 0.63              |
| 1:ZH:78:SER:O     | 1:ZH:354:GLY:HA3  | 1.99                     | 0.62              |
| 1:ZK:167:LYS:NZ   | 1:ZK:168:THR:O    | 2.31                     | 0.62              |
| 1:ZW:285:LYS:O    | 1:ZW:306:ASN:ND2  | 2.29                     | 0.62              |
| 2:s:82:SER:OG     | 2:s:223:ASN:ND2   | 2.32                     | 0.62              |
| 2:z:22:ILE:HD11   | 2:z:232:ASN:HB3   | 1.81                     | 0.62              |
| 2:8:36:ARG:HB3    | 2:8:224:VAL:HG22  | 1.81                     | 0.62              |
| 2:x:88:GLN:HB2    | 2:x:218:TYR:CE1   | 2.34                     | 0.62              |
| 1:ZI:111:MET:CE   | 1:ZN:58:THR:HB    | 2.29                     | 0.62              |
| 1:ZM:223:PRO:HD2  | 1:ZM:223:PRO:O    | 1.97                     | 0.62              |
| 1:ZX:242:GLY:O    | 1:ZX:263:PHE:N    | 2.30                     | 0.62              |
| 2:ZA:70:THR:HG22  | 2:ZA:71:GLY:H     | 1.64                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZD:237:GLN:O    | 2:ZD:241:GLU:HG2  | 2.00                     | 0.62              |
| 2:ZA:259:GLN:O    | 2:ZA:260:LEU:C    | 2.42                     | 0.62              |
| 1:ZL:367:ASP:HB3  | 1:ZL:370:LYS:HG2  | 1.82                     | 0.62              |
| 1:ZR:180:LYS:HB3  | 1:ZR:200:PHE:CD1  | 2.34                     | 0.62              |
| 2:7:22:ILE:HG21   | 2:7:233:MET:HG3   | 1.81                     | 0.62              |
| 1:ZN:34:SER:HB3   | 1:ZN:366:VAL:HG22 | 1.82                     | 0.62              |
| 2:2:42:GLU:HB3    | 2:2:75:VAL:HG23   | 1.81                     | 0.62              |
| 2:5:70:THR:HG22   | 2:5:71:GLY:H      | 1.65                     | 0.62              |
| 1:ZH:238:LEU:HD21 | 1:ZH:242:GLY:HA3  | 1.81                     | 0.62              |
| 1:ZX:17:LEU:HD13  | 1:Zc:395:ILE:HD11 | 1.81                     | 0.62              |
| 1:ZL:331:ASP:HA   | 1:ZQ:40:ALA:HB1   | 1.80                     | 0.62              |
| 1:ZP:146:ALA:HB2  | 1:ZP:286:PRO:HD3  | 1.81                     | 0.62              |
| 1:Zb:97:ASN:OD1   | 1:Zb:99:GLN:NE2   | 2.32                     | 0.62              |
| 1:ZF:43:PHE:HE1   | 2:ZA:37:GLN:HE22  | 1.48                     | 0.62              |
| 1:ZS:319:ASN:ND2  | 1:ZS:352:ASN:OD1  | 2.33                     | 0.62              |
| 2:ZB:24:ASN:OD1   | 2:ZB:37:GLN:NE2   | 2.33                     | 0.62              |
| 2:ZB:163:GLY:O    | 2:ZB:164:GLN:C    | 2.43                     | 0.62              |
| 2:v:142:ILE:HD13  | 2:v:149:ILE:HG12  | 1.82                     | 0.62              |
| 1:ZN:53:LYS:HB2   | 2:ZC:88:GLN:HE21  | 1.63                     | 0.61              |
| 1:ZY:104:GLU:OE2  | 1:ZY:104:GLU:N    | 2.26                     | 0.61              |
| 2:8:70:THR:HG22   | 2:8:71:GLY:H      | 1.65                     | 0.61              |
| 2:ZB:175:LEU:HG   | 2:ZB:206:PRO:HG3  | 1.82                     | 0.61              |
| 2:x:49:ILE:HD12   | 2:x:66:LEU:HD11   | 1.81                     | 0.61              |
| 1:ZT:27:SER:OG    | 1:ZY:381:ASN:OD1  | 2.13                     | 0.61              |
| 2:1:100:GLN:OE1   | 2:1:100:GLN:N     | 2.30                     | 0.61              |
| 1:ZO:18:ASP:HA    | 1:ZT:5:GLN:HE22   | 1.64                     | 0.61              |
| 2:2:49:ILE:HG21   | 2:2:66:LEU:HD23   | 1.82                     | 0.61              |
| 2:4:254:LEU:O     | 2:4:258:THR:HG23  | 2.01                     | 0.61              |
| 2:x:3:SER:O       | 2:x:5:LEU:N       | 2.32                     | 0.61              |
| 1:ZH:281:GLN:OE1  | 1:ZH:283:GLY:N    | 2.31                     | 0.61              |
| 1:ZW:322:ASN:HB3  | 1:ZW:340:SER:HA   | 1.82                     | 0.61              |
| 1:Zc:396:LEU:O    | 1:Zc:400:VAL:HG23 | 2.00                     | 0.61              |
| 2:4:50:ARG:HD3    | 2:4:62:LEU:HD11   | 1.82                     | 0.61              |
| 2:5:94:ASP:OD2    | 2:ZA:38:ARG:NH1   | 2.32                     | 0.61              |
| 1:ZK:7:VAL:HG22   | 2:ZE:231:VAL:HG11 | 1.82                     | 0.61              |
| 1:ZK:112:GLN:N    | 1:ZK:112:GLN:OE1  | 2.33                     | 0.61              |
| 1:ZQ:355:LYS:NZ   | 1:ZW:87:ASP:OD1   | 2.31                     | 0.61              |
| 2:ZC:10:THR:HG21  | 2:ZC:71:GLY:HA3   | 1.83                     | 0.61              |
| 2:s:256:LYS:HD2   | 2:s:259:GLN:HE21  | 1.63                     | 0.61              |
| 2:y:109:ASP:OD2   | 2:y:111:THR:OG1   | 2.15                     | 0.61              |
| 1:Za:2:SER:OG     | 1:Za:3:PHE:N      | 2.34                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zg:385:ASN:O    | 1:Zg:388:THR:N    | 2.33                     | 0.61              |
| 2:r:79:ARG:NH2    | 2:r:186:SER:OG    | 2.33                     | 0.61              |
| 2:t:52:PRO:HA     | 2:t:64:SER:O      | 2.00                     | 0.61              |
| 1:ZU:294:ILE:O    | 1:ZU:358:ASN:ND2  | 2.30                     | 0.61              |
| 1:ZV:178:TYR:HA   | 1:ZV:201:VAL:HG22 | 1.83                     | 0.61              |
| 2:9:20:ASP:OD1    | 2:ZE:4:SER:OG     | 2.18                     | 0.61              |
| 2:ZA:34:PHE:HB3   | 2:ZA:222:SER:HB3  | 1.82                     | 0.61              |
| 1:ZJ:370:LYS:HE3  | 1:ZP:11:ASN:ND2   | 2.14                     | 0.61              |
| 1:ZL:83:PHE:HB2   | 1:ZL:95:SER:O     | 2.01                     | 0.61              |
| 1:ZN:165:PRO:HG2  | 1:ZN:201:VAL:HG23 | 1.82                     | 0.61              |
| 1:ZN:379:GLN:HG3  | 1:ZS:391:THR:HG23 | 1.82                     | 0.61              |
| 1:ZR:146:ALA:HB2  | 1:ZR:286:PRO:HD3  | 1.83                     | 0.61              |
| 1:ZW:178:TYR:HA   | 1:ZW:201:VAL:HG22 | 1.83                     | 0.61              |
| 1:ZF:107:ASN:ND2  | 1:ZF:138:THR:OG1  | 2.33                     | 0.61              |
| 1:ZO:170:PHE:HE2  | 1:ZO:178:TYR:HB3  | 1.65                     | 0.61              |
| 1:ZW:349:GLY:O    | 1:Zc:89:ASN:ND2   | 2.34                     | 0.61              |
| 1:ZY:383:GLN:HG2  | 1:Zd:398:THR:HG21 | 1.82                     | 0.61              |
| 1:Zc:42:MET:HG2   | 1:Zc:53:LYS:HE3   | 1.83                     | 0.61              |
| 2:1:99:GLY:O      | 2:1:116:ARG:NH2   | 2.29                     | 0.61              |
| 1:ZS:295:ASN:ND2  | 1:ZS:299:THR:OG1  | 2.34                     | 0.60              |
| 1:ZT:187:TYR:HE2  | 1:ZT:285:LYS:HB2  | 1.65                     | 0.60              |
| 2:3:88:GLN:HB2    | 2:3:218:TYR:CE2   | 2.37                     | 0.60              |
| 2:4:50:ARG:NH1    | 2:z:75:VAL:HG13   | 2.16                     | 0.60              |
| 2:9:259:GLN:O     | 2:9:260:LEU:C     | 2.44                     | 0.60              |
| 2:s:178:PHE:CE2   | 2:s:184:LEU:HD21  | 2.36                     | 0.60              |
| 1:ZV:281:GLN:NE2  | 1:ZV:283:GLY:O    | 2.34                     | 0.60              |
| 2:5:75:VAL:O      | 2:ZA:50:ARG:NH1   | 2.33                     | 0.60              |
| 1:ZO:248:THR:OG1  | 1:ZO:257:ALA:N    | 2.34                     | 0.60              |
| 1:ZP:338:GLN:HE22 | 2:ZE:167:PRO:HG2  | 1.65                     | 0.60              |
| 1:ZU:17:LEU:HD13  | 1:ZZ:395:ILE:HD11 | 1.82                     | 0.60              |
| 2:s:140:ILE:HG23  | 2:s:170:VAL:HG12  | 1.82                     | 0.60              |
| 1:ZW:17:LEU:CD1   | 1:Zb:395:ILE:HD11 | 2.31                     | 0.60              |
| 1:ZY:194:HIS:HB3  | 1:ZY:196:MET:HE3  | 1.82                     | 0.60              |
| 2:3:22:ILE:HG21   | 2:3:233:MET:HG3   | 1.83                     | 0.60              |
| 2:4:242:ILE:HD13  | 2:ZA:258:THR:HG23 | 1.83                     | 0.60              |
| 2:r:143:PRO:HG2   | 2:r:161:GLN:HE22  | 1.65                     | 0.60              |
| 2:t:22:ILE:HG21   | 2:t:233:MET:HG2   | 1.84                     | 0.60              |
| 1:ZH:5:GLN:HE21   | 2:ZC:24:ASN:HB2   | 1.67                     | 0.60              |
| 1:ZJ:65:THR:HG22  | 1:ZU:50:LEU:HD12  | 1.82                     | 0.60              |
| 1:ZL:144:MET:SD   | 1:ZL:310:GLN:NE2  | 2.75                     | 0.60              |
| 1:ZV:196:MET:HA   | 1:ZV:196:MET:HE3  | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZD:208:LEU:O    | 2:ZD:210:GLY:N    | 2.35                     | 0.60              |
| 2:u:50:ARG:HG2    | 2:u:65:GLY:HA2    | 1.84                     | 0.60              |
| 1:ZU:331:ASP:HA   | 1:ZZ:40:ALA:HB1   | 1.82                     | 0.60              |
| 1:ZX:80:ASN:OD1   | 1:ZX:81:GLY:N     | 2.34                     | 0.60              |
| 1:ZZ:394:GLN:O    | 1:ZZ:398:THR:HG23 | 2.01                     | 0.60              |
| 2:8:215:TYR:OH    | 2:ZE:189:GLU:OE2  | 2.19                     | 0.60              |
| 1:ZZ:184:VAL:HG13 | 1:ZZ:196:MET:HB2  | 1.83                     | 0.60              |
| 2:4:40:VAL:O      | 2:4:75:VAL:N      | 2.30                     | 0.60              |
| 2:9:64:SER:O      | 2:9:64:SER:OG     | 2.19                     | 0.60              |
| 1:ZH:11:ASN:O     | 1:ZH:15:THR:HG23  | 2.00                     | 0.60              |
| 1:Zc:71:ARG:NH1   | 1:Zc:74:ASP:OD1   | 2.35                     | 0.60              |
| 2:6:180:ASN:OD1   | 2:6:183:GLY:N     | 2.35                     | 0.60              |
| 2:y:86:LEU:HD12   | 2:y:218:TYR:HB3   | 1.84                     | 0.60              |
| 1:ZF:346:GLY:HA3  | 1:ZF:353:PHE:CE2  | 2.37                     | 0.60              |
| 1:ZG:399:LEU:HD11 | 2:ZB:240:TYR:CZ   | 2.37                     | 0.60              |
| 1:ZO:71:ARG:HB2   | 1:ZO:74:ASP:OD1   | 2.02                     | 0.60              |
| 1:ZP:50:LEU:CD2   | 2:ZE:85:ASN:CG    | 2.75                     | 0.60              |
| 1:ZU:150:THR:H    | 1:ZU:282:ASN:HD21 | 1.48                     | 0.60              |
| 2:3:34:PHE:HB3    | 2:3:222:SER:HB3   | 1.83                     | 0.60              |
| 2:3:248:SER:O     | 2:3:252:GLN:HG2   | 2.02                     | 0.60              |
| 1:ZH:322:ASN:CB   | 2:ZC:122:VAL:O    | 2.50                     | 0.59              |
| 1:ZO:146:ALA:HB2  | 1:ZO:286:PRO:HD3  | 1.83                     | 0.59              |
| 1:ZX:114:MET:HE1  | 1:ZX:333:VAL:HG21 | 1.82                     | 0.59              |
| 1:Ze:233:ASN:HD21 | 1:Ze:237:ILE:HB   | 1.67                     | 0.59              |
| 1:Zg:114:MET:HA   | 1:Zg:114:MET:HE3  | 1.82                     | 0.59              |
| 2:5:35:LYS:NZ     | 2:5:220:GLU:OE2   | 2.35                     | 0.59              |
| 2:t:90:ASN:O      | 2:t:91:ASN:C      | 2.45                     | 0.59              |
| 1:ZG:39:PHE:HB2   | 2:ZB:31:THR:HG22  | 1.83                     | 0.59              |
| 1:ZJ:17:LEU:HD13  | 1:ZO:395:ILE:HD11 | 1.84                     | 0.59              |
| 1:ZZ:309:GLU:N    | 1:ZZ:309:GLU:OE2  | 2.34                     | 0.59              |
| 2:ZB:40:VAL:HG23  | 2:ZB:75:VAL:HB    | 1.84                     | 0.59              |
| 2:ZC:54:ALA:HB1   | 2:w:150:THR:HG21  | 1.83                     | 0.59              |
| 1:ZI:338:GLN:OE1  | 2:7:167:PRO:CG    | 2.50                     | 0.59              |
| 1:ZQ:188:ASP:HA   | 1:ZQ:257:ALA:HB2  | 1.82                     | 0.59              |
| 1:ZS:289:LEU:HA   | 1:ZS:304:TYR:HA   | 1.84                     | 0.59              |
| 2:r:93:LYS:HE3    | 2:r:149:ILE:HG21  | 1.84                     | 0.59              |
| 1:Za:24:ILE:O     | 1:Za:27:SER:OG    | 2.20                     | 0.59              |
| 2:9:137:GLN:HE21  | 2:9:138:PRO:HA    | 1.67                     | 0.59              |
| 2:z:115:THR:HB    | 2:z:191:LEU:HD23  | 1.85                     | 0.59              |
| 1:ZJ:399:LEU:CD1  | 2:ZE:240:TYR:CE2  | 2.83                     | 0.59              |
| 1:ZK:165:PRO:HG2  | 1:ZK:201:VAL:HG13 | 1.84                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:ZT:42:MET:HE3  | 1:ZT:53:LYS:HB3   | 1.84                     | 0.59              |
| 1:Zh:217:ASP:HB3 | 1:Zh:220:ALA:HB2  | 1.85                     | 0.59              |
| 2:x:22:ILE:HG21  | 2:x:233:MET:HG3   | 1.84                     | 0.59              |
| 1:ZJ:393:ASP:OD1 | 2:ZD:238:ARG:CZ   | 2.50                     | 0.59              |
| 1:ZM:156:ILE:HB  | 1:ZM:276:ILE:HG23 | 1.84                     | 0.59              |
| 1:ZQ:6:ALA:HB1   | 1:ZQ:389:ILE:HG12 | 1.85                     | 0.59              |
| 1:ZV:101:LYS:HZ1 | 1:ZV:111:MET:HA   | 1.66                     | 0.59              |
| 2:t:241:GLU:HG3  | 2:y:256:LYS:HE3   | 1.84                     | 0.59              |
| 2:x:3:SER:O      | 2:x:6:TRP:N       | 2.35                     | 0.59              |
| 1:ZM:18:ASP:O    | 1:ZR:5:GLN:NE2    | 2.36                     | 0.59              |
| 2:5:208:LEU:O    | 2:5:210:GLY:N     | 2.34                     | 0.59              |
| 1:ZT:180:LYS:HD3 | 1:ZT:274:ASN:HB3  | 1.85                     | 0.59              |
| 1:ZW:208:TRP:NE1 | 1:ZW:268:GLN:OE1  | 2.35                     | 0.59              |
| 1:ZT:314:GLN:NE2 | 1:ZT:347:THR:OG1  | 2.35                     | 0.59              |
| 1:Zc:101:LYS:HE2 | 1:Zh:322:ASN:HD21 | 1.67                     | 0.59              |
| 1:Zc:150:THR:OG1 | 1:Zc:282:ASN:ND2  | 2.35                     | 0.59              |
| 2:5:115:THR:HB   | 2:5:191:LEU:HD23  | 1.85                     | 0.59              |
| 1:ZH:160:SER:O   | 1:ZN:252:ASN:ND2  | 2.35                     | 0.59              |
| 1:ZO:211:TYR:CE2 | 1:ZO:226:ALA:HA   | 2.38                     | 0.59              |
| 2:8:45:LEU:HD21  | 2:x:98:LYS:HG3    | 1.85                     | 0.59              |
| 2:ZA:49:ILE:HG21 | 2:ZA:66:LEU:HD23  | 1.85                     | 0.59              |
| 2:0:180:ASN:ND2  | 2:v:122:VAL:O     | 2.35                     | 0.59              |
| 1:ZK:393:ASP:OD1 | 2:ZE:238:ARG:CZ   | 2.51                     | 0.58              |
| 1:Zb:57:ILE:HD12 | 1:Zg:47:LYS:HB2   | 1.85                     | 0.58              |
| 2:t:75:VAL:HA    | 2:y:51:GLN:HE22   | 1.68                     | 0.58              |
| 1:ZZ:71:ARG:HG2  | 1:ZZ:73:LEU:H     | 1.68                     | 0.58              |
| 1:Zc:281:GLN:NE2 | 1:Zc:283:GLY:O    | 2.36                     | 0.58              |
| 2:2:40:VAL:O     | 2:2:75:VAL:N      | 2.33                     | 0.58              |
| 2:ZD:46:TYR:HA   | 2:ZD:69:GLY:HA2   | 1.84                     | 0.58              |
| 1:ZJ:217:ASP:HB3 | 1:ZJ:220:ALA:HB2  | 1.84                     | 0.58              |
| 1:ZL:22:ASN:ND2  | 1:ZQ:49:GLY:HA3   | 2.18                     | 0.58              |
| 1:ZS:33:LYS:O    | 1:ZS:59:GLN:NE2   | 2.36                     | 0.58              |
| 1:Zd:144:MET:HE3 | 1:Zd:145:ALA:N    | 2.19                     | 0.58              |
| 1:Zf:159:ASN:ND2 | 1:Zf:161:THR:OG1  | 2.34                     | 0.58              |
| 1:ZQ:22:ASN:OD1  | 1:ZQ:26:ASN:ND2   | 2.35                     | 0.58              |
| 1:ZT:248:THR:OG1 | 1:ZT:257:ALA:N    | 2.37                     | 0.58              |
| 2:2:1:MET:HB2    | 2:w:235:GLN:HE21  | 1.68                     | 0.58              |
| 2:7:137:GLN:HA   | 2:7:139:ALA:H     | 1.69                     | 0.58              |
| 2:9:127:GLN:NE2  | 2:9:135:GLN:OE1   | 2.37                     | 0.58              |
| 2:1:49:ILE:HB    | 2:1:66:LEU:HD23   | 1.85                     | 0.58              |
| 1:ZI:53:LYS:CE   | 2:ZD:189:GLU:OE1  | 2.51                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZS:105:ASN:HB2  | 1:ZS:107:ASN:HD21 | 1.68                     | 0.58              |
| 1:ZX:146:ALA:HB2  | 1:ZX:286:PRO:HD3  | 1.85                     | 0.58              |
| 1:Zd:208:TRP:NE1  | 1:Zd:268:GLN:OE1  | 2.37                     | 0.58              |
| 2:r:76:ALA:HA     | 2:w:66:LEU:HB3    | 1.84                     | 0.58              |
| 1:ZK:75:VAL:HG21  | 1:ZK:356:LEU:HD23 | 1.85                     | 0.58              |
| 1:ZS:228:THR:HB   | 1:ZS:244:VAL:HG11 | 1.86                     | 0.58              |
| 1:ZU:154:MET:HE1  | 1:ZU:198:VAL:HG21 | 1.86                     | 0.58              |
| 1:ZZ:69:THR:OG1   | 1:ZZ:74:ASP:OD2   | 2.21                     | 0.58              |
| 1:Zb:107:ASN:ND2  | 1:Zb:138:THR:OG1  | 2.37                     | 0.58              |
| 2:8:230:LEU:HD21  | 2:ZD:242:ILE:HG23 | 1.86                     | 0.58              |
| 2:y:66:LEU:H      | 2:y:66:LEU:HD23   | 1.69                     | 0.58              |
| 1:ZI:99:GLN:HG3   | 1:ZI:361:LEU:HD21 | 1.84                     | 0.58              |
| 1:ZU:373:VAL:O    | 1:ZU:376:ILE:N    | 2.36                     | 0.58              |
| 1:Zf:101:LYS:HD3  | 1:Zf:102:LEU:H    | 1.67                     | 0.58              |
| 2:4:64:SER:O      | 2:4:64:SER:OG     | 2.19                     | 0.58              |
| 2:6:35:LYS:HB2    | 2:6:79:ARG:HD2    | 1.85                     | 0.58              |
| 2:8:47:GLN:N      | 2:8:68:ILE:O      | 2.37                     | 0.58              |
| 1:ZI:195:ASP:OD2  | 1:ZI:216:SER:OG   | 2.22                     | 0.58              |
| 1:ZJ:89:ASN:ND2   | 2:ZD:207:GLY:O    | 2.36                     | 0.58              |
| 1:ZK:27:SER:OG    | 1:ZP:381:ASN:ND2  | 2.37                     | 0.58              |
| 1:ZK:150:THR:OG1  | 1:ZK:282:ASN:ND2  | 2.36                     | 0.58              |
| 1:ZO:140:PRO:HD2  | 1:ZO:312:LEU:CD2  | 2.34                     | 0.58              |
| 1:ZX:178:TYR:HA   | 1:ZX:201:VAL:HG22 | 1.85                     | 0.58              |
| 1:Zb:380:ARG:NH2  | 1:Zh:393:ASP:OD1  | 2.36                     | 0.58              |
| 1:ZI:49:GLY:HA3   | 2:ZD:24:ASN:HD21  | 1.69                     | 0.58              |
| 1:ZJ:393:ASP:CG   | 2:ZD:238:ARG:HH21 | 2.12                     | 0.58              |
| 1:ZO:367:ASP:O    | 1:ZO:371:GLU:HG2  | 2.04                     | 0.58              |
| 1:ZS:17:LEU:HD13  | 1:ZX:395:ILE:HD11 | 1.85                     | 0.58              |
| 2:8:1:MET:HE3     | 2:x:226:VAL:HG21  | 1.84                     | 0.58              |
| 2:ZD:115:THR:HB   | 2:ZD:191:LEU:HD23 | 1.84                     | 0.58              |
| 2:u:6:TRP:O       | 2:u:10:THR:HG23   | 2.04                     | 0.58              |
| 1:ZU:112:GLN:OE1  | 1:ZU:112:GLN:N    | 2.36                     | 0.58              |
| 1:ZX:50:LEU:H     | 1:ZX:50:LEU:HD22  | 1.69                     | 0.58              |
| 2:ZE:154:ASP:OD2  | 2:ZE:154:ASP:N    | 2.37                     | 0.58              |
| 1:ZH:319:ASN:HB2  | 1:ZH:353:PHE:HE1  | 1.69                     | 0.57              |
| 1:ZI:373:VAL:HG21 | 1:ZO:10:LEU:HD22  | 1.86                     | 0.57              |
| 1:ZP:178:TYR:HA   | 1:ZP:201:VAL:HG12 | 1.86                     | 0.57              |
| 1:Ze:129:GLN:OE1  | 1:Ze:132:ALA:N    | 2.34                     | 0.57              |
| 2:2:98:LYS:HB3    | 2:2:213:LEU:H     | 1.68                     | 0.57              |
| 2:2:232:ASN:O     | 2:2:236:VAL:HG13  | 2.04                     | 0.57              |
| 1:ZF:322:ASN:CG   | 2:ZA:122:VAL:O    | 2.46                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZJ:49:GLY:HA3   | 2:ZE:24:ASN:ND2   | 2.19                     | 0.57              |
| 1:Zb:80:ASN:OD1   | 1:Zb:81:GLY:N     | 2.37                     | 0.57              |
| 2:8:24:ASN:ND2    | 2:ZD:70:THR:O     | 2.36                     | 0.57              |
| 2:9:83:GLN:NE2    | 2:9:97:ILE:O      | 2.37                     | 0.57              |
| 2:v:129:VAL:HG12  | 2:v:135:GLN:HA    | 1.84                     | 0.57              |
| 1:ZG:263:PHE:O    | 1:ZG:266:SER:OG   | 2.18                     | 0.57              |
| 1:ZQ:155:GLN:HG3  | 1:ZQ:278:ALA:HB3  | 1.86                     | 0.57              |
| 1:ZQ:155:GLN:NE2  | 1:ZQ:277:VAL:HB   | 2.19                     | 0.57              |
| 1:ZQ:196:MET:HA   | 1:ZQ:196:MET:HE3  | 1.86                     | 0.57              |
| 1:ZJ:373:VAL:O    | 1:ZJ:377:VAL:HG23 | 2.04                     | 0.57              |
| 1:ZO:65:THR:HG22  | 1:ZZ:50:LEU:HD22  | 1.86                     | 0.57              |
| 1:ZX:367:ASP:O    | 1:ZX:371:GLU:HG2  | 2.05                     | 0.57              |
| 1:ZZ:104:GLU:OE1  | 1:Ze:338:GLN:NE2  | 2.38                     | 0.57              |
| 2:3:122:VAL:O     | 2:8:180:ASN:ND2   | 2.37                     | 0.57              |
| 2:ZB:7:ILE:HG23   | 2:ZB:71:GLY:HA2   | 1.86                     | 0.57              |
| 2:ZC:208:LEU:O    | 2:ZC:210:GLY:N    | 2.37                     | 0.57              |
| 2:0:151:ILE:HG12  | 2:0:157:VAL:HG22  | 1.86                     | 0.57              |
| 2:1:178:PHE:HE1   | 2:1:201:PRO:HB3   | 1.67                     | 0.57              |
| 1:ZG:180:LYS:HD2  | 1:ZG:181:LYS:H    | 1.70                     | 0.57              |
| 1:ZH:40:ALA:HB1   | 2:ZC:189:GLU:HA   | 1.86                     | 0.57              |
| 1:ZL:167:LYS:HA   | 1:ZL:167:LYS:HE3  | 1.86                     | 0.57              |
| 1:Zc:217:ASP:HB3  | 1:Zc:220:ALA:HB2  | 1.86                     | 0.57              |
| 2:2:85:ASN:O      | 2:2:221:THR:OG1   | 2.21                     | 0.57              |
| 2:3:52:PRO:HB3    | 2:3:65:GLY:H      | 1.70                     | 0.57              |
| 2:8:22:ILE:HG21   | 2:8:233:MET:HG3   | 1.87                     | 0.57              |
| 1:ZI:212:THR:HG21 | 1:ZI:246:ILE:HD13 | 1.86                     | 0.57              |
| 1:ZJ:159:ASN:ND2  | 1:ZJ:161:THR:OG1  | 2.38                     | 0.57              |
| 1:ZQ:281:GLN:NE2  | 1:ZQ:283:GLY:O    | 2.38                     | 0.57              |
| 1:Zd:71:ARG:NH1   | 1:Zd:74:ASP:OD1   | 2.38                     | 0.57              |
| 2:t:142:ILE:HD13  | 2:t:149:ILE:HG12  | 1.86                     | 0.57              |
| 2:z:49:ILE:HD12   | 2:z:66:LEU:HD11   | 1.86                     | 0.57              |
| 1:ZM:196:MET:HA   | 1:ZM:196:MET:HE3  | 1.86                     | 0.57              |
| 1:ZM:270:ASN:HD22 | 1:ZS:192:ASN:HA   | 1.69                     | 0.57              |
| 1:ZP:50:LEU:CD1   | 2:ZE:85:ASN:HA    | 2.35                     | 0.57              |
| 1:ZY:17:LEU:HD13  | 1:Zd:395:ILE:HD11 | 1.86                     | 0.57              |
| 1:ZZ:196:MET:HE3  | 1:ZZ:196:MET:HA   | 1.87                     | 0.57              |
| 2:ZA:257:LEU:HG   | 2:z:230:LEU:HD12  | 1.87                     | 0.57              |
| 2:t:140:ILE:HD12  | 2:t:171:GLY:HA2   | 1.86                     | 0.57              |
| 1:ZV:349:GLY:O    | 1:Zb:89:ASN:ND2   | 2.38                     | 0.57              |
| 1:ZZ:83:PHE:HB2   | 1:ZZ:95:SER:O     | 2.05                     | 0.57              |
| 1:Ze:34:SER:HB3   | 1:Ze:366:VAL:HG12 | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:67:GLN:HE22   | 2:w:186:SER:H     | 1.53                     | 0.57              |
| 1:ZI:183:THR:OG1  | 1:ZT:131:GLY:O    | 2.16                     | 0.57              |
| 1:Zb:349:GLY:O    | 1:Zh:89:ASN:ND2   | 2.35                     | 0.57              |
| 1:Ze:106:ARG:HH22 | 1:Ze:141:ASN:HB3  | 1.68                     | 0.57              |
| 2:6:77:THR:HG23   | 2:ZB:66:LEU:HD12  | 1.87                     | 0.57              |
| 2:ZB:208:LEU:O    | 2:ZB:210:GLY:N    | 2.38                     | 0.57              |
| 2:x:1:MET:HG3     | 2:x:2:ILE:H       | 1.69                     | 0.57              |
| 1:ZG:165:PRO:HG2  | 1:ZG:201:VAL:HG13 | 1.86                     | 0.57              |
| 1:ZH:395:ILE:HG21 | 2:ZC:240:TYR:CD2  | 2.37                     | 0.57              |
| 1:ZN:319:ASN:ND2  | 1:ZN:352:ASN:O    | 2.38                     | 0.57              |
| 1:ZS:322:ASN:HB3  | 1:ZS:340:SER:HA   | 1.87                     | 0.57              |
| 1:Zd:102:LEU:HD11 | 1:Zd:139:ILE:HD12 | 1.87                     | 0.57              |
| 1:Ze:156:ILE:HG13 | 1:Ze:276:ILE:HA   | 1.87                     | 0.57              |
| 2:3:7:ILE:HG23    | 2:3:71:GLY:HA2    | 1.86                     | 0.57              |
| 2:7:98:LYS:NZ     | 2:ZD:187:ILE:O    | 2.37                     | 0.57              |
| 2:7:241:GLU:HG2   | 2:ZC:256:LYS:HG3  | 1.87                     | 0.57              |
| 2:r:241:GLU:OE1   | 2:x:258:THR:OG1   | 2.22                     | 0.57              |
| 1:ZS:235:ASN:OD1  | 1:ZY:189:SER:OG   | 2.23                     | 0.56              |
| 1:ZW:6:ALA:HB1    | 1:ZW:389:ILE:HG12 | 1.87                     | 0.56              |
| 1:Ze:95:SER:HB2   | 1:Ze:333:VAL:HG23 | 1.87                     | 0.56              |
| 2:6:1:MET:HE2     | 2:v:226:VAL:HG11  | 1.87                     | 0.56              |
| 2:ZC:123:ASP:OD1  | 2:ZC:123:ASP:N    | 2.38                     | 0.56              |
| 1:ZJ:165:PRO:HG2  | 1:ZJ:201:VAL:HG13 | 1.85                     | 0.56              |
| 1:Zc:395:ILE:O    | 1:Zc:398:THR:HG22 | 2.06                     | 0.56              |
| 2:ZC:22:ILE:HG21  | 2:ZC:233:MET:HG3  | 1.87                     | 0.56              |
| 1:ZJ:399:LEU:HD22 | 2:8:227:ALA:CB    | 2.35                     | 0.56              |
| 1:ZM:24:ILE:O     | 1:ZM:27:SER:OG    | 2.22                     | 0.56              |
| 1:ZO:53:LYS:HB2   | 2:ZD:88:GLN:HE21  | 1.69                     | 0.56              |
| 1:ZR:107:ASN:ND2  | 1:ZR:138:THR:OG1  | 2.38                     | 0.56              |
| 1:ZR:267:MET:HE2  | 1:ZR:269:GLN:NE2  | 2.19                     | 0.56              |
| 1:ZU:159:ASN:N    | 1:ZU:274:ASN:OD1  | 2.32                     | 0.56              |
| 1:ZW:228:THR:HB   | 1:ZW:244:VAL:HG21 | 1.87                     | 0.56              |
| 1:Zd:159:ASN:ND2  | 1:Zd:162:ASP:OD2  | 2.38                     | 0.56              |
| 1:Zf:69:THR:OG1   | 1:Zf:74:ASP:OD2   | 2.20                     | 0.56              |
| 2:2:128:LEU:HD12  | 2:2:140:ILE:HB    | 1.88                     | 0.56              |
| 2:3:19:MET:HB2    | 2:3:236:VAL:HG11  | 1.87                     | 0.56              |
| 2:9:115:THR:HB    | 2:9:191:LEU:HD23  | 1.87                     | 0.56              |
| 2:ZD:52:PRO:HG3   | 2:ZD:67:GLN:HE21  | 1.70                     | 0.56              |
| 2:ZD:70:THR:HG22  | 2:ZD:71:GLY:H     | 1.70                     | 0.56              |
| 1:ZV:144:MET:HG2  | 1:ZV:287:GLY:H    | 1.71                     | 0.56              |
| 2:3:49:ILE:HG21   | 2:3:66:LEU:HD23   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:255:GLN:O     | 2:r:259:GLN:HG2   | 2.05                     | 0.56              |
| 1:ZF:331:ASP:HA   | 1:ZK:40:ALA:HB1   | 1.88                     | 0.56              |
| 1:ZJ:41:ASP:HB2   | 1:ZJ:43:PHE:CE2   | 2.40                     | 0.56              |
| 1:ZK:310:GLN:O    | 1:ZK:312:LEU:HD12 | 2.05                     | 0.56              |
| 1:ZN:65:THR:HA    | 1:ZY:50:LEU:HD23  | 1.88                     | 0.56              |
| 1:ZS:180:LYS:HD2  | 1:ZS:181:LYS:H    | 1.71                     | 0.56              |
| 2:6:185:GLU:OE1   | 2:ZB:51:GLN:NE2   | 2.38                     | 0.56              |
| 2:8:122:VAL:O     | 2:ZD:180:ASN:ND2  | 2.39                     | 0.56              |
| 1:ZH:75:VAL:CG1   | 1:ZH:356:LEU:HB3  | 2.35                     | 0.56              |
| 1:ZI:322:ASN:CG   | 2:ZD:122:VAL:O    | 2.48                     | 0.56              |
| 1:ZJ:195:ASP:OD2  | 1:ZJ:216:SER:OG   | 2.17                     | 0.56              |
| 1:ZK:102:LEU:HD21 | 1:ZK:106:ARG:HD3  | 1.86                     | 0.56              |
| 1:ZK:379:GLN:HG3  | 1:ZP:391:THR:HG23 | 1.87                     | 0.56              |
| 1:ZO:156:ILE:HG21 | 1:ZO:200:PHE:HE2  | 1.71                     | 0.56              |
| 1:ZT:294:ILE:O    | 1:ZT:358:ASN:ND2  | 2.39                     | 0.56              |
| 2:5:66:LEU:HD12   | 2:0:77:THR:HG23   | 1.87                     | 0.56              |
| 2:9:45:LEU:HD22   | 2:y:98:LYS:CG     | 2.30                     | 0.56              |
| 2:ZB:19:MET:HE1   | 2:ZB:233:MET:HG3  | 1.86                     | 0.56              |
| 2:w:22:ILE:HG21   | 2:w:233:MET:HG3   | 1.88                     | 0.56              |
| 1:ZK:99:GLN:HG3   | 1:ZK:361:LEU:HD11 | 1.88                     | 0.56              |
| 1:ZM:171:SER:O    | 1:ZM:177:SER:OG   | 2.23                     | 0.56              |
| 1:ZO:304:TYR:HE1  | 1:ZO:310:GLN:HB3  | 1.71                     | 0.56              |
| 1:ZS:159:ASN:ND2  | 1:ZS:162:ASP:OD1  | 2.38                     | 0.56              |
| 1:ZF:388:THR:HB   | 2:ZA:233:MET:SD   | 2.46                     | 0.56              |
| 1:ZF:402:LEU:HD22 | 2:ZA:248:SER:HB2  | 1.87                     | 0.56              |
| 1:ZL:53:LYS:HB2   | 2:ZA:218:TYR:HH   | 1.71                     | 0.56              |
| 1:ZL:165:PRO:HG3  | 1:ZL:179:ASN:ND2  | 2.20                     | 0.56              |
| 1:ZP:50:LEU:HD11  | 2:ZE:85:ASN:HA    | 1.88                     | 0.56              |
| 1:ZQ:390:LYS:HB2  | 1:ZV:402:LEU:HD22 | 1.86                     | 0.56              |
| 1:ZX:159:ASN:ND2  | 1:ZX:161:THR:OG1  | 2.35                     | 0.56              |
| 2:2:9:LYS:HE3     | 2:w:228:GLU:HG3   | 1.87                     | 0.56              |
| 2:ZA:99:GLY:O     | 2:ZA:116:ARG:NH2  | 2.39                     | 0.56              |
| 1:ZI:53:LYS:HE2   | 2:ZD:189:GLU:OE1  | 2.06                     | 0.56              |
| 1:ZI:71:ARG:NH1   | 1:ZI:74:ASP:OD1   | 2.39                     | 0.56              |
| 1:ZK:118:GLY:HA2  | 1:ZK:316:VAL:HG12 | 1.87                     | 0.56              |
| 1:ZP:107:ASN:HD22 | 1:ZP:138:THR:HG22 | 1.69                     | 0.56              |
| 1:ZP:164:VAL:HG22 | 1:ZP:202:LYS:HG2  | 1.87                     | 0.56              |
| 1:Zc:331:ASP:HA   | 1:Zh:40:ALA:HB1   | 1.87                     | 0.56              |
| 2:ZE:128:LEU:HD13 | 2:ZE:140:ILE:HB   | 1.87                     | 0.56              |
| 1:ZG:112:GLN:HG2  | 1:ZG:331:ASP:HB3  | 1.87                     | 0.56              |
| 1:ZI:382:TYR:CE1  | 1:ZN:395:ILE:HG23 | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZM:105:ASN:HB2  | 1:ZM:107:ASN:HD21 | 1.70                     | 0.56              |
| 1:ZS:247:THR:HG23 | 1:ZS:258:THR:HG22 | 1.88                     | 0.56              |
| 1:Zb:217:ASP:HB3  | 1:Zb:220:ALA:HB2  | 1.88                     | 0.56              |
| 2:1:91:ASN:ND2    | 2:1:94:ASP:OD1    | 2.39                     | 0.56              |
| 2:t:241:GLU:OE1   | 2:z:258:THR:OG1   | 2.20                     | 0.56              |
| 1:ZH:380:ARG:NH1  | 1:ZN:393:ASP:OD1  | 2.40                     | 0.55              |
| 1:ZH:393:ASP:OD1  | 2:ZB:238:ARG:NH1  | 2.39                     | 0.55              |
| 1:ZI:269:GLN:HE22 | 1:ZO:146:ALA:H    | 1.53                     | 0.55              |
| 1:ZO:186:VAL:HG23 | 1:ZO:194:HIS:HB2  | 1.87                     | 0.55              |
| 2:8:241:GLU:HB3   | 2:ZE:258:THR:HG21 | 1.87                     | 0.55              |
| 2:v:38:ARG:NH2    | 2:v:78:GLU:OE1    | 2.36                     | 0.55              |
| 1:ZL:8:SER:OG     | 1:ZL:52:VAL:O     | 2.23                     | 0.55              |
| 1:ZY:217:ASP:HB3  | 1:ZY:220:ALA:HB2  | 1.89                     | 0.55              |
| 1:Ze:130:GLN:H    | 1:Ze:130:GLN:CD   | 2.14                     | 0.55              |
| 2:4:22:ILE:HG21   | 2:4:233:MET:HG2   | 1.88                     | 0.55              |
| 1:ZG:397:ASN:OD1  | 1:ZG:401:ASN:ND2  | 2.39                     | 0.55              |
| 1:ZV:330:GLY:O    | 1:ZV:333:VAL:HG12 | 2.06                     | 0.55              |
| 1:ZX:80:ASN:ND2   | 1:ZX:352:ASN:OD1  | 2.39                     | 0.55              |
| 1:ZZ:33:LYS:O     | 1:ZZ:59:GLN:NE2   | 2.38                     | 0.55              |
| 1:Zd:381:ASN:OD1  | 1:Zd:385:ASN:ND2  | 2.39                     | 0.55              |
| 2:2:34:PHE:HB3    | 2:2:222:SER:HB3   | 1.88                     | 0.55              |
| 2:4:55:GLN:NE2    | 2:4:57:SER:O      | 2.40                     | 0.55              |
| 2:5:9:LYS:HE3     | 2:z:228:GLU:HG3   | 1.89                     | 0.55              |
| 1:ZI:47:LYS:CE    | 2:ZD:76:ALA:HB1   | 2.29                     | 0.55              |
| 1:ZJ:41:ASP:HB2   | 1:ZJ:43:PHE:HE2   | 1.71                     | 0.55              |
| 1:ZO:236:GLY:O    | 1:ZO:237:ILE:C    | 2.49                     | 0.55              |
| 1:ZS:117:THR:HG22 | 1:ZS:136:PRO:HA   | 1.88                     | 0.55              |
| 1:ZV:111:MET:N    | 1:ZV:111:MET:SD   | 2.79                     | 0.55              |
| 1:Zh:97:ASN:OD1   | 1:Zh:99:GLN:NE2   | 2.40                     | 0.55              |
| 2:3:107:LEU:HD12  | 2:3:111:THR:HG23  | 1.88                     | 0.55              |
| 1:ZN:112:GLN:HG2  | 1:ZN:331:ASP:HB3  | 1.88                     | 0.55              |
| 1:ZU:16:ASN:O     | 1:ZU:20:ILE:HG13  | 2.06                     | 0.55              |
| 1:ZZ:160:SER:O    | 1:ZZ:202:LYS:NZ   | 2.39                     | 0.55              |
| 2:3:9:LYS:HE3     | 2:x:228:GLU:HG3   | 1.89                     | 0.55              |
| 2:9:45:LEU:HD21   | 2:y:215:TYR:CE2   | 2.42                     | 0.55              |
| 2:0:22:ILE:HG21   | 2:0:233:MET:HG3   | 1.87                     | 0.55              |
| 1:ZI:388:THR:HG23 | 2:ZD:233:MET:CE   | 2.36                     | 0.55              |
| 1:ZM:129:GLN:HE21 | 1:ZM:132:ALA:HB2  | 1.71                     | 0.55              |
| 1:ZT:319:ASN:OD1  | 1:ZT:320:PHE:N    | 2.39                     | 0.55              |
| 1:ZW:210:VAL:O    | 1:ZW:227:SER:OG   | 2.23                     | 0.55              |
| 2:0:6:TRP:O       | 2:0:10:THR:HG23   | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:95:VAL:HG12   | 2:r:216:GLN:HA    | 1.89                     | 0.55              |
| 2:z:229:GLU:O     | 2:z:233:MET:HG3   | 2.06                     | 0.55              |
| 1:ZJ:397:ASN:HD22 | 2:ZD:238:ARG:NH1  | 2.03                     | 0.55              |
| 1:ZK:233:ASN:ND2  | 1:ZK:237:ILE:O    | 2.38                     | 0.55              |
| 1:Zb:105:ASN:O    | 1:Zb:106:ARG:HB2  | 2.05                     | 0.55              |
| 1:Zc:379:GLN:NE2  | 1:Zh:394:GLN:HE21 | 2.05                     | 0.55              |
| 1:ZF:18:ASP:OD1   | 1:ZK:2:SER:HB2    | 2.07                     | 0.55              |
| 1:ZF:352:ASN:OD1  | 1:ZF:352:ASN:N    | 2.39                     | 0.55              |
| 1:ZG:212:THR:HG21 | 1:ZG:246:ILE:HD13 | 1.87                     | 0.55              |
| 1:ZN:107:ASN:ND2  | 1:ZN:138:THR:OG1  | 2.39                     | 0.55              |
| 2:2:35:LYS:NZ     | 2:2:220:GLU:OE2   | 2.40                     | 0.55              |
| 2:3:240:TYR:HE1   | 2:8:257:LEU:HD13  | 1.72                     | 0.55              |
| 2:s:185:GLU:HG3   | 2:x:67:GLN:NE2    | 2.21                     | 0.55              |
| 2:ZE:208:LEU:O    | 2:ZE:210:GLY:N    | 2.40                     | 0.55              |
| 1:ZM:184:VAL:HG13 | 1:ZM:196:MET:HB2  | 1.88                     | 0.55              |
| 1:ZN:248:THR:OG1  | 1:ZN:257:ALA:N    | 2.40                     | 0.55              |
| 1:ZU:146:ALA:HB2  | 1:ZU:286:PRO:HD3  | 1.88                     | 0.55              |
| 1:ZY:251:ILE:HG22 | 1:ZY:252:ASN:OD1  | 2.07                     | 0.55              |
| 2:8:79:ARG:NH2    | 2:8:184:LEU:O     | 2.40                     | 0.55              |
| 2:ZD:35:LYS:HB2   | 2:ZD:79:ARG:HD3   | 1.88                     | 0.55              |
| 2:v:126:GLY:O     | 2:v:127:GLN:HB2   | 2.05                     | 0.55              |
| 2:z:22:ILE:HG21   | 2:z:233:MET:HG2   | 1.89                     | 0.55              |
| 1:ZG:395:ILE:HG22 | 2:ZB:240:TYR:HE2  | 1.68                     | 0.54              |
| 1:ZN:71:ARG:NH1   | 1:ZN:74:ASP:OD1   | 2.40                     | 0.54              |
| 1:ZN:93:PHE:HB3   | 1:ZN:333:VAL:HG13 | 1.89                     | 0.54              |
| 1:ZW:196:MET:HE1  | 1:ZW:214:ASP:HB2  | 1.88                     | 0.54              |
| 1:ZY:299:THR:HG22 | 1:ZY:314:GLN:HG3  | 1.89                     | 0.54              |
| 2:3:45:LEU:HD21   | 2:s:215:TYR:CE2   | 2.42                     | 0.54              |
| 2:ZC:111:THR:HG21 | 2:1:163:GLY:HA2   | 1.88                     | 0.54              |
| 1:ZK:331:ASP:HA   | 1:ZP:40:ALA:HB1   | 1.88                     | 0.54              |
| 1:ZU:180:LYS:HZ1  | 1:ZU:274:ASN:C    | 2.15                     | 0.54              |
| 2:8:205:THR:OG1   | 2:8:208:LEU:HD23  | 2.08                     | 0.54              |
| 1:ZH:285:LYS:O    | 1:ZH:306:ASN:ND2  | 2.40                     | 0.54              |
| 1:ZM:367:ASP:O    | 1:ZM:371:GLU:HG2  | 2.07                     | 0.54              |
| 1:ZR:210:VAL:HB   | 1:ZR:228:THR:HG22 | 1.88                     | 0.54              |
| 1:ZY:16:ASN:HB2   | 1:ZY:39:PHE:HZ    | 1.72                     | 0.54              |
| 2:r:147:LEU:HD11  | 2:r:162:GLN:HA    | 1.88                     | 0.54              |
| 2:u:3:SER:O       | 2:u:7:ILE:HD12    | 2.06                     | 0.54              |
| 1:ZI:190:GLN:OE1  | 1:ZI:192:ASN:ND2  | 2.36                     | 0.54              |
| 1:ZT:187:TYR:CE2  | 1:ZT:285:LYS:HB2  | 2.41                     | 0.54              |
| 1:ZX:128:ILE:H    | 1:ZX:128:ILE:HD12 | 1.71                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zf:79:GLN:O     | 1:Zf:96:ARG:NH2   | 2.40                     | 0.54              |
| 2:z:180:ASN:ND2   | 2:z:197:SER:O     | 2.38                     | 0.54              |
| 1:ZH:42:MET:O     | 1:ZH:50:LEU:HB2   | 2.08                     | 0.54              |
| 1:ZP:201:VAL:HG23 | 1:ZP:209:ALA:HB3  | 1.90                     | 0.54              |
| 1:ZR:71:ARG:O     | 1:ZR:359:GLY:HA2  | 2.08                     | 0.54              |
| 1:ZT:83:PHE:HB2   | 1:ZT:95:SER:O     | 2.08                     | 0.54              |
| 1:ZV:383:GLN:O    | 1:ZV:387:GLN:HG2  | 2.07                     | 0.54              |
| 1:Zf:109:VAL:HG12 | 1:Zf:115:GLN:HA   | 1.88                     | 0.54              |
| 2:4:50:ARG:HH12   | 2:z:75:VAL:HG13   | 1.71                     | 0.54              |
| 2:ZC:254:LEU:O    | 2:ZC:258:THR:HG23 | 2.07                     | 0.54              |
| 2:ZE:22:ILE:HG21  | 2:ZE:233:MET:HG3  | 1.89                     | 0.54              |
| 1:ZM:150:THR:OG1  | 1:ZM:282:ASN:ND2  | 2.39                     | 0.54              |
| 1:ZN:53:LYS:HD3   | 2:ZC:218:TYR:OH   | 2.08                     | 0.54              |
| 1:ZT:281:GLN:NE2  | 1:ZT:283:GLY:O    | 2.35                     | 0.54              |
| 1:ZX:349:GLY:O    | 1:Zd:89:ASN:ND2   | 2.32                     | 0.54              |
| 1:ZZ:337:THR:HG22 | 1:ZZ:339:ALA:H    | 1.72                     | 0.54              |
| 1:Ze:322:ASN:HB3  | 1:Ze:340:SER:HA   | 1.89                     | 0.54              |
| 2:3:184:LEU:HB3   | 2:3:192:TYR:HB3   | 1.90                     | 0.54              |
| 2:4:52:PRO:HB3    | 2:4:65:GLY:H      | 1.73                     | 0.54              |
| 2:y:44:LEU:HD23   | 2:y:73:ARG:HD2    | 1.88                     | 0.54              |
| 1:ZF:102:LEU:O    | 1:ZK:322:ASN:ND2  | 2.40                     | 0.54              |
| 1:ZS:65:THR:HG22  | 1:Zd:50:LEU:HD12  | 1.90                     | 0.54              |
| 1:ZT:158:LEU:HB2  | 1:ZT:268:GLN:HG3  | 1.90                     | 0.54              |
| 1:Zc:93:PHE:HD1   | 1:Zc:114:MET:HE1  | 1.71                     | 0.54              |
| 1:Zf:111:MET:HA   | 1:Zf:111:MET:HE3  | 1.90                     | 0.54              |
| 2:9:248:SER:HB2   | 2:ZE:260:LEU:HD22 | 1.90                     | 0.54              |
| 2:ZC:151:ILE:HG12 | 2:ZC:157:VAL:HG22 | 1.90                     | 0.54              |
| 2:1:78:GLU:HG2    | 2:w:121:GLN:HE22  | 1.70                     | 0.54              |
| 2:s:187:ILE:HD11  | 2:s:193:ILE:HD13  | 1.90                     | 0.54              |
| 1:ZJ:399:LEU:HD21 | 2:8:227:ALA:HB1   | 1.89                     | 0.54              |
| 1:ZX:331:ASP:O    | 1:ZX:333:VAL:HG23 | 2.08                     | 0.54              |
| 1:Ze:397:ASN:O    | 1:Ze:398:THR:C    | 2.48                     | 0.54              |
| 1:Zh:294:ILE:O    | 1:Zh:358:ASN:ND2  | 2.40                     | 0.54              |
| 2:4:78:GLU:OE1    | 2:z:121:GLN:NE2   | 2.41                     | 0.54              |
| 2:s:19:MET:HE1    | 2:s:233:MET:HG2   | 1.90                     | 0.54              |
| 1:ZF:288:ASP:OD2  | 1:ZF:288:ASP:N    | 2.40                     | 0.54              |
| 1:ZO:288:ASP:OD1  | 1:ZO:289:LEU:N    | 2.41                     | 0.54              |
| 1:ZZ:14:ALA:HB2   | 1:ZZ:382:TYR:HE2  | 1.73                     | 0.54              |
| 1:Zb:83:PHE:HB2   | 1:Zb:95:SER:O     | 2.08                     | 0.54              |
| 2:8:35:LYS:NZ     | 2:8:220:GLU:OE2   | 2.38                     | 0.54              |
| 2:v:187:ILE:HG13  | 2:v:191:LEU:HB2   | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZF:399:LEU:HD22 | 2:ZA:240:TYR:OH   | 2.07                     | 0.54              |
| 1:ZM:81:GLY:HA3   | 1:ZM:317:LEU:HD23 | 1.89                     | 0.54              |
| 1:ZP:93:PHE:HB3   | 1:ZP:333:VAL:HG13 | 1.90                     | 0.54              |
| 1:ZY:150:THR:OG1  | 1:ZY:282:ASN:ND2  | 2.35                     | 0.54              |
| 2:4:19:MET:HB2    | 2:4:236:VAL:HG11  | 1.90                     | 0.54              |
| 2:ZB:40:VAL:O     | 2:ZB:75:VAL:N     | 2.41                     | 0.54              |
| 2:s:77:THR:HG23   | 2:x:66:LEU:HB2    | 1.89                     | 0.54              |
| 2:s:178:PHE:CE1   | 2:s:201:PRO:HB3   | 2.42                     | 0.54              |
| 2:x:2:ILE:CG2     | 2:x:254:LEU:HD11  | 2.37                     | 0.54              |
| 1:ZG:97:ASN:OD1   | 1:ZG:98:GLY:N     | 2.40                     | 0.53              |
| 1:ZH:395:ILE:HG22 | 2:ZC:240:TYR:CE2  | 2.42                     | 0.53              |
| 1:ZL:18:ASP:OD1   | 1:ZQ:2:SER:N      | 2.41                     | 0.53              |
| 1:ZO:53:LYS:CD    | 2:ZD:218:TYR:OH   | 2.47                     | 0.53              |
| 1:ZV:128:ILE:HD12 | 1:ZV:314:GLN:HB2  | 1.90                     | 0.53              |
| 1:ZW:382:TYR:CE1  | 1:Zb:395:ILE:HG23 | 2.43                     | 0.53              |
| 1:Za:14:ALA:HB2   | 1:Za:382:TYR:HE2  | 1.72                     | 0.53              |
| 1:Ze:137:ILE:HG21 | 1:Ze:300:VAL:HG21 | 1.90                     | 0.53              |
| 2:u:76:ALA:HA     | 2:z:66:LEU:HB3    | 1.90                     | 0.53              |
| 1:ZG:109:VAL:HG12 | 1:ZG:115:GLN:HA   | 1.91                     | 0.53              |
| 1:ZJ:43:PHE:HE1   | 2:ZE:37:GLN:NE2   | 2.06                     | 0.53              |
| 1:ZM:44:ALA:CB    | 2:ZB:98:LYS:HE3   | 2.38                     | 0.53              |
| 1:ZP:87:ASP:OD1   | 1:ZP:87:ASP:N     | 2.35                     | 0.53              |
| 1:ZS:349:GLY:O    | 1:ZY:89:ASN:ND2   | 2.42                     | 0.53              |
| 1:ZU:165:PRO:HG2  | 1:ZU:201:VAL:HG13 | 1.89                     | 0.53              |
| 1:ZY:188:ASP:OD1  | 1:ZY:194:HIS:NE2  | 2.39                     | 0.53              |
| 1:Zd:33:LYS:NZ    | 1:Zd:362:GLU:OE1  | 2.39                     | 0.53              |
| 2:t:91:ASN:HB3    | 2:t:94:ASP:OD2    | 2.09                     | 0.53              |
| 2:z:43:ASP:OD1    | 2:z:43:ASP:N      | 2.41                     | 0.53              |
| 1:ZJ:231:LYS:NZ   | 1:ZJ:239:GLU:OE1  | 2.38                     | 0.53              |
| 1:Zc:29:THR:HG23  | 1:Zh:39:PHE:HB2   | 1.89                     | 0.53              |
| 1:Zd:281:GLN:NE2  | 1:Zd:283:GLY:O    | 2.39                     | 0.53              |
| 2:6:52:PRO:HB3    | 2:6:65:GLY:H      | 1.74                     | 0.53              |
| 2:7:256:LYS:HD2   | 2:7:256:LYS:O     | 2.08                     | 0.53              |
| 2:ZA:97:ILE:HD12  | 2:ZA:116:ARG:HG3  | 1.91                     | 0.53              |
| 2:1:19:MET:HB2    | 2:1:236:VAL:HG11  | 1.91                     | 0.53              |
| 1:ZO:156:ILE:HG13 | 1:ZO:276:ILE:HA   | 1.91                     | 0.53              |
| 1:ZU:170:PHE:HE2  | 1:ZU:223:PRO:HG2  | 1.73                     | 0.53              |
| 1:ZX:71:ARG:NH1   | 1:ZX:100:PHE:O    | 2.36                     | 0.53              |
| 2:7:49:ILE:HG21   | 2:7:66:LEU:HD23   | 1.91                     | 0.53              |
| 2:ZD:42:GLU:OE2   | 2:ZD:73:ARG:NE    | 2.35                     | 0.53              |
| 1:ZJ:151:THR:OG1  | 1:ZJ:282:ASN:ND2  | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZP:74:ASP:O     | 1:ZP:359:GLY:N    | 2.40                     | 0.53              |
| 1:ZP:112:GLN:HG2  | 1:ZP:331:ASP:HB3  | 1.89                     | 0.53              |
| 1:ZX:319:ASN:OD1  | 1:ZX:320:PHE:N    | 2.42                     | 0.53              |
| 1:Zf:397:ASN:O    | 1:Zf:398:THR:C    | 2.51                     | 0.53              |
| 2:7:57:SER:OG     | 2:r:154:ASP:OD1   | 2.27                     | 0.53              |
| 2:9:22:ILE:HG21   | 2:9:233:MET:HG3   | 1.91                     | 0.53              |
| 2:ZB:120:PHE:HB3  | 2:ZB:128:LEU:HD22 | 1.90                     | 0.53              |
| 1:ZO:148:SER:HA   | 1:ZO:187:TYR:O    | 2.08                     | 0.53              |
| 1:ZU:293:GLN:NE2  | 1:ZU:303:ASN:HD21 | 2.07                     | 0.53              |
| 1:ZY:106:ARG:HH12 | 1:ZY:141:ASN:HB3  | 1.74                     | 0.53              |
| 2:3:33:GLY:N      | 2:3:220:GLU:O     | 2.40                     | 0.53              |
| 2:4:256:LYS:HG2   | 2:z:241:GLU:HG2   | 1.90                     | 0.53              |
| 2:5:257:LEU:HG    | 2:u:230:LEU:CD1   | 2.34                     | 0.53              |
| 2:0:116:ARG:NH1   | 2:0:220:GLU:OE2   | 2.41                     | 0.53              |
| 1:ZF:7:VAL:HG22   | 2:9:231:VAL:HG11  | 1.90                     | 0.53              |
| 1:ZK:146:ALA:HB2  | 1:ZK:286:PRO:HD3  | 1.91                     | 0.53              |
| 1:ZL:399:LEU:CD2  | 2:ZA:227:ALA:HB1  | 2.39                     | 0.53              |
| 1:ZO:201:VAL:HG23 | 1:ZO:209:ALA:HB3  | 1.91                     | 0.53              |
| 1:ZQ:112:GLN:NE2  | 1:ZQ:331:ASP:HB3  | 2.24                     | 0.53              |
| 1:ZQ:184:VAL:HG13 | 1:ZQ:196:MET:HB2  | 1.89                     | 0.53              |
| 1:Zc:84:ARG:HD2   | 1:Zc:345:LEU:HD21 | 1.90                     | 0.53              |
| 2:6:197:SER:HB3   | 2:ZB:53:GLY:HA2   | 1.88                     | 0.53              |
| 2:s:76:ALA:HA     | 2:x:66:LEU:HB3    | 1.89                     | 0.53              |
| 1:ZK:270:ASN:HD22 | 1:ZQ:192:ASN:HA   | 1.73                     | 0.53              |
| 1:ZO:374:ASN:O    | 1:ZO:377:VAL:N    | 2.42                     | 0.53              |
| 1:ZT:196:MET:HA   | 1:ZT:196:MET:HE3  | 1.89                     | 0.53              |
| 1:ZU:156:ILE:HG13 | 1:ZU:276:ILE:HA   | 1.91                     | 0.53              |
| 1:ZV:112:GLN:HG2  | 1:ZV:331:ASP:HB3  | 1.89                     | 0.53              |
| 2:6:153:ARG:HH12  | 2:6:213:LEU:HD22  | 1.74                     | 0.53              |
| 2:6:175:LEU:HD21  | 2:6:214:LEU:HD21  | 1.89                     | 0.53              |
| 2:u:188:GLY:O     | 2:u:190:ASN:N     | 2.40                     | 0.53              |
| 1:ZG:382:TYR:HE1  | 1:ZL:399:LEU:HD11 | 1.73                     | 0.53              |
| 1:ZP:396:LEU:O    | 1:ZP:400:VAL:HG23 | 2.09                     | 0.53              |
| 1:ZS:367:ASP:O    | 1:ZS:371:GLU:HG2  | 2.09                     | 0.53              |
| 1:ZV:3:PHE:O      | 1:ZV:7:VAL:HG23   | 2.09                     | 0.53              |
| 1:ZW:112:GLN:OE1  | 1:ZW:112:GLN:N    | 2.42                     | 0.53              |
| 2:3:145:ASN:O     | 2:3:161:GLN:NE2   | 2.42                     | 0.53              |
| 2:5:174:ASN:ND2   | 2:5:203:GLU:OE2   | 2.36                     | 0.53              |
| 2:ZC:137:GLN:HA   | 2:ZC:138:PRO:C    | 2.34                     | 0.53              |
| 2:ZE:122:VAL:HG13 | 2:ZE:126:GLY:HA2  | 1.91                     | 0.53              |
| 2:0:83:GLN:NE2    | 2:0:97:ILE:O      | 2.20                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZG:217:ASP:HB3  | 1:ZG:220:ALA:HB2  | 1.90                     | 0.53              |
| 1:ZH:391:THR:CG2  | 2:ZC:19:MET:CE    | 2.87                     | 0.53              |
| 1:ZR:44:ALA:HB3   | 1:ZR:50:LEU:HD12  | 1.91                     | 0.53              |
| 1:ZX:42:MET:HG2   | 1:ZX:53:LYS:HE3   | 1.91                     | 0.53              |
| 1:Za:287:GLY:N    | 1:Za:306:ASN:HD22 | 2.07                     | 0.53              |
| 1:Ze:99:GLN:HE22  | 1:Ze:111:MET:HG2  | 1.73                     | 0.53              |
| 1:Zf:139:ILE:HA   | 1:Zf:312:LEU:HD13 | 1.91                     | 0.53              |
| 2:r:19:MET:HE1    | 2:r:233:MET:HE2   | 1.90                     | 0.53              |
| 1:ZF:397:ASN:HB2  | 2:9:238:ARG:CZ    | 2.39                     | 0.52              |
| 1:ZH:399:LEU:O    | 1:ZH:400:VAL:C    | 2.51                     | 0.52              |
| 1:ZP:208:TRP:NE1  | 1:ZP:268:GLN:OE1  | 2.36                     | 0.52              |
| 1:ZU:178:TYR:HA   | 1:ZU:201:VAL:HG22 | 1.89                     | 0.52              |
| 1:Zb:233:ASN:HD21 | 1:Zb:237:ILE:HB   | 1.74                     | 0.52              |
| 1:Zc:10:LEU:HD22  | 1:Zc:389:ILE:HD12 | 1.91                     | 0.52              |
| 1:Ze:165:PRO:HG2  | 1:Ze:201:VAL:HG13 | 1.91                     | 0.52              |
| 1:Zg:85:LEU:HD13  | 1:Zg:114:MET:HB3  | 1.91                     | 0.52              |
| 2:5:245:LYS:HE3   | 2:ZB:258:THR:O    | 2.09                     | 0.52              |
| 2:6:42:GLU:OE1    | 2:6:73:ARG:NH2    | 2.32                     | 0.52              |
| 2:1:115:THR:HB    | 2:1:191:LEU:HD23  | 1.91                     | 0.52              |
| 1:ZG:380:ARG:NE   | 1:ZM:393:ASP:OD2  | 2.33                     | 0.52              |
| 1:ZW:33:LYS:NZ    | 1:ZW:362:GLU:OE1  | 2.42                     | 0.52              |
| 1:ZZ:33:LYS:NZ    | 1:ZZ:362:GLU:OE1  | 2.42                     | 0.52              |
| 2:2:208:LEU:O     | 2:2:210:GLY:N     | 2.42                     | 0.52              |
| 2:ZA:111:THR:HG21 | 2:z:163:GLY:HA2   | 1.90                     | 0.52              |
| 2:ZD:47:GLN:N     | 2:ZD:68:ILE:O     | 2.41                     | 0.52              |
| 1:ZR:288:ASP:H    | 1:ZR:305:SER:HG   | 1.57                     | 0.52              |
| 1:ZS:379:GLN:NE2  | 1:ZX:394:GLN:OE1  | 2.37                     | 0.52              |
| 1:ZU:71:ARG:NH1   | 1:ZZ:324:GLU:OE2  | 2.42                     | 0.52              |
| 2:6:57:SER:O      | 2:6:59:GLN:N      | 2.35                     | 0.52              |
| 2:1:78:GLU:HG2    | 2:w:121:GLN:NE2   | 2.23                     | 0.52              |
| 2:u:185:GLU:HB3   | 2:u:193:ILE:HG13  | 1.92                     | 0.52              |
| 2:y:254:LEU:O     | 2:y:258:THR:HG23  | 2.08                     | 0.52              |
| 1:ZF:84:ARG:NH1   | 1:ZF:134:PRO:HB2  | 2.23                     | 0.52              |
| 1:ZJ:393:ASP:OD1  | 2:ZD:238:ARG:NH2  | 2.43                     | 0.52              |
| 1:ZL:93:PHE:CD2   | 1:ZL:114:MET:HE1  | 2.45                     | 0.52              |
| 1:ZR:83:PHE:HB2   | 1:ZR:95:SER:O     | 2.10                     | 0.52              |
| 1:ZY:125:PRO:HD2  | 1:ZY:125:PRO:O    | 2.08                     | 0.52              |
| 2:x:254:LEU:O     | 2:x:258:THR:HG23  | 2.09                     | 0.52              |
| 1:ZM:160:SER:O    | 1:ZM:202:LYS:NZ   | 2.41                     | 0.52              |
| 1:ZQ:102:LEU:HD21 | 1:ZQ:106:ARG:HA   | 1.90                     | 0.52              |
| 1:Zd:180:LYS:HB3  | 1:Zd:200:PHE:HB2  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zd:397:ASN:O    | 1:Zd:399:LEU:N    | 2.43                     | 0.52              |
| 2:4:130:THR:OG1   | 2:4:131:ALA:N     | 2.42                     | 0.52              |
| 2:0:251:ASP:OD1   | 2:u:238:ARG:NH2   | 2.33                     | 0.52              |
| 2:1:16:GLN:OE1    | 2:1:16:GLN:HA     | 2.10                     | 0.52              |
| 1:ZL:27:SER:O     | 1:ZL:364:SER:OG   | 2.27                     | 0.52              |
| 1:ZR:200:PHE:CE2  | 1:ZR:263:PHE:HE1  | 2.26                     | 0.52              |
| 1:ZR:331:ASP:HA   | 1:ZW:40:ALA:HB1   | 1.92                     | 0.52              |
| 1:ZU:160:SER:HA   | 1:ZU:268:GLN:HE21 | 1.74                     | 0.52              |
| 1:Zd:397:ASN:C    | 1:Zd:399:LEU:N    | 2.63                     | 0.52              |
| 2:2:178:PHE:CE1   | 2:2:184:LEU:HD21  | 2.45                     | 0.52              |
| 2:7:257:LEU:HG    | 2:w:230:LEU:HD12  | 1.92                     | 0.52              |
| 1:ZF:139:ILE:HG12 | 1:ZF:312:LEU:HD22 | 1.92                     | 0.52              |
| 1:ZK:322:ASN:OD1  | 1:ZK:325:GLY:N    | 2.43                     | 0.52              |
| 1:ZO:2:SER:OG     | 1:ZO:3:PHE:N      | 2.37                     | 0.52              |
| 1:ZQ:200:PHE:HE2  | 1:ZQ:263:PHE:HE2  | 1.57                     | 0.52              |
| 1:ZU:144:MET:HE3  | 1:ZU:306:ASN:HD21 | 1.73                     | 0.52              |
| 1:ZZ:210:VAL:HB   | 1:ZZ:228:THR:HG22 | 1.90                     | 0.52              |
| 1:Za:188:ASP:OD1  | 1:Za:192:ASN:N    | 2.42                     | 0.52              |
| 2:3:219:VAL:HG11  | 2:8:38:ARG:HH12   | 1.75                     | 0.52              |
| 2:4:42:GLU:OE2    | 2:4:73:ARG:NE     | 2.28                     | 0.52              |
| 2:7:235:GLN:HG2   | 2:ZD:5:LEU:HD21   | 1.91                     | 0.52              |
| 2:y:116:ARG:NH2   | 2:y:220:GLU:OE1   | 2.42                     | 0.52              |
| 1:ZI:53:LYS:HG3   | 2:7:218:TYR:OH    | 2.10                     | 0.52              |
| 1:ZR:267:MET:HE2  | 1:ZR:269:GLN:HE22 | 1.74                     | 0.52              |
| 1:ZS:151:THR:OG1  | 1:ZS:282:ASN:ND2  | 2.43                     | 0.52              |
| 1:ZW:331:ASP:HA   | 1:Zb:40:ALA:HB1   | 1.92                     | 0.52              |
| 1:ZX:331:ASP:HA   | 1:Zc:40:ALA:HB1   | 1.91                     | 0.52              |
| 1:Zf:397:ASN:O    | 1:Zf:400:VAL:N    | 2.43                     | 0.52              |
| 1:Zg:157:ASN:HB3  | 1:Zg:271:THR:HG21 | 1.90                     | 0.52              |
| 2:2:151:ILE:HG12  | 2:2:157:VAL:HG22  | 1.92                     | 0.52              |
| 2:5:77:THR:HG23   | 2:ZA:66:LEU:HD12  | 1.90                     | 0.52              |
| 2:5:257:LEU:HD21  | 2:u:227:ALA:HA    | 1.91                     | 0.52              |
| 2:8:226:VAL:HG11  | 2:ZD:242:ILE:HD12 | 1.90                     | 0.52              |
| 2:ZC:5:LEU:O      | 2:ZC:9:LYS:HG3    | 2.09                     | 0.52              |
| 1:ZI:367:ASP:O    | 1:ZI:371:GLU:HG2  | 2.10                     | 0.52              |
| 1:ZK:4:SER:CB     | 2:9:85:ASN:ND2    | 2.43                     | 0.52              |
| 1:ZN:41:ASP:N     | 1:ZN:41:ASP:OD2   | 2.42                     | 0.52              |
| 1:ZP:380:ARG:NE   | 1:ZV:393:ASP:OD2  | 2.43                     | 0.52              |
| 1:ZW:93:PHE:HB3   | 1:ZW:333:VAL:HG13 | 1.92                     | 0.52              |
| 1:ZY:230:LEU:HD21 | 1:ZY:263:PHE:HD2  | 1.74                     | 0.52              |
| 1:Za:116:LEU:HD21 | 1:Za:315:ILE:HD13 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zb:109:VAL:HG12 | 1:Zb:115:GLN:HA   | 1.92                     | 0.52              |
| 1:Zf:317:LEU:HD21 | 1:Zf:356:LEU:HD11 | 1.91                     | 0.52              |
| 2:7:75:VAL:O      | 2:ZC:50:ARG:NH1   | 2.37                     | 0.52              |
| 2:ZA:40:VAL:HG23  | 2:ZA:75:VAL:HB    | 1.92                     | 0.52              |
| 2:z:3:SER:O       | 2:z:7:ILE:HG13    | 2.09                     | 0.52              |
| 1:ZF:398:THR:HG21 | 2:ZA:241:GLU:HG2  | 1.91                     | 0.52              |
| 1:ZH:380:ARG:HB3  | 1:ZN:396:LEU:HD13 | 1.91                     | 0.52              |
| 1:ZK:170:PHE:HE2  | 1:ZK:223:PRO:HG2  | 1.74                     | 0.52              |
| 1:ZN:212:THR:HG21 | 1:ZN:246:ILE:HD11 | 1.91                     | 0.52              |
| 1:ZP:331:ASP:HA   | 1:ZU:40:ALA:HB1   | 1.91                     | 0.52              |
| 1:ZV:34:SER:HB3   | 1:ZV:366:VAL:HG12 | 1.91                     | 0.52              |
| 1:ZV:180:LYS:HD3  | 1:ZV:274:ASN:HB3  | 1.91                     | 0.52              |
| 1:ZZ:381:ASN:O    | 1:ZZ:385:ASN:ND2  | 2.43                     | 0.52              |
| 1:Za:150:THR:OG1  | 1:Za:282:ASN:ND2  | 2.34                     | 0.52              |
| 1:ZG:30:TYR:HD1   | 1:ZG:363:ALA:HA   | 1.75                     | 0.51              |
| 1:ZM:80:ASN:OD1   | 1:ZM:81:GLY:N     | 2.43                     | 0.51              |
| 1:ZS:118:GLY:HA2  | 1:ZS:316:VAL:HG12 | 1.92                     | 0.51              |
| 1:ZS:180:LYS:HB2  | 1:ZS:274:ASN:HD22 | 1.76                     | 0.51              |
| 1:Zg:111:MET:HE2  | 1:Zg:111:MET:N    | 2.25                     | 0.51              |
| 2:4:7:ILE:HG23    | 2:4:71:GLY:HA2    | 1.92                     | 0.51              |
| 2:7:18:ASN:O      | 2:7:22:ILE:HG13   | 2.10                     | 0.51              |
| 2:w:107:LEU:HD12  | 2:w:111:THR:HG23  | 1.92                     | 0.51              |
| 1:ZI:154:MET:HG3  | 1:ZI:279:THR:HG22 | 1.91                     | 0.51              |
| 1:ZM:374:ASN:O    | 1:ZM:377:VAL:N    | 2.43                     | 0.51              |
| 1:ZR:162:ASP:OD2  | 1:ZR:274:ASN:ND2  | 2.42                     | 0.51              |
| 1:ZR:288:ASP:N    | 1:ZR:305:SER:OG   | 2.43                     | 0.51              |
| 1:ZV:211:TYR:CE2  | 1:ZV:226:ALA:HA   | 2.45                     | 0.51              |
| 1:Zc:146:ALA:HB2  | 1:Zc:286:PRO:HD3  | 1.91                     | 0.51              |
| 2:8:127:GLN:HE22  | 2:8:139:ALA:HB1   | 1.75                     | 0.51              |
| 2:ZE:37:GLN:HG2   | 2:ZE:79:ARG:HD2   | 1.92                     | 0.51              |
| 1:ZI:338:GLN:OE1  | 2:7:167:PRO:HG2   | 2.10                     | 0.51              |
| 1:ZJ:34:SER:HB3   | 1:ZJ:366:VAL:HG22 | 1.92                     | 0.51              |
| 1:ZV:184:VAL:HG13 | 1:ZV:196:MET:HB2  | 1.93                     | 0.51              |
| 1:ZZ:332:ASN:N    | 1:Ze:41:ASP:OD2   | 2.34                     | 0.51              |
| 2:ZC:34:PHE:HB3   | 2:ZC:222:SER:HB3  | 1.91                     | 0.51              |
| 2:y:129:VAL:HG12  | 2:y:135:GLN:HA    | 1.91                     | 0.51              |
| 1:ZH:384:SER:OG   | 2:ZC:26:LEU:HD22  | 2.09                     | 0.51              |
| 1:ZP:234:GLU:OE1  | 1:ZV:255:THR:N    | 2.42                     | 0.51              |
| 2:9:155:GLY:HA2   | 2:9:214:LEU:HD12  | 1.92                     | 0.51              |
| 2:ZB:25:ASN:HD21  | 2:ZB:37:GLN:H     | 1.56                     | 0.51              |
| 2:ZD:151:ILE:HG23 | 2:ZD:157:VAL:HG22 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZG:150:THR:OG1  | 1:ZG:282:ASN:ND2  | 2.38                     | 0.51              |
| 1:ZJ:331:ASP:HA   | 1:ZO:40:ALA:HB1   | 1.91                     | 0.51              |
| 1:ZS:307:GLU:N    | 1:ZS:307:GLU:OE2  | 2.43                     | 0.51              |
| 1:ZU:150:THR:HG23 | 1:ZU:151:THR:HG23 | 1.93                     | 0.51              |
| 1:ZV:2:SER:OG     | 1:ZV:392:GLN:OE1  | 2.21                     | 0.51              |
| 1:Zf:314:GLN:NE2  | 1:Zf:347:THR:OG1  | 2.44                     | 0.51              |
| 2:ZB:130:THR:HG22 | 2:ZB:131:ALA:H    | 1.75                     | 0.51              |
| 2:ZC:174:ASN:ND2  | 2:ZC:203:GLU:OE2  | 2.42                     | 0.51              |
| 2:x:79:ARG:HH22   | 2:x:184:LEU:HB2   | 1.74                     | 0.51              |
| 1:ZG:4:SER:CB     | 2:5:85:ASN:ND2    | 2.73                     | 0.51              |
| 1:ZI:39:PHE:HB2   | 2:ZD:31:THR:HG22  | 1.91                     | 0.51              |
| 1:ZI:75:VAL:O     | 1:ZI:98:GLY:HA3   | 2.10                     | 0.51              |
| 1:ZJ:57:ILE:HG13  | 1:ZO:47:LYS:HB2   | 1.93                     | 0.51              |
| 1:ZL:269:GLN:NE2  | 1:ZR:190:GLN:HA   | 2.25                     | 0.51              |
| 1:ZM:399:LEU:HD23 | 2:ZB:227:ALA:HA   | 1.91                     | 0.51              |
| 1:ZQ:379:GLN:HE21 | 1:ZV:394:GLN:HE22 | 1.58                     | 0.51              |
| 1:ZR:114:MET:HE1  | 1:ZR:333:VAL:HG11 | 1.93                     | 0.51              |
| 1:ZR:200:PHE:HE2  | 1:ZR:263:PHE:HE1  | 1.58                     | 0.51              |
| 1:ZU:33:LYS:NZ    | 1:ZU:362:GLU:OE1  | 2.41                     | 0.51              |
| 1:ZV:211:TYR:HE2  | 1:ZV:226:ALA:HA   | 1.75                     | 0.51              |
| 1:ZW:210:VAL:HB   | 1:ZW:228:THR:HG22 | 1.93                     | 0.51              |
| 1:Zg:144:MET:HE2  | 1:Zg:310:GLN:HE21 | 1.76                     | 0.51              |
| 2:0:120:PHE:HB3   | 2:0:128:LEU:HD22  | 1.92                     | 0.51              |
| 2:x:2:ILE:HG23    | 2:x:254:LEU:HD11  | 1.92                     | 0.51              |
| 2:x:89:THR:OG1    | 2:x:94:ASP:OD2    | 2.28                     | 0.51              |
| 1:ZH:391:THR:HG22 | 2:ZC:19:MET:CE    | 2.41                     | 0.51              |
| 1:ZI:374:ASN:O    | 1:ZI:375:MET:C    | 2.54                     | 0.51              |
| 1:ZJ:306:ASN:O    | 1:ZJ:307:GLU:HG2  | 2.10                     | 0.51              |
| 1:ZM:144:MET:HE3  | 1:ZM:306:ASN:HD21 | 1.76                     | 0.51              |
| 1:ZP:139:ILE:HA   | 1:ZP:312:LEU:HD13 | 1.91                     | 0.51              |
| 1:ZS:5:GLN:HG3    | 1:ZS:50:LEU:O     | 2.11                     | 0.51              |
| 1:ZS:93:PHE:HB3   | 1:ZS:333:VAL:HG13 | 1.93                     | 0.51              |
| 1:ZS:102:LEU:HD21 | 1:ZS:106:ARG:HD3  | 1.93                     | 0.51              |
| 2:0:150:THR:OG1   | 2:0:158:SER:OG    | 2.29                     | 0.51              |
| 2:v:98:LYS:HG3    | 2:v:215:TYR:HE2   | 1.76                     | 0.51              |
| 1:ZH:112:GLN:HG2  | 1:ZH:331:ASP:HB3  | 1.93                     | 0.51              |
| 1:ZK:27:SER:HA    | 1:ZK:366:VAL:HG21 | 1.93                     | 0.51              |
| 1:ZM:165:PRO:HG2  | 1:ZM:201:VAL:HG13 | 1.92                     | 0.51              |
| 1:ZO:199:TYR:O    | 1:ZO:210:VAL:HA   | 2.11                     | 0.51              |
| 1:ZT:196:MET:SD   | 1:ZT:248:THR:HG22 | 2.51                     | 0.51              |
| 1:ZV:95:SER:OG    | 1:ZV:333:VAL:HG23 | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Za:112:GLN:NE2  | 1:Za:331:ASP:O    | 2.44                     | 0.51              |
| 1:Zg:317:LEU:HD11 | 1:Zg:356:LEU:HD21 | 1.92                     | 0.51              |
| 1:Zh:284:TYR:HB2  | 1:Zh:306:ASN:HD22 | 1.76                     | 0.51              |
| 2:r:233:MET:HE1   | 2:w:246:ALA:HA    | 1.93                     | 0.51              |
| 2:z:21:VAL:HG21   | 2:z:39:ALA:HB2    | 1.91                     | 0.51              |
| 1:ZG:150:THR:HG1  | 1:ZG:282:ASN:HD21 | 1.59                     | 0.51              |
| 1:ZG:208:TRP:NE1  | 1:ZG:268:GLN:OE1  | 2.41                     | 0.51              |
| 1:ZQ:74:ASP:HB3   | 1:ZQ:361:LEU:HG   | 1.93                     | 0.51              |
| 1:Zb:95:SER:HB2   | 1:Zb:333:VAL:HG22 | 1.92                     | 0.51              |
| 1:Zh:77:ILE:HD13  | 1:Zh:96:ARG:HD2   | 1.92                     | 0.51              |
| 2:5:49:ILE:HG22   | 2:5:50:ARG:HG3    | 1.93                     | 0.51              |
| 2:5:248:SER:HB3   | 2:ZA:260:LEU:HD22 | 1.93                     | 0.51              |
| 2:6:115:THR:HB    | 2:6:191:LEU:HD23  | 1.93                     | 0.51              |
| 2:s:31:THR:HG23   | 2:x:42:GLU:HA     | 1.92                     | 0.51              |
| 2:u:178:PHE:CE1   | 2:u:201:PRO:HB3   | 2.46                     | 0.51              |
| 1:ZT:71:ARG:HB3   | 1:ZT:74:ASP:OD1   | 2.11                     | 0.51              |
| 1:ZZ:204:LYS:HG3  | 1:ZZ:205:ASP:H    | 1.76                     | 0.51              |
| 2:4:151:ILE:HG12  | 2:4:157:VAL:HG22  | 1.93                     | 0.51              |
| 2:4:255:GLN:HE21  | 2:4:259:GLN:NE2   | 2.09                     | 0.51              |
| 2:ZE:115:THR:HB   | 2:ZE:191:LEU:HD23 | 1.93                     | 0.51              |
| 2:v:19:MET:HG2    | 2:v:236:VAL:HG11  | 1.93                     | 0.51              |
| 1:ZH:390:LYS:HB2  | 1:ZM:402:LEU:HD22 | 1.92                     | 0.50              |
| 1:ZK:348:ALA:HB2  | 1:ZK:356:LEU:HD13 | 1.94                     | 0.50              |
| 1:ZL:42:MET:HG2   | 1:ZL:53:LYS:HD3   | 1.93                     | 0.50              |
| 1:ZN:44:ALA:CB    | 2:ZC:98:LYS:CE    | 2.89                     | 0.50              |
| 1:ZP:17:LEU:HD13  | 1:ZU:395:ILE:HD11 | 1.92                     | 0.50              |
| 1:ZQ:71:ARG:HG2   | 1:ZQ:73:LEU:H     | 1.76                     | 0.50              |
| 1:ZQ:156:ILE:HG22 | 1:ZQ:276:ILE:HG23 | 1.93                     | 0.50              |
| 1:ZT:165:PRO:HG2  | 1:ZT:201:VAL:HG13 | 1.92                     | 0.50              |
| 1:Za:41:ASP:N     | 1:Za:41:ASP:OD1   | 2.44                     | 0.50              |
| 1:Zh:392:GLN:HA   | 1:Zh:395:ILE:HG22 | 1.93                     | 0.50              |
| 2:7:164:GLN:HE22  | 2:7:166:ALA:HB3   | 1.76                     | 0.50              |
| 2:ZE:59:GLN:HG2   | 2:ZE:60:THR:HG23  | 1.92                     | 0.50              |
| 1:ZG:264:LEU:HD12 | 1:ZG:265:ASN:H    | 1.75                     | 0.50              |
| 1:ZJ:109:VAL:HG12 | 1:ZJ:115:GLN:HG3  | 1.93                     | 0.50              |
| 1:ZM:206:ASN:ND2  | 1:ZM:233:ASN:O    | 2.44                     | 0.50              |
| 1:ZS:139:ILE:HA   | 1:ZS:312:LEU:HD23 | 1.94                     | 0.50              |
| 1:Zb:154:MET:HE3  | 1:Zb:156:ILE:HB   | 1.93                     | 0.50              |
| 1:Zg:83:PHE:HB2   | 1:Zg:95:SER:O     | 2.11                     | 0.50              |
| 2:ZB:175:LEU:HD21 | 2:ZB:214:LEU:HD21 | 1.94                     | 0.50              |
| 2:u:189:GLU:O     | 2:u:191:LEU:HG    | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZF:379:GLN:HG3  | 1:ZK:391:THR:HG23 | 1.92                     | 0.50              |
| 1:ZG:65:THR:HG22  | 1:ZR:50:LEU:HD22  | 1.92                     | 0.50              |
| 1:ZG:104:GLU:HA   | 1:ZG:104:GLU:OE2  | 2.10                     | 0.50              |
| 1:ZH:52:VAL:HB    | 2:ZC:28:ASN:OD1   | 2.11                     | 0.50              |
| 1:ZK:103:ASP:OD1  | 1:ZK:107:ASN:N    | 2.40                     | 0.50              |
| 1:ZO:236:GLY:CA   | 1:ZO:268:GLN:H    | 2.21                     | 0.50              |
| 1:ZO:373:VAL:O    | 1:ZO:374:ASN:C    | 2.54                     | 0.50              |
| 1:ZV:159:ASN:ND2  | 1:ZV:162:ASP:OD2  | 2.38                     | 0.50              |
| 1:Za:109:VAL:HG12 | 1:Za:115:GLN:HA   | 1.92                     | 0.50              |
| 1:Za:171:SER:O    | 1:Za:177:SER:OG   | 2.28                     | 0.50              |
| 2:ZA:128:LEU:HD12 | 2:ZA:140:ILE:HB   | 1.92                     | 0.50              |
| 2:ZC:10:THR:HG23  | 2:ZC:71:GLY:HA3   | 1.94                     | 0.50              |
| 2:0:108:PRO:HG2   | 2:u:153:ARG:HH21  | 1.76                     | 0.50              |
| 2:1:248:SER:O     | 2:1:252:GLN:HG3   | 2.11                     | 0.50              |
| 2:y:205:THR:OG1   | 2:y:208:LEU:HB2   | 2.11                     | 0.50              |
| 1:ZF:324:GLU:HG3  | 2:ZA:121:GLN:OE1  | 2.10                     | 0.50              |
| 1:ZJ:43:PHE:CE1   | 2:ZE:37:GLN:NE2   | 2.80                     | 0.50              |
| 1:ZP:96:ARG:NH2   | 1:ZP:362:GLU:OE2  | 2.39                     | 0.50              |
| 1:Zd:349:GLY:HA3  | 1:Zd:355:LYS:HD3  | 1.92                     | 0.50              |
| 2:5:56:SER:H      | 2:5:61:THR:HA     | 1.77                     | 0.50              |
| 2:ZC:77:THR:O     | 2:ZC:77:THR:OG1   | 2.28                     | 0.50              |
| 2:0:19:MET:HB2    | 2:0:236:VAL:HG11  | 1.94                     | 0.50              |
| 1:ZG:146:ALA:HB2  | 1:ZG:286:PRO:HD3  | 1.92                     | 0.50              |
| 1:ZH:84:ARG:HD2   | 1:ZH:345:LEU:HD21 | 1.93                     | 0.50              |
| 1:ZH:352:ASN:HD22 | 2:ZC:145:ASN:HA   | 1.75                     | 0.50              |
| 1:ZM:271:THR:OG1  | 1:ZM:273:ALA:O    | 2.27                     | 0.50              |
| 1:ZM:399:LEU:CD2  | 2:ZB:227:ALA:HA   | 2.41                     | 0.50              |
| 1:ZQ:30:TYR:HD1   | 1:ZQ:363:ALA:HA   | 1.75                     | 0.50              |
| 1:ZQ:367:ASP:O    | 1:ZQ:371:GLU:HG2  | 2.10                     | 0.50              |
| 1:ZR:180:LYS:NZ   | 1:ZR:181:LYS:O    | 2.45                     | 0.50              |
| 1:ZS:271:THR:OG1  | 1:ZS:273:ALA:O    | 2.29                     | 0.50              |
| 1:Ze:362:GLU:OE1  | 1:Ze:362:GLU:N    | 2.38                     | 0.50              |
| 1:Zf:381:ASN:O    | 1:Zf:385:ASN:ND2  | 2.44                     | 0.50              |
| 2:4:240:TYR:HE2   | 2:9:257:LEU:HG    | 1.76                     | 0.50              |
| 2:6:35:LYS:NZ     | 2:6:220:GLU:OE2   | 2.39                     | 0.50              |
| 2:r:82:SER:OG     | 2:r:223:ASN:ND2   | 2.36                     | 0.50              |
| 2:s:79:ARG:NH2    | 2:s:186:SER:OG    | 2.44                     | 0.50              |
| 2:u:164:GLN:C     | 2:u:166:ALA:H     | 2.19                     | 0.50              |
| 1:ZH:144:MET:HE3  | 1:ZH:306:ASN:HD21 | 1.77                     | 0.50              |
| 1:ZJ:7:VAL:HG22   | 2:ZD:231:VAL:HG11 | 1.93                     | 0.50              |
| 1:ZK:109:VAL:HG12 | 1:ZK:115:GLN:HA   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZN:65:THR:HG21  | 1:ZY:4:SER:HB2    | 1.93                     | 0.50              |
| 1:ZO:102:LEU:HD21 | 1:ZO:106:ARG:HD2  | 1.93                     | 0.50              |
| 2:4:226:VAL:HG11  | 2:9:242:ILE:HD13  | 1.93                     | 0.50              |
| 2:5:173:LEU:HD23  | 2:5:214:LEU:HD13  | 1.93                     | 0.50              |
| 1:ZF:22:ASN:ND2   | 1:ZK:48:VAL:O     | 2.40                     | 0.50              |
| 1:ZF:322:ASN:OD1  | 2:ZA:122:VAL:O    | 2.30                     | 0.50              |
| 1:ZH:52:VAL:CB    | 2:ZC:28:ASN:OD1   | 2.58                     | 0.50              |
| 1:ZI:388:THR:CG2  | 2:ZD:233:MET:CE   | 2.89                     | 0.50              |
| 1:ZJ:237:ILE:H    | 1:ZJ:237:ILE:HD12 | 1.77                     | 0.50              |
| 1:ZP:6:ALA:HB1    | 1:ZP:389:ILE:HG13 | 1.94                     | 0.50              |
| 1:ZP:391:THR:O    | 1:ZP:395:ILE:HG23 | 2.12                     | 0.50              |
| 1:ZU:270:ASN:ND2  | 1:Za:286:PRO:HD2  | 2.27                     | 0.50              |
| 1:Zb:86:VAL:HG13  | 1:Zb:115:GLN:HB2  | 1.92                     | 0.50              |
| 1:Zb:114:MET:HE1  | 1:Zb:333:VAL:HG11 | 1.94                     | 0.50              |
| 1:Zb:373:VAL:O    | 1:Zb:377:VAL:HG23 | 2.12                     | 0.50              |
| 1:Zc:188:ASP:OD1  | 1:Zc:192:ASN:N    | 2.44                     | 0.50              |
| 1:Zd:317:LEU:HD11 | 1:Zd:356:LEU:HD21 | 1.93                     | 0.50              |
| 2:2:227:ALA:HA    | 2:ZD:257:LEU:HD21 | 1.93                     | 0.50              |
| 2:5:76:ALA:HB1    | 2:ZA:64:SER:O     | 2.12                     | 0.50              |
| 2:ZA:37:GLN:HG2   | 2:ZA:79:ARG:HD3   | 1.93                     | 0.50              |
| 2:ZD:40:VAL:HG23  | 2:ZD:75:VAL:HB    | 1.94                     | 0.50              |
| 1:ZJ:399:LEU:CD2  | 2:8:227:ALA:CB    | 2.90                     | 0.50              |
| 1:ZO:178:TYR:HA   | 1:ZO:201:VAL:HG12 | 1.92                     | 0.50              |
| 1:ZY:27:SER:O     | 1:ZY:364:SER:OG   | 2.30                     | 0.50              |
| 1:Zd:397:ASN:O    | 1:Zd:398:THR:C    | 2.53                     | 0.50              |
| 2:4:184:LEU:HB3   | 2:4:192:TYR:HB3   | 1.93                     | 0.50              |
| 2:ZB:5:LEU:O      | 2:ZB:9:LYS:HG3    | 2.11                     | 0.50              |
| 2:1:72:VAL:HB     | 2:w:28:ASN:ND2    | 2.26                     | 0.50              |
| 2:t:129:VAL:HG12  | 2:t:135:GLN:HA    | 1.93                     | 0.50              |
| 2:x:184:LEU:HB3   | 2:x:192:TYR:HB3   | 1.94                     | 0.50              |
| 2:y:19:MET:HB2    | 2:y:236:VAL:HG11  | 1.93                     | 0.50              |
| 1:ZG:300:VAL:HG13 | 1:ZG:312:LEU:HB2  | 1.93                     | 0.50              |
| 1:ZK:34:SER:HB3   | 1:ZK:366:VAL:HG12 | 1.94                     | 0.50              |
| 1:ZN:102:LEU:O    | 1:ZS:322:ASN:ND2  | 2.44                     | 0.50              |
| 1:ZV:314:GLN:NE2  | 1:ZV:347:THR:OG1  | 2.44                     | 0.50              |
| 1:ZX:208:TRP:NE1  | 1:ZX:268:GLN:OE1  | 2.36                     | 0.50              |
| 1:Zf:319:ASN:OD1  | 1:Zf:320:PHE:N    | 2.44                     | 0.50              |
| 2:4:123:ASP:OD1   | 2:4:127:GLN:N     | 2.45                     | 0.50              |
| 2:7:56:SER:O      | 2:r:153:ARG:N     | 2.39                     | 0.50              |
| 1:ZF:99:GLN:HG2   | 1:ZF:111:MET:HE2  | 1.93                     | 0.49              |
| 1:ZH:397:ASN:OD1  | 1:ZH:401:ASN:ND2  | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZO:80:ASN:OD1   | 1:ZO:81:GLY:N     | 2.45                     | 0.49              |
| 1:ZO:129:GLN:O    | 1:ZO:129:GLN:HG3  | 2.11                     | 0.49              |
| 1:Zh:391:THR:O    | 1:Zh:395:ILE:HG22 | 2.12                     | 0.49              |
| 2:5:7:ILE:HG23    | 2:5:71:GLY:HA2    | 1.92                     | 0.49              |
| 2:7:52:PRO:HB3    | 2:7:65:GLY:H      | 1.77                     | 0.49              |
| 2:7:151:ILE:HG12  | 2:7:157:VAL:HG22  | 1.94                     | 0.49              |
| 1:ZO:141:ASN:O    | 1:ZO:142:THR:C    | 2.56                     | 0.49              |
| 1:ZP:50:LEU:CD2   | 2:ZE:85:ASN:ND2   | 2.75                     | 0.49              |
| 1:ZS:116:LEU:HD21 | 1:ZS:315:ILE:HD13 | 1.94                     | 0.49              |
| 1:ZT:337:THR:OG1  | 1:ZT:338:GLN:N    | 2.44                     | 0.49              |
| 2:3:185:GLU:OE1   | 2:8:51:GLN:NE2    | 2.45                     | 0.49              |
| 2:6:46:TYR:HA     | 2:6:69:GLY:HA2    | 1.93                     | 0.49              |
| 2:y:2:ILE:HG13    | 2:y:254:LEU:HD21  | 1.93                     | 0.49              |
| 1:ZJ:171:SER:O    | 1:ZJ:177:SER:OG   | 2.28                     | 0.49              |
| 1:ZL:84:ARG:HH12  | 1:ZL:92:VAL:HG22  | 1.77                     | 0.49              |
| 1:ZN:139:ILE:HA   | 1:ZN:312:LEU:HD22 | 1.93                     | 0.49              |
| 1:ZP:181:LYS:HD3  | 1:Za:129:GLN:HE22 | 1.77                     | 0.49              |
| 1:ZQ:65:THR:HA    | 1:Zb:50:LEU:HD13  | 1.94                     | 0.49              |
| 1:Zb:179:ASN:OD1  | 1:Zb:202:LYS:N    | 2.35                     | 0.49              |
| 1:Zf:126:PRO:HB2  | 1:Zf:311:VAL:HG12 | 1.94                     | 0.49              |
| 2:2:70:THR:HG22   | 2:2:71:GLY:H      | 1.77                     | 0.49              |
| 2:6:180:ASN:ND2   | 2:1:122:VAL:O     | 2.35                     | 0.49              |
| 2:s:241:GLU:OE1   | 2:y:258:THR:OG1   | 2.26                     | 0.49              |
| 1:ZH:2:SER:HB2    | 2:ZC:20:ASP:OD1   | 2.12                     | 0.49              |
| 1:ZJ:395:ILE:CG2  | 2:ZE:240:TYR:CD2  | 2.80                     | 0.49              |
| 1:ZK:89:ASN:ND2   | 2:ZE:207:GLY:O    | 2.46                     | 0.49              |
| 1:ZK:175:ALA:HA   | 1:ZK:178:TYR:CZ   | 2.47                     | 0.49              |
| 1:ZL:30:TYR:HD1   | 1:ZL:363:ALA:HA   | 1.77                     | 0.49              |
| 1:ZS:322:ASN:OD1  | 1:ZS:325:GLY:N    | 2.45                     | 0.49              |
| 1:ZT:396:LEU:O    | 1:ZT:400:VAL:HG23 | 2.12                     | 0.49              |
| 1:ZV:387:GLN:CD   | 1:Zb:400:VAL:HG13 | 2.38                     | 0.49              |
| 1:Zg:159:ASN:ND2  | 1:Zg:161:THR:OG1  | 2.44                     | 0.49              |
| 2:2:66:LEU:HD12   | 2:x:77:THR:HG23   | 1.94                     | 0.49              |
| 2:6:230:LEU:HA    | 2:6:233:MET:HG3   | 1.95                     | 0.49              |
| 2:ZB:151:ILE:HG23 | 2:ZB:157:VAL:HG22 | 1.93                     | 0.49              |
| 1:ZG:160:SER:HA   | 1:ZG:268:GLN:HE21 | 1.76                     | 0.49              |
| 1:ZM:390:LYS:HB2  | 1:ZR:402:LEU:HD22 | 1.94                     | 0.49              |
| 1:ZU:141:ASN:HA   | 1:ZU:289:LEU:HD13 | 1.94                     | 0.49              |
| 1:ZV:147:LYS:NZ   | 1:ZV:148:SER:O    | 2.43                     | 0.49              |
| 1:Zb:96:ARG:HG3   | 1:Zb:334:TRP:HZ3  | 1.76                     | 0.49              |
| 1:Zb:322:ASN:OD1  | 1:Zb:325:GLY:N    | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zc:139:ILE:HA   | 1:Zc:312:LEU:HD22 | 1.93                     | 0.49              |
| 1:Zc:317:LEU:HD21 | 1:Zc:356:LEU:HD21 | 1.95                     | 0.49              |
| 1:Zh:2:SER:C      | 1:Zh:392:GLN:HE22 | 2.21                     | 0.49              |
| 2:0:51:GLN:NE2    | 2:0:65:GLY:HA3    | 2.27                     | 0.49              |
| 2:u:129:VAL:HG12  | 2:u:135:GLN:HA    | 1.94                     | 0.49              |
| 1:ZF:47:LYS:CD    | 2:ZA:77:THR:H     | 2.22                     | 0.49              |
| 1:ZH:175:ALA:HA   | 1:ZH:178:TYR:CZ   | 2.47                     | 0.49              |
| 1:ZM:269:GLN:OE1  | 1:ZS:146:ALA:N    | 2.45                     | 0.49              |
| 1:ZT:17:LEU:HD13  | 1:ZY:395:ILE:HD11 | 1.95                     | 0.49              |
| 1:ZT:210:VAL:HB   | 1:ZT:228:THR:HG22 | 1.93                     | 0.49              |
| 1:ZU:65:THR:HA    | 1:Zf:50:LEU:HD13  | 1.94                     | 0.49              |
| 1:ZU:182:GLY:HA2  | 1:Zf:131:GLY:HA3  | 1.93                     | 0.49              |
| 1:ZW:102:LEU:O    | 1:Zb:322:ASN:ND2  | 2.46                     | 0.49              |
| 1:Za:348:ALA:HB1  | 1:Za:355:LYS:HA   | 1.94                     | 0.49              |
| 1:Zh:386:ALA:O    | 1:Zh:389:ILE:HG22 | 2.13                     | 0.49              |
| 2:9:252:GLN:O     | 2:9:256:LYS:HG2   | 2.12                     | 0.49              |
| 2:ZE:49:ILE:HB    | 2:ZE:66:LEU:HB3   | 1.93                     | 0.49              |
| 2:r:185:GLU:HB3   | 2:r:193:ILE:HG23  | 1.95                     | 0.49              |
| 1:ZH:3:PHE:HB3    | 2:ZB:235:GLN:HE22 | 1.77                     | 0.49              |
| 1:ZI:46:SER:CB    | 2:ZD:185:GLU:CD   | 2.66                     | 0.49              |
| 1:ZN:156:ILE:HD12 | 1:ZN:276:ILE:HG13 | 1.93                     | 0.49              |
| 1:ZY:21:GLY:HA2   | 1:ZY:24:ILE:HG22  | 1.94                     | 0.49              |
| 1:Za:68:ASN:OD1   | 1:Za:68:ASN:N     | 2.44                     | 0.49              |
| 1:Zd:389:ILE:O    | 1:Zd:390:LYS:C    | 2.55                     | 0.49              |
| 2:4:76:ALA:HB1    | 2:9:64:SER:O      | 2.13                     | 0.49              |
| 2:ZB:163:GLY:O    | 2:ZB:165:ALA:N    | 2.46                     | 0.49              |
| 2:ZB:172:GLN:HE22 | 2:ZB:205:THR:HG23 | 1.78                     | 0.49              |
| 2:0:80:LEU:HD13   | 2:v:91:ASN:HB2    | 1.94                     | 0.49              |
| 2:u:36:ARG:NH2    | 2:u:229:GLU:OE2   | 2.45                     | 0.49              |
| 1:ZH:351:GLY:O    | 2:ZC:162:GLN:OE1  | 2.30                     | 0.49              |
| 1:ZJ:397:ASN:ND2  | 2:ZD:238:ARG:HH12 | 2.11                     | 0.49              |
| 1:ZK:228:THR:HB   | 1:ZK:244:VAL:HG11 | 1.95                     | 0.49              |
| 1:ZM:399:LEU:HD21 | 2:ZB:227:ALA:HB1  | 1.95                     | 0.49              |
| 1:ZT:188:ASP:HA   | 1:ZT:257:ALA:HB2  | 1.93                     | 0.49              |
| 1:ZX:195:ASP:OD2  | 1:ZX:216:SER:OG   | 2.31                     | 0.49              |
| 1:ZZ:373:VAL:HG11 | 1:Zf:7:VAL:HG22   | 1.95                     | 0.49              |
| 1:Zg:196:MET:HE3  | 1:Zg:248:THR:HG22 | 1.95                     | 0.49              |
| 2:9:175:LEU:HD13  | 2:9:206:PRO:HG3   | 1.93                     | 0.49              |
| 2:ZB:50:ARG:HB2   | 2:ZB:66:LEU:H     | 1.76                     | 0.49              |
| 2:0:231:VAL:O     | 2:0:235:GLN:HG3   | 2.12                     | 0.49              |
| 2:r:238:ARG:NH2   | 2:x:251:ASP:OD1   | 2.40                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:t:126:GLY:HA2   | 2:y:179:MET:HE3   | 1.95                     | 0.49              |
| 2:y:82:SER:HB2    | 2:y:223:ASN:HD21  | 1.78                     | 0.49              |
| 1:ZG:395:ILE:HG21 | 2:ZB:240:TYR:CE2  | 2.31                     | 0.49              |
| 1:ZH:39:PHE:HB2   | 2:ZC:31:THR:HG22  | 1.93                     | 0.49              |
| 1:ZR:199:TYR:HB2  | 1:ZR:211:TYR:HB2  | 1.95                     | 0.49              |
| 1:ZT:69:THR:HG21  | 1:ZT:361:LEU:HD12 | 1.93                     | 0.49              |
| 1:ZT:243:THR:HG22 | 1:ZT:262:SER:HB2  | 1.94                     | 0.49              |
| 1:ZT:380:ARG:HD2  | 1:ZZ:396:LEU:HB3  | 1.94                     | 0.49              |
| 1:Zb:144:MET:SD   | 1:Zb:306:ASN:ND2  | 2.85                     | 0.49              |
| 2:3:151:ILE:HG12  | 2:3:157:VAL:HG22  | 1.93                     | 0.49              |
| 2:ZB:29:VAL:O     | 2:ZB:222:SER:OG   | 2.31                     | 0.49              |
| 2:r:238:ARG:HG3   | 2:x:254:LEU:HD13  | 1.95                     | 0.49              |
| 2:x:198:SER:O     | 2:x:198:SER:OG    | 2.27                     | 0.49              |
| 1:ZH:24:ILE:O     | 1:ZH:27:SER:OG    | 2.25                     | 0.49              |
| 1:ZN:233:ASN:HD21 | 1:ZN:237:ILE:HB   | 1.77                     | 0.49              |
| 1:ZP:159:ASN:OD1  | 1:ZP:161:THR:N    | 2.46                     | 0.49              |
| 1:ZT:95:SER:OG    | 1:ZT:332:ASN:O    | 2.23                     | 0.49              |
| 1:ZU:293:GLN:HE21 | 1:ZU:303:ASN:HD21 | 1.61                     | 0.49              |
| 1:ZW:104:GLU:HG2  | 1:ZW:105:ASN:OD1  | 2.13                     | 0.49              |
| 1:ZX:41:ASP:OD1   | 1:ZX:41:ASP:N     | 2.42                     | 0.49              |
| 1:Zc:107:ASN:ND2  | 1:Zc:138:THR:OG1  | 2.46                     | 0.49              |
| 2:4:35:LYS:HE3    | 2:4:81:HIS:HA     | 1.95                     | 0.49              |
| 2:6:10:THR:OG1    | 2:6:71:GLY:HA3    | 2.12                     | 0.49              |
| 2:1:142:ILE:HD11  | 2:1:149:ILE:HD12  | 1.93                     | 0.49              |
| 1:ZG:27:SER:O     | 1:ZG:364:SER:OG   | 2.30                     | 0.48              |
| 1:ZH:3:PHE:CB     | 2:ZB:235:GLN:HE22 | 2.25                     | 0.48              |
| 1:ZH:210:VAL:O    | 1:ZH:227:SER:N    | 2.45                     | 0.48              |
| 1:ZP:83:PHE:HB2   | 1:ZP:95:SER:O     | 2.13                     | 0.48              |
| 1:ZS:103:ASP:OD2  | 1:ZS:105:ASN:N    | 2.44                     | 0.48              |
| 1:ZU:285:LYS:O    | 1:ZU:306:ASN:ND2  | 2.42                     | 0.48              |
| 1:ZV:5:GLN:HB2    | 1:ZV:50:LEU:O     | 2.13                     | 0.48              |
| 1:Ze:178:TYR:HA   | 1:Ze:201:VAL:HG22 | 1.94                     | 0.48              |
| 2:6:122:VAL:O     | 2:ZB:180:ASN:ND2  | 2.46                     | 0.48              |
| 2:8:34:PHE:HB3    | 2:8:222:SER:HB3   | 1.94                     | 0.48              |
| 2:ZD:184:LEU:HB3  | 2:ZD:192:TYR:HB3  | 1.95                     | 0.48              |
| 2:v:123:ASP:OD2   | 2:v:127:GLN:HB2   | 2.13                     | 0.48              |
| 1:ZI:198:VAL:HG22 | 1:ZI:212:THR:HG22 | 1.95                     | 0.48              |
| 1:ZK:204:LYS:HZ2  | 1:ZK:207:GLU:HG3  | 1.78                     | 0.48              |
| 1:ZM:203:THR:OG1  | 1:ZM:207:GLU:OE1  | 2.23                     | 0.48              |
| 1:ZS:188:ASP:HA   | 1:ZS:257:ALA:HB2  | 1.96                     | 0.48              |
| 1:ZX:83:PHE:HB2   | 1:ZX:95:SER:O     | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zc:188:ASP:HA   | 1:Zc:257:ALA:HB2  | 1.95                     | 0.48              |
| 1:Zd:154:MET:HB2  | 1:Zd:279:THR:HG22 | 1.95                     | 0.48              |
| 2:3:155:GLY:HA2   | 2:3:214:LEU:HD12  | 1.94                     | 0.48              |
| 2:5:5:LEU:HD23    | 2:z:235:GLN:HG3   | 1.95                     | 0.48              |
| 2:8:185:GLU:HG3   | 2:ZD:67:GLN:NE2   | 2.28                     | 0.48              |
| 2:9:184:LEU:HB3   | 2:9:192:TYR:HB3   | 1.95                     | 0.48              |
| 2:ZD:105:VAL:HA   | 2:ZD:136:VAL:HA   | 1.95                     | 0.48              |
| 2:0:185:GLU:HB3   | 2:0:193:ILE:HG13  | 1.94                     | 0.48              |
| 2:r:190:ASN:ND2   | 2:w:42:GLU:HG3    | 2.29                     | 0.48              |
| 1:ZH:319:ASN:HB2  | 1:ZH:353:PHE:CE1  | 2.47                     | 0.48              |
| 1:ZW:18:ASP:HB3   | 1:Zb:5:GLN:HE22   | 1.77                     | 0.48              |
| 1:ZW:144:MET:SD   | 1:ZW:310:GLN:NE2  | 2.86                     | 0.48              |
| 1:ZY:102:LEU:HD11 | 1:ZY:139:ILE:HD12 | 1.95                     | 0.48              |
| 1:Zb:24:ILE:O     | 1:Zb:27:SER:OG    | 2.31                     | 0.48              |
| 1:Zb:85:LEU:HD13  | 1:Zb:114:MET:HB3  | 1.94                     | 0.48              |
| 1:Zb:293:GLN:NE2  | 1:Zb:303:ASN:OD1  | 2.45                     | 0.48              |
| 1:Zb:331:ASP:HA   | 1:Zg:40:ALA:HB1   | 1.95                     | 0.48              |
| 2:4:44:LEU:HB3    | 2:4:70:THR:HB     | 1.95                     | 0.48              |
| 2:7:34:PHE:HB3    | 2:7:222:SER:HB3   | 1.95                     | 0.48              |
| 1:ZI:93:PHE:HB3   | 1:ZI:333:VAL:HG13 | 1.95                     | 0.48              |
| 1:ZM:17:LEU:HD13  | 1:ZR:395:ILE:HD11 | 1.94                     | 0.48              |
| 1:ZR:180:LYS:HB3  | 1:ZR:200:PHE:HD1  | 1.79                     | 0.48              |
| 1:ZY:319:ASN:ND2  | 1:ZY:352:ASN:O    | 2.46                     | 0.48              |
| 1:ZZ:180:LYS:HB3  | 1:ZZ:200:PHE:HB2  | 1.96                     | 0.48              |
| 2:6:20:ASP:OD1    | 2:ZB:3:SER:HB3    | 2.14                     | 0.48              |
| 2:y:35:LYS:NZ     | 2:y:220:GLU:OE2   | 2.44                     | 0.48              |
| 1:ZG:99:GLN:HG3   | 1:ZG:361:LEU:HD11 | 1.95                     | 0.48              |
| 1:ZG:399:LEU:HD11 | 2:ZB:240:TYR:CE2  | 2.49                     | 0.48              |
| 1:ZG:402:LEU:HD22 | 2:ZB:248:SER:HB3  | 1.94                     | 0.48              |
| 1:ZL:316:VAL:HG22 | 1:ZL:345:LEU:HD12 | 1.96                     | 0.48              |
| 1:ZP:122:THR:OG1  | 1:ZP:129:GLN:NE2  | 2.46                     | 0.48              |
| 1:ZR:186:VAL:HG22 | 1:ZR:194:HIS:HB2  | 1.95                     | 0.48              |
| 1:ZV:367:ASP:HB3  | 1:ZV:370:LYS:HD2  | 1.95                     | 0.48              |
| 1:ZY:373:VAL:HG11 | 1:Ze:7:VAL:HG22   | 1.94                     | 0.48              |
| 1:ZZ:331:ASP:HA   | 1:Ze:40:ALA:HB1   | 1.96                     | 0.48              |
| 1:Zb:68:ASN:OD1   | 1:Zb:68:ASN:N     | 2.47                     | 0.48              |
| 2:5:129:VAL:HG12  | 2:5:135:GLN:HA    | 1.96                     | 0.48              |
| 2:5:238:ARG:NH1   | 2:5:241:GLU:OE2   | 2.45                     | 0.48              |
| 2:8:42:GLU:CB     | 2:8:75:VAL:HG23   | 2.41                     | 0.48              |
| 2:ZA:95:VAL:HG11  | 2:ZA:214:LEU:HD23 | 1.95                     | 0.48              |
| 1:ZG:390:LYS:HB2  | 1:ZL:402:LEU:HD22 | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZH:18:ASP:HB3   | 1:ZM:5:GLN:HE22   | 1.78                     | 0.48              |
| 1:ZH:355:LYS:N    | 1:ZH:355:LYS:HD3  | 2.29                     | 0.48              |
| 1:ZK:248:THR:HG1  | 1:ZK:257:ALA:N    | 2.10                     | 0.48              |
| 1:ZL:165:PRO:HG2  | 1:ZL:201:VAL:HG13 | 1.94                     | 0.48              |
| 1:ZS:201:VAL:HG22 | 1:ZS:209:ALA:HB3  | 1.96                     | 0.48              |
| 1:ZT:228:THR:HB   | 1:ZT:244:VAL:HG11 | 1.94                     | 0.48              |
| 1:ZZ:93:PHE:HB3   | 1:ZZ:333:VAL:HG13 | 1.94                     | 0.48              |
| 1:Zb:170:PHE:HE2  | 1:Zb:223:PRO:HG2  | 1.79                     | 0.48              |
| 1:Zb:299:THR:HG22 | 1:Zb:314:GLN:HG3  | 1.95                     | 0.48              |
| 1:Zf:297:ASP:OD1  | 1:Zf:297:ASP:N    | 2.36                     | 0.48              |
| 1:Zg:95:SER:OG    | 1:Zg:332:ASN:O    | 2.19                     | 0.48              |
| 2:9:123:ASP:OD2   | 2:9:125:ASN:ND2   | 2.47                     | 0.48              |
| 2:ZE:36:ARG:HB3   | 2:ZE:224:VAL:HG22 | 1.95                     | 0.48              |
| 2:ZE:140:ILE:HG23 | 2:ZE:171:GLY:HA3  | 1.96                     | 0.48              |
| 2:z:2:ILE:HG21    | 2:z:254:LEU:HD11  | 1.96                     | 0.48              |
| 1:ZG:52:VAL:HG23  | 2:ZB:28:ASN:ND2   | 2.28                     | 0.48              |
| 1:ZG:159:ASN:ND2  | 1:ZG:272:GLY:O    | 2.45                     | 0.48              |
| 1:ZP:156:ILE:HD12 | 1:ZP:276:ILE:HG12 | 1.96                     | 0.48              |
| 1:ZT:233:ASN:HD21 | 1:ZT:237:ILE:HB   | 1.77                     | 0.48              |
| 1:ZT:269:GLN:HB3  | 1:ZZ:286:PRO:HG2  | 1.95                     | 0.48              |
| 1:Ze:196:MET:SD   | 1:Ze:212:THR:HB   | 2.54                     | 0.48              |
| 1:Zf:294:ILE:HG12 | 1:Zf:300:VAL:HG22 | 1.96                     | 0.48              |
| 1:Zg:3:PHE:O      | 1:Zg:7:VAL:HG22   | 2.13                     | 0.48              |
| 2:3:50:ARG:HH21   | 2:y:73:ARG:NH2    | 2.12                     | 0.48              |
| 2:4:22:ILE:HD11   | 2:4:232:ASN:HB3   | 1.95                     | 0.48              |
| 2:5:205:THR:HB    | 2:5:208:LEU:HD23  | 1.94                     | 0.48              |
| 2:5:215:TYR:HB3   | 2:5:218:TYR:HD2   | 1.78                     | 0.48              |
| 1:ZM:331:ASP:HA   | 1:ZR:40:ALA:HB1   | 1.95                     | 0.48              |
| 1:ZQ:22:ASN:N     | 1:ZV:5:GLN:HE21   | 2.11                     | 0.48              |
| 1:ZU:195:ASP:OD2  | 1:ZU:195:ASP:N    | 2.40                     | 0.48              |
| 1:Zb:288:ASP:O    | 1:Zb:305:SER:N    | 2.45                     | 0.48              |
| 1:Zg:146:ALA:HB2  | 1:Zg:286:PRO:HD3  | 1.95                     | 0.48              |
| 2:2:121:GLN:NE2   | 2:7:78:GLU:OE1    | 2.38                     | 0.48              |
| 2:5:44:LEU:HB3    | 2:5:70:THR:HB     | 1.95                     | 0.48              |
| 2:8:19:MET:HB2    | 2:8:236:VAL:HG11  | 1.96                     | 0.48              |
| 2:ZA:95:VAL:O     | 2:ZA:118:GLY:HA3  | 2.13                     | 0.48              |
| 2:0:33:GLY:N      | 2:0:220:GLU:O     | 2.47                     | 0.48              |
| 2:0:195:THR:HG22  | 2:0:196:GLN:H     | 1.79                     | 0.48              |
| 2:x:19:MET:HB2    | 2:x:236:VAL:HG11  | 1.96                     | 0.48              |
| 1:ZF:47:LYS:HE3   | 1:ZF:47:LYS:HB3   | 1.67                     | 0.48              |
| 1:ZH:298:GLY:HA2  | 1:ZH:356:LEU:HD12 | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZI:17:LEU:HD13  | 1:ZN:395:ILE:HD11 | 1.95                     | 0.48              |
| 1:ZI:147:LYS:HE2  | 1:ZI:282:ASN:HD22 | 1.79                     | 0.48              |
| 1:ZO:5:GLN:HG2    | 1:ZO:50:LEU:O     | 2.14                     | 0.48              |
| 1:ZQ:317:LEU:HD11 | 1:ZQ:356:LEU:HD21 | 1.96                     | 0.48              |
| 1:ZR:390:LYS:O    | 1:ZR:394:GLN:HG2  | 2.14                     | 0.48              |
| 1:ZU:69:THR:HG22  | 1:ZU:71:ARG:H     | 1.79                     | 0.48              |
| 1:ZU:181:LYS:HZ3  | 1:ZU:197:ASN:HB3  | 1.79                     | 0.48              |
| 1:ZW:186:VAL:HG23 | 1:ZW:194:HIS:HB2  | 1.95                     | 0.48              |
| 1:ZW:294:ILE:HG12 | 1:ZW:300:VAL:HG22 | 1.96                     | 0.48              |
| 1:Zd:20:ILE:O     | 1:Zd:24:ILE:HG13  | 2.14                     | 0.48              |
| 1:Ze:33:LYS:HG3   | 1:Ze:61:PHE:CD2   | 2.49                     | 0.48              |
| 1:Zf:2:SER:OG     | 1:Zf:3:PHE:N      | 2.46                     | 0.48              |
| 2:4:97:ILE:HD11   | 2:4:103:PHE:CE2   | 2.49                     | 0.48              |
| 2:6:47:GLN:N      | 2:6:68:ILE:O      | 2.45                     | 0.48              |
| 2:6:64:SER:O      | 2:6:64:SER:OG     | 2.23                     | 0.48              |
| 2:ZE:34:PHE:HB3   | 2:ZE:222:SER:HB3  | 1.95                     | 0.48              |
| 1:ZH:78:SER:OG    | 1:ZH:355:LYS:N    | 2.35                     | 0.48              |
| 1:ZI:402:LEU:HD22 | 2:ZD:248:SER:HB2  | 1.95                     | 0.48              |
| 1:ZW:159:ASN:ND2  | 1:ZW:162:ASP:OD1  | 2.45                     | 0.48              |
| 1:ZZ:367:ASP:HB2  | 1:ZZ:370:LYS:HG3  | 1.94                     | 0.48              |
| 2:2:76:ALA:HB1    | 2:7:64:SER:O      | 2.14                     | 0.48              |
| 2:6:210:GLY:O     | 2:6:211:ALA:C     | 2.53                     | 0.48              |
| 2:9:130:THR:HG22  | 2:9:132:GLY:H     | 1.79                     | 0.48              |
| 2:s:115:THR:HB    | 2:s:191:LEU:HD23  | 1.96                     | 0.48              |
| 2:t:190:ASN:ND2   | 2:y:42:GLU:HG3    | 2.29                     | 0.48              |
| 1:ZO:14:ALA:HB2   | 1:ZO:382:TYR:HE2  | 1.78                     | 0.47              |
| 1:ZO:33:LYS:HD2   | 1:ZO:61:PHE:HA    | 1.95                     | 0.47              |
| 1:ZR:126:PRO:HG2  | 1:ZR:310:GLN:HE21 | 1.78                     | 0.47              |
| 1:ZR:261:LEU:HD21 | 1:ZR:263:PHE:HE2  | 1.78                     | 0.47              |
| 1:ZS:170:PHE:HE2  | 1:ZS:223:PRO:HG2  | 1.79                     | 0.47              |
| 1:ZW:211:TYR:CD1  | 1:ZW:226:ALA:HA   | 2.49                     | 0.47              |
| 1:ZW:317:LEU:HD11 | 1:ZW:356:LEU:HD21 | 1.96                     | 0.47              |
| 1:Zb:154:MET:HE1  | 1:Zb:276:ILE:HG12 | 1.96                     | 0.47              |
| 2:3:230:LEU:HA    | 2:3:233:MET:HE2   | 1.95                     | 0.47              |
| 2:3:240:TYR:CE1   | 2:8:257:LEU:HD13  | 2.49                     | 0.47              |
| 2:6:153:ARG:HH22  | 2:6:213:LEU:HD13  | 1.78                     | 0.47              |
| 2:ZB:95:VAL:O     | 2:ZB:118:GLY:HA3  | 2.14                     | 0.47              |
| 2:ZC:230:LEU:O    | 2:ZC:234:ILE:HG12 | 2.14                     | 0.47              |
| 2:u:185:GLU:HG3   | 2:z:67:GLN:NE2    | 2.22                     | 0.47              |
| 1:ZG:318:ALA:HB2  | 1:ZG:345:LEU:HD23 | 1.96                     | 0.47              |
| 1:ZH:33:LYS:HA    | 1:ZH:365:ASN:HD21 | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZJ:110:ASN:ND2  | 1:ZJ:112:GLN:OE1  | 2.47                     | 0.47              |
| 1:ZJ:380:ARG:HD3  | 1:ZJ:380:ARG:HA   | 1.71                     | 0.47              |
| 1:ZM:235:ASN:ND2  | 1:ZS:189:SER:OG   | 2.47                     | 0.47              |
| 1:ZS:380:ARG:HH21 | 1:ZY:397:ASN:HD21 | 1.61                     | 0.47              |
| 1:ZT:184:VAL:HG13 | 1:ZT:196:MET:HB2  | 1.96                     | 0.47              |
| 1:Zf:59:GLN:HB3   | 1:Zf:61:PHE:CE1   | 2.49                     | 0.47              |
| 2:ZD:50:ARG:HB2   | 2:ZD:66:LEU:H     | 1.78                     | 0.47              |
| 2:0:42:GLU:HB3    | 2:0:75:VAL:HG21   | 1.96                     | 0.47              |
| 2:0:73:ARG:HH11   | 2:0:73:ARG:HB2    | 1.78                     | 0.47              |
| 2:1:66:LEU:HD12   | 2:w:77:THR:HG23   | 1.95                     | 0.47              |
| 1:ZH:114:MET:HE1  | 1:ZH:333:VAL:HG11 | 1.97                     | 0.47              |
| 1:ZX:17:LEU:HD13  | 1:Zc:395:ILE:CD1  | 2.44                     | 0.47              |
| 1:Zd:116:LEU:HD12 | 1:Zd:117:THR:N    | 2.29                     | 0.47              |
| 2:4:241:GLU:OE1   | 2:ZA:258:THR:HB   | 2.15                     | 0.47              |
| 2:5:22:ILE:HG21   | 2:5:233:MET:HG3   | 1.96                     | 0.47              |
| 2:x:142:ILE:HD13  | 2:x:149:ILE:HD13  | 1.96                     | 0.47              |
| 1:ZG:52:VAL:HB    | 2:ZB:28:ASN:ND2   | 2.29                     | 0.47              |
| 1:ZI:83:PHE:HB2   | 1:ZI:95:SER:O     | 2.14                     | 0.47              |
| 1:ZL:373:VAL:O    | 1:ZL:375:MET:N    | 2.47                     | 0.47              |
| 1:ZN:44:ALA:HB1   | 2:ZC:98:LYS:HE2   | 1.95                     | 0.47              |
| 1:ZN:331:ASP:HA   | 1:ZS:40:ALA:HB1   | 1.96                     | 0.47              |
| 1:ZP:14:ALA:HB2   | 1:ZP:382:TYR:HE2  | 1.79                     | 0.47              |
| 1:ZP:314:GLN:NE2  | 1:ZP:347:THR:OG1  | 2.47                     | 0.47              |
| 1:ZU:99:GLN:NE2   | 1:ZZ:38:SER:OG    | 2.46                     | 0.47              |
| 1:Za:16:ASN:O     | 1:Za:20:ILE:HG12  | 2.14                     | 0.47              |
| 1:Zc:83:PHE:HB2   | 1:Zc:95:SER:O     | 2.13                     | 0.47              |
| 1:Zg:87:ASP:OD1   | 1:Zg:91:SER:N     | 2.46                     | 0.47              |
| 2:3:22:ILE:HD11   | 2:3:232:ASN:HB3   | 1.95                     | 0.47              |
| 2:5:34:PHE:HB3    | 2:5:222:SER:HB3   | 1.95                     | 0.47              |
| 2:5:100:GLN:HG3   | 2:5:100:GLN:O     | 2.14                     | 0.47              |
| 2:8:95:VAL:O      | 2:8:118:GLY:HA3   | 2.14                     | 0.47              |
| 2:8:238:ARG:NH1   | 2:8:241:GLU:OE1   | 2.47                     | 0.47              |
| 2:ZD:97:ILE:HD11  | 2:ZD:103:PHE:CE2  | 2.49                     | 0.47              |
| 2:1:18:ASN:O      | 2:1:22:ILE:HG13   | 2.15                     | 0.47              |
| 2:t:98:LYS:HD3    | 2:t:213:LEU:HD12  | 1.95                     | 0.47              |
| 2:u:18:ASN:HB2    | 2:u:41:PHE:HZ     | 1.79                     | 0.47              |
| 2:x:3:SER:C       | 2:x:5:LEU:N       | 2.72                     | 0.47              |
| 1:ZF:162:ASP:OD2  | 1:ZF:274:ASN:ND2  | 2.30                     | 0.47              |
| 1:ZI:47:LYS:HE3   | 2:ZD:76:ALA:CA    | 2.43                     | 0.47              |
| 1:ZM:93:PHE:HB3   | 1:ZM:333:VAL:HG13 | 1.95                     | 0.47              |
| 1:ZQ:228:THR:HG21 | 1:ZQ:244:VAL:HG11 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZS:6:ALA:O      | 1:ZS:9:GLY:N      | 2.48                     | 0.47              |
| 1:ZT:144:MET:HG3  | 1:ZT:310:GLN:NE2  | 2.29                     | 0.47              |
| 1:Zb:309:GLU:OE1  | 1:Zb:309:GLU:N    | 2.41                     | 0.47              |
| 2:3:215:TYR:HE2   | 2:ZE:45:LEU:HD21  | 1.80                     | 0.47              |
| 2:5:1:MET:HE2     | 2:u:226:VAL:HG21  | 1.96                     | 0.47              |
| 2:6:56:SER:O      | 2:6:57:SER:C      | 2.57                     | 0.47              |
| 2:r:43:ASP:OD1    | 2:r:43:ASP:N      | 2.45                     | 0.47              |
| 1:ZF:210:VAL:O    | 1:ZF:227:SER:N    | 2.48                     | 0.47              |
| 1:ZO:140:PRO:HD2  | 1:ZO:312:LEU:HD23 | 1.95                     | 0.47              |
| 1:ZP:27:SER:O     | 1:ZP:364:SER:OG   | 2.32                     | 0.47              |
| 1:ZW:171:SER:HB3  | 1:ZW:174:ASP:HB2  | 1.96                     | 0.47              |
| 1:ZX:6:ALA:HB1    | 1:ZX:389:ILE:HG12 | 1.95                     | 0.47              |
| 1:Zc:6:ALA:HB1    | 1:Zc:389:ILE:HG13 | 1.96                     | 0.47              |
| 1:Zc:80:ASN:OD1   | 1:Zc:81:GLY:N     | 2.46                     | 0.47              |
| 1:Ze:58:THR:OG1   | 1:Ze:59:GLN:N     | 2.47                     | 0.47              |
| 2:6:158:SER:HB3   | 2:6:167:PRO:HB2   | 1.96                     | 0.47              |
| 2:9:50:ARG:HD3    | 2:9:66:LEU:HD12   | 1.96                     | 0.47              |
| 2:v:208:LEU:O     | 2:v:209:ASN:HB3   | 2.15                     | 0.47              |
| 2:y:115:THR:HB    | 2:y:191:LEU:HD23  | 1.97                     | 0.47              |
| 1:ZF:52:VAL:CB    | 2:ZA:28:ASN:OD1   | 2.61                     | 0.47              |
| 1:ZG:358:ASN:OD1  | 1:ZG:359:GLY:N    | 2.47                     | 0.47              |
| 1:ZH:233:ASN:OD1  | 1:ZH:234:GLU:N    | 2.47                     | 0.47              |
| 1:ZJ:87:ASP:OD2   | 1:ZJ:88:SER:N     | 2.45                     | 0.47              |
| 1:ZK:373:VAL:HG11 | 1:ZQ:7:VAL:HG22   | 1.96                     | 0.47              |
| 1:ZL:84:ARG:HG2   | 1:ZL:117:THR:OG1  | 2.14                     | 0.47              |
| 1:ZL:234:GLU:OE2  | 1:ZR:255:THR:OG1  | 2.31                     | 0.47              |
| 1:ZM:399:LEU:CD2  | 2:ZB:227:ALA:CB   | 2.92                     | 0.47              |
| 1:ZO:18:ASP:HA    | 1:ZT:5:GLN:NE2    | 2.28                     | 0.47              |
| 1:ZO:74:ASP:OD1   | 1:ZO:74:ASP:N     | 2.48                     | 0.47              |
| 1:ZQ:97:ASN:HD22  | 1:ZQ:332:ASN:ND2  | 2.13                     | 0.47              |
| 1:ZR:295:ASN:ND2  | 1:ZR:299:THR:OG1  | 2.38                     | 0.47              |
| 1:ZR:390:LYS:HB2  | 1:ZW:402:LEU:HD22 | 1.97                     | 0.47              |
| 1:ZV:107:ASN:HD22 | 1:ZV:138:THR:HG22 | 1.79                     | 0.47              |
| 1:ZW:233:ASN:HD21 | 1:ZW:237:ILE:HB   | 1.79                     | 0.47              |
| 1:ZW:396:LEU:HD23 | 1:ZW:396:LEU:HA   | 1.73                     | 0.47              |
| 1:ZX:245:ASN:C    | 1:ZX:246:ILE:HD13 | 2.40                     | 0.47              |
| 1:ZX:317:LEU:HD11 | 1:ZX:356:LEU:HD21 | 1.97                     | 0.47              |
| 1:Za:149:THR:HG21 | 1:Za:186:VAL:HB   | 1.97                     | 0.47              |
| 1:Zg:194:HIS:CE1  | 1:Zg:251:ILE:HD12 | 2.50                     | 0.47              |
| 1:Zg:294:ILE:HG12 | 1:Zg:300:VAL:HG22 | 1.97                     | 0.47              |
| 2:ZE:48:THR:HG22  | 2:ZE:67:GLN:HE22  | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:r:98:LYS:HE2    | 2:x:187:ILE:O     | 2.14                     | 0.47              |
| 2:r:155:GLY:HA2   | 2:r:214:LEU:HD12  | 1.97                     | 0.47              |
| 2:w:85:ASN:O      | 2:w:221:THR:OG1   | 2.32                     | 0.47              |
| 2:w:142:ILE:HD13  | 2:w:149:ILE:HD13  | 1.96                     | 0.47              |
| 2:x:188:GLY:O     | 2:x:190:ASN:N     | 2.48                     | 0.47              |
| 1:ZG:160:SER:O    | 1:ZM:252:ASN:ND2  | 2.48                     | 0.47              |
| 1:ZG:195:ASP:O    | 1:ZG:215:SER:OG   | 2.33                     | 0.47              |
| 1:ZJ:183:THR:HG22 | 1:ZU:131:GLY:O    | 2.15                     | 0.47              |
| 1:ZJ:195:ASP:OD2  | 1:ZJ:195:ASP:N    | 2.36                     | 0.47              |
| 1:ZL:383:GLN:O    | 1:ZL:387:GLN:HG2  | 2.15                     | 0.47              |
| 1:ZN:382:TYR:CE1  | 1:ZS:395:ILE:HG23 | 2.50                     | 0.47              |
| 1:ZQ:233:ASN:HD21 | 1:ZQ:239:GLU:HB3  | 1.79                     | 0.47              |
| 1:ZU:195:ASP:OD2  | 1:ZU:216:SER:OG   | 2.22                     | 0.47              |
| 1:Zd:60:ASP:O     | 1:Zd:365:ASN:ND2  | 2.48                     | 0.47              |
| 1:Ze:269:GLN:HG2  | 1:Ze:270:ASN:H    | 1.80                     | 0.47              |
| 1:Zg:328:SER:HG   | 1:Zg:334:TRP:CD1  | 2.32                     | 0.47              |
| 2:6:57:SER:HB3    | 2:w:108:PRO:CB    | 2.39                     | 0.47              |
| 2:t:153:ARG:HH21  | 2:z:108:PRO:HG2   | 1.79                     | 0.47              |
| 2:x:7:ILE:HG12    | 2:x:70:THR:O      | 2.13                     | 0.47              |
| 2:y:7:ILE:HG23    | 2:y:71:GLY:HA2    | 1.96                     | 0.47              |
| 1:ZM:86:VAL:HG13  | 1:ZM:117:THR:HG21 | 1.97                     | 0.47              |
| 1:ZN:87:ASP:OD2   | 1:ZN:88:SER:N     | 2.39                     | 0.47              |
| 1:ZP:195:ASP:OD2  | 1:ZP:216:SER:OG   | 2.25                     | 0.47              |
| 1:ZZ:10:LEU:HG    | 1:ZZ:382:TYR:CZ   | 2.49                     | 0.47              |
| 1:Zb:171:SER:HB3  | 1:Zb:174:ASP:HB2  | 1.97                     | 0.47              |
| 2:4:238:ARG:O     | 2:4:242:ILE:HG12  | 2.15                     | 0.47              |
| 2:9:128:LEU:HD12  | 2:9:140:ILE:HB    | 1.95                     | 0.47              |
| 2:ZC:40:VAL:HG23  | 2:ZC:75:VAL:HB    | 1.97                     | 0.47              |
| 2:u:113:ALA:HB1   | 2:u:191:LEU:HB3   | 1.96                     | 0.47              |
| 2:x:2:ILE:HG12    | 2:x:254:LEU:HD11  | 1.97                     | 0.47              |
| 1:ZF:384:SER:OG   | 2:ZA:26:LEU:HD22  | 2.14                     | 0.47              |
| 1:ZQ:33:LYS:O     | 1:ZQ:59:GLN:NE2   | 2.48                     | 0.47              |
| 1:ZS:392:GLN:HA   | 1:ZS:395:ILE:HD12 | 1.97                     | 0.47              |
| 1:ZT:143:LEU:HD21 | 1:ZT:286:PRO:HB3  | 1.97                     | 0.47              |
| 1:ZX:71:ARG:HB3   | 1:ZX:74:ASP:CG    | 2.39                     | 0.47              |
| 1:ZX:307:GLU:OE1  | 1:ZX:307:GLU:O    | 2.32                     | 0.47              |
| 1:ZY:184:VAL:HG13 | 1:ZY:196:MET:HB2  | 1.97                     | 0.47              |
| 1:ZZ:99:GLN:HB3   | 1:ZZ:111:MET:HE3  | 1.96                     | 0.47              |
| 1:Zd:171:SER:O    | 1:Zd:177:SER:OG   | 2.30                     | 0.47              |
| 1:Ze:352:ASN:OD1  | 1:Ze:352:ASN:N    | 2.43                     | 0.47              |
| 2:6:95:VAL:O      | 2:6:118:GLY:HA3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZA:70:THR:HG22  | 2:ZA:71:GLY:N     | 2.29                     | 0.47              |
| 2:v:98:LYS:N      | 2:v:213:LEU:O     | 2.40                     | 0.47              |
| 2:w:188:GLY:O     | 2:w:190:ASN:N     | 2.47                     | 0.47              |
| 1:ZG:185:THR:OG1  | 1:ZR:133:ASN:OD1  | 2.33                     | 0.46              |
| 1:ZK:397:ASN:HB2  | 2:ZE:238:ARG:HH22 | 1.80                     | 0.46              |
| 1:Zh:269:GLN:HG2  | 1:Zh:270:ASN:H    | 1.80                     | 0.46              |
| 2:4:173:LEU:HD23  | 2:4:214:LEU:HD13  | 1.97                     | 0.46              |
| 2:r:122:VAL:HG23  | 2:w:180:ASN:HD22  | 1.80                     | 0.46              |
| 2:t:122:VAL:HG11  | 2:t:142:ILE:HD12  | 1.97                     | 0.46              |
| 1:ZG:264:LEU:HD12 | 1:ZG:265:ASN:N    | 2.30                     | 0.46              |
| 1:ZI:52:VAL:HG13  | 2:ZD:28:ASN:OD1   | 2.15                     | 0.46              |
| 1:ZI:183:THR:HG22 | 1:ZI:197:ASN:ND2  | 2.30                     | 0.46              |
| 1:ZM:267:MET:HE2  | 1:ZM:269:GLN:NE2  | 2.29                     | 0.46              |
| 1:ZX:96:ARG:NH2   | 1:ZX:362:GLU:OE2  | 2.40                     | 0.46              |
| 1:ZY:194:HIS:CE1  | 1:ZY:251:ILE:HD12 | 2.51                     | 0.46              |
| 1:Zg:79:GLN:HB2   | 1:Zg:354:GLY:HA3  | 1.96                     | 0.46              |
| 2:8:111:THR:HG21  | 2:x:163:GLY:HA2   | 1.96                     | 0.46              |
| 2:x:153:ARG:HE    | 2:x:213:LEU:HD13  | 1.80                     | 0.46              |
| 1:ZF:50:LEU:CD2   | 2:4:85:ASN:OD1    | 2.64                     | 0.46              |
| 1:ZI:374:ASN:O    | 1:ZI:376:ILE:N    | 2.48                     | 0.46              |
| 1:ZP:367:ASP:O    | 1:ZP:371:GLU:HG2  | 2.15                     | 0.46              |
| 1:ZS:149:THR:HG21 | 1:ZS:186:VAL:HG12 | 1.97                     | 0.46              |
| 1:ZS:182:GLY:HA2  | 1:Zd:131:GLY:HA3  | 1.97                     | 0.46              |
| 1:ZY:210:VAL:HB   | 1:ZY:228:THR:HG22 | 1.97                     | 0.46              |
| 2:3:194:GLU:OE2   | 2:3:201:PRO:HD3   | 2.16                     | 0.46              |
| 2:6:45:LEU:HD21   | 2:v:215:TYR:CE2   | 2.50                     | 0.46              |
| 2:ZB:257:LEU:HD21 | 2:0:227:ALA:HA    | 1.97                     | 0.46              |
| 1:ZF:50:LEU:HD22  | 2:4:85:ASN:HA     | 1.97                     | 0.46              |
| 1:ZI:204:LYS:O    | 1:ZI:205:ASP:C    | 2.58                     | 0.46              |
| 1:ZL:318:ALA:HB1  | 1:ZL:343:ALA:HB1  | 1.98                     | 0.46              |
| 1:ZM:374:ASN:O    | 1:ZM:375:MET:C    | 2.59                     | 0.46              |
| 1:ZQ:155:GLN:HE21 | 1:ZQ:277:VAL:HB   | 1.79                     | 0.46              |
| 1:ZT:185:THR:OG1  | 1:Ze:133:ASN:OD1  | 2.34                     | 0.46              |
| 1:ZV:93:PHE:HB3   | 1:ZV:333:VAL:CG2  | 2.46                     | 0.46              |
| 1:ZW:16:ASN:HB2   | 1:ZW:39:PHE:HZ    | 1.80                     | 0.46              |
| 2:5:219:VAL:HG11  | 2:ZA:38:ARG:HH22  | 1.80                     | 0.46              |
| 2:8:41:PHE:HA     | 2:8:74:PRO:HA     | 1.96                     | 0.46              |
| 2:r:61:THR:OG1    | 2:r:62:LEU:N      | 2.46                     | 0.46              |
| 2:r:122:VAL:HG11  | 2:r:142:ILE:HD12  | 1.97                     | 0.46              |
| 2:s:22:ILE:HG21   | 2:s:233:MET:HG3   | 1.98                     | 0.46              |
| 2:t:11:GLY:O      | 2:t:15:GLN:HG2    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:x:95:VAL:O      | 2:x:118:GLY:HA3   | 2.15                     | 0.46              |
| 1:ZF:233:ASN:HD21 | 1:ZF:237:ILE:HB   | 1.80                     | 0.46              |
| 1:ZG:319:ASN:OD1  | 1:ZG:344:LEU:HB3  | 2.16                     | 0.46              |
| 1:ZH:159:ASN:ND2  | 1:ZH:162:ASP:OD2  | 2.46                     | 0.46              |
| 1:ZJ:24:ILE:O     | 1:ZJ:27:SER:OG    | 2.32                     | 0.46              |
| 1:ZJ:159:ASN:HB3  | 1:ZJ:162:ASP:OD2  | 2.15                     | 0.46              |
| 1:ZJ:367:ASP:OD2  | 1:ZJ:370:LYS:HB2  | 2.15                     | 0.46              |
| 1:ZU:107:ASN:ND2  | 1:ZU:138:THR:HG22 | 2.31                     | 0.46              |
| 2:2:184:LEU:HB3   | 2:2:192:TYR:HB3   | 1.96                     | 0.46              |
| 2:5:44:LEU:HD23   | 2:5:44:LEU:HA     | 1.77                     | 0.46              |
| 2:7:115:THR:HB    | 2:7:191:LEU:HD23  | 1.96                     | 0.46              |
| 2:ZC:7:ILE:HG23   | 2:ZC:71:GLY:HA2   | 1.97                     | 0.46              |
| 2:x:42:GLU:OE1    | 2:x:75:VAL:HG21   | 2.15                     | 0.46              |
| 1:ZL:208:TRP:HE1  | 1:ZL:268:GLN:CD   | 2.23                     | 0.46              |
| 1:ZO:331:ASP:HA   | 1:ZT:40:ALA:HB1   | 1.97                     | 0.46              |
| 1:ZP:16:ASN:HB2   | 1:ZP:39:PHE:HZ    | 1.80                     | 0.46              |
| 1:ZP:144:MET:SD   | 1:ZP:306:ASN:ND2  | 2.77                     | 0.46              |
| 1:ZQ:160:SER:O    | 1:ZW:252:ASN:ND2  | 2.48                     | 0.46              |
| 1:ZQ:194:HIS:CE1  | 1:ZQ:251:ILE:HD12 | 2.50                     | 0.46              |
| 1:ZR:212:THR:HG21 | 1:ZR:246:ILE:HG13 | 1.97                     | 0.46              |
| 1:ZR:373:VAL:HG11 | 1:ZX:7:VAL:HG22   | 1.97                     | 0.46              |
| 1:ZS:143:LEU:HD23 | 1:ZS:143:LEU:H    | 1.80                     | 0.46              |
| 1:ZS:317:LEU:HD11 | 1:ZS:356:LEU:HD21 | 1.98                     | 0.46              |
| 1:Ze:110:ASN:OD1  | 1:Ze:114:MET:N    | 2.49                     | 0.46              |
| 2:6:57:SER:CB     | 2:w:108:PRO:HG3   | 2.46                     | 0.46              |
| 2:1:258:THR:OG1   | 2:v:241:GLU:OE2   | 2.26                     | 0.46              |
| 2:u:32:ASN:HD22   | 2:u:219:VAL:HB    | 1.80                     | 0.46              |
| 1:ZG:388:THR:HG1  | 2:ZB:233:MET:HE1  | 1.79                     | 0.46              |
| 1:ZR:281:GLN:NE2  | 1:ZR:283:GLY:O    | 2.47                     | 0.46              |
| 1:ZS:180:LYS:HD2  | 1:ZS:181:LYS:N    | 2.30                     | 0.46              |
| 1:ZS:394:GLN:O    | 1:ZS:398:THR:HG22 | 2.16                     | 0.46              |
| 1:ZT:16:ASN:HB2   | 1:ZT:39:PHE:HZ    | 1.81                     | 0.46              |
| 1:ZW:199:TYR:HB2  | 1:ZW:211:TYR:HB2  | 1.98                     | 0.46              |
| 1:Za:93:PHE:HB3   | 1:Za:333:VAL:HG13 | 1.97                     | 0.46              |
| 1:Ze:95:SER:OG    | 1:Ze:332:ASN:O    | 2.24                     | 0.46              |
| 1:Zh:374:ASN:HA   | 1:Zh:377:VAL:HG12 | 1.98                     | 0.46              |
| 2:2:3:SER:OG      | 2:r:85:ASN:ND2    | 2.39                     | 0.46              |
| 2:5:19:MET:HB2    | 2:5:236:VAL:HG11  | 1.97                     | 0.46              |
| 2:7:7:ILE:HG23    | 2:7:71:GLY:HA2    | 1.95                     | 0.46              |
| 2:8:255:GLN:O     | 2:8:259:GLN:HG2   | 2.16                     | 0.46              |
| 2:0:89:THR:HG23   | 2:0:91:ASN:H      | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:w:184:LEU:HB3   | 2:w:192:TYR:HB3   | 1.97                     | 0.46              |
| 1:ZI:109:VAL:HG12 | 1:ZI:115:GLN:HA   | 1.97                     | 0.46              |
| 1:ZL:140:PRO:HD2  | 1:ZL:312:LEU:HD22 | 1.98                     | 0.46              |
| 1:ZM:109:VAL:HG12 | 1:ZM:115:GLN:HA   | 1.98                     | 0.46              |
| 1:ZO:196:MET:HE3  | 1:ZO:248:THR:HG22 | 1.98                     | 0.46              |
| 1:ZS:34:SER:HB3   | 1:ZS:366:VAL:HG22 | 1.98                     | 0.46              |
| 1:ZV:391:THR:O    | 1:ZV:395:ILE:HG12 | 2.16                     | 0.46              |
| 1:ZW:373:VAL:HG11 | 1:Zc:7:VAL:HG22   | 1.98                     | 0.46              |
| 1:ZY:109:VAL:HG12 | 1:ZY:115:GLN:HA   | 1.98                     | 0.46              |
| 1:ZZ:5:GLN:HG2    | 1:ZZ:50:LEU:O     | 2.16                     | 0.46              |
| 1:ZZ:109:VAL:HG12 | 1:ZZ:115:GLN:HA   | 1.98                     | 0.46              |
| 1:Za:139:ILE:HA   | 1:Za:312:LEU:HD22 | 1.98                     | 0.46              |
| 2:1:135:GLN:NE2   | 2:1:137:GLN:HG2   | 2.30                     | 0.46              |
| 1:ZH:43:PHE:HD2   | 1:ZH:49:GLY:HA2   | 1.81                     | 0.46              |
| 1:ZP:245:ASN:C    | 1:ZP:246:ILE:HD13 | 2.40                     | 0.46              |
| 1:ZQ:93:PHE:HB3   | 1:ZQ:333:VAL:HG13 | 1.97                     | 0.46              |
| 1:ZS:105:ASN:HB2  | 1:ZS:107:ASN:ND2  | 2.30                     | 0.46              |
| 1:Ze:44:ALA:HB3   | 1:Ze:50:LEU:HD11  | 1.98                     | 0.46              |
| 1:Zh:69:THR:OG1   | 1:Zh:74:ASP:OD1   | 2.29                     | 0.46              |
| 2:4:45:LEU:CD2    | 2:t:98:LYS:HG2    | 2.45                     | 0.46              |
| 2:ZE:5:LEU:HB2    | 2:ZE:250:THR:HG21 | 1.98                     | 0.46              |
| 2:z:151:ILE:HG12  | 2:z:157:VAL:HG22  | 1.97                     | 0.46              |
| 1:ZG:230:LEU:HB3  | 1:ZG:238:LEU:HD11 | 1.98                     | 0.46              |
| 1:ZH:83:PHE:HB2   | 1:ZH:95:SER:O     | 2.15                     | 0.46              |
| 1:ZK:262:SER:OG   | 1:ZK:264:LEU:HG   | 2.15                     | 0.46              |
| 1:ZL:106:ARG:HD3  | 1:ZL:140:PRO:HA   | 1.97                     | 0.46              |
| 1:ZO:156:ILE:HA   | 1:ZO:277:VAL:HG23 | 1.98                     | 0.46              |
| 1:ZR:184:VAL:HG13 | 1:ZR:196:MET:HB2  | 1.98                     | 0.46              |
| 1:ZS:156:ILE:HG13 | 1:ZS:276:ILE:HA   | 1.98                     | 0.46              |
| 1:ZT:18:ASP:HB3   | 1:ZY:5:GLN:HE22   | 1.80                     | 0.46              |
| 1:ZU:10:LEU:HD23  | 1:ZU:10:LEU:HA    | 1.84                     | 0.46              |
| 1:ZY:17:LEU:HD13  | 1:Zd:395:ILE:CD1  | 2.45                     | 0.46              |
| 1:ZY:57:ILE:HD12  | 1:Zd:47:LYS:HB2   | 1.98                     | 0.46              |
| 1:ZY:83:PHE:HB2   | 1:ZY:95:SER:O     | 2.16                     | 0.46              |
| 2:4:95:VAL:O      | 2:4:118:GLY:HA3   | 2.16                     | 0.46              |
| 2:s:188:GLY:O     | 2:s:190:ASN:N     | 2.49                     | 0.46              |
| 2:t:135:GLN:NE2   | 2:t:137:GLN:OE1   | 2.49                     | 0.46              |
| 2:u:115:THR:HB    | 2:u:191:LEU:HD23  | 1.97                     | 0.46              |
| 1:ZH:75:VAL:HG13  | 1:ZH:356:LEU:HB3  | 1.98                     | 0.45              |
| 1:ZI:197:ASN:HD22 | 1:ZI:197:ASN:N    | 2.14                     | 0.45              |
| 1:ZW:74:ASP:O     | 1:ZW:359:GLY:N    | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZW:314:GLN:NE2  | 1:ZW:347:THR:OG1  | 2.49                     | 0.45              |
| 1:ZY:268:GLN:NE2  | 1:Ze:190:GLN:HE22 | 2.12                     | 0.45              |
| 1:ZZ:99:GLN:HE21  | 1:ZZ:111:MET:HE3  | 1.82                     | 0.45              |
| 1:ZZ:208:TRP:NE1  | 1:ZZ:268:GLN:OE1  | 2.38                     | 0.45              |
| 1:Zf:5:GLN:HG2    | 1:Zf:50:LEU:O     | 2.15                     | 0.45              |
| 2:2:79:ARG:HH11   | 2:2:79:ARG:HG3    | 1.81                     | 0.45              |
| 2:3:215:TYR:CE2   | 2:ZE:45:LEU:HD21  | 2.52                     | 0.45              |
| 2:5:29:VAL:O      | 2:5:222:SER:OG    | 2.33                     | 0.45              |
| 2:8:40:VAL:O      | 2:8:75:VAL:N      | 2.45                     | 0.45              |
| 2:8:56:SER:O      | 2:s:152:GLY:HA3   | 2.17                     | 0.45              |
| 2:1:252:GLN:NE2   | 2:w:237:GLN:HE22  | 2.14                     | 0.45              |
| 2:r:205:THR:HB    | 2:r:208:LEU:HD12  | 1.99                     | 0.45              |
| 2:s:36:ARG:HD3    | 2:s:80:LEU:HD22   | 1.97                     | 0.45              |
| 1:ZG:181:LYS:HE2  | 1:ZR:129:GLN:HE21 | 1.80                     | 0.45              |
| 1:ZJ:233:ASN:ND2  | 1:ZJ:235:ASN:H    | 2.14                     | 0.45              |
| 1:ZK:93:PHE:HB3   | 1:ZK:333:VAL:HG13 | 1.98                     | 0.45              |
| 1:ZL:104:GLU:H    | 1:ZL:104:GLU:CD   | 2.23                     | 0.45              |
| 1:ZM:213:HIS:HB2  | 1:ZM:223:PRO:HG3  | 1.99                     | 0.45              |
| 1:ZU:109:VAL:HG12 | 1:ZU:115:GLN:HA   | 1.98                     | 0.45              |
| 1:Za:81:GLY:HA3   | 1:Za:317:LEU:HD23 | 1.97                     | 0.45              |
| 1:Za:104:GLU:OE2  | 1:Zf:341:GLY:HA2  | 2.15                     | 0.45              |
| 1:Zc:93:PHE:CD1   | 1:Zc:114:MET:HE1  | 2.50                     | 0.45              |
| 1:Zd:5:GLN:HG2    | 1:Zd:50:LEU:O     | 2.17                     | 0.45              |
| 1:Zd:93:PHE:HB3   | 1:Zd:333:VAL:HG13 | 1.98                     | 0.45              |
| 2:2:244:SER:HG    | 2:7:256:LYS:NZ    | 2.10                     | 0.45              |
| 2:5:184:LEU:HB3   | 2:5:192:TYR:HB3   | 1.99                     | 0.45              |
| 2:6:1:MET:HE3     | 2:6:1:MET:HB2     | 1.86                     | 0.45              |
| 2:6:57:SER:OG     | 2:w:108:PRO:HG3   | 2.17                     | 0.45              |
| 2:7:19:MET:HB2    | 2:7:236:VAL:HG11  | 1.98                     | 0.45              |
| 2:u:229:GLU:O     | 2:u:233:MET:HG3   | 2.15                     | 0.45              |
| 2:v:130:THR:OG1   | 2:v:131:ALA:N     | 2.50                     | 0.45              |
| 2:x:249:THR:O     | 2:x:253:MET:HG3   | 2.16                     | 0.45              |
| 1:ZN:159:ASN:ND2  | 1:ZN:162:ASP:OD2  | 2.49                     | 0.45              |
| 1:ZP:83:PHE:O     | 1:ZP:94:TYR:HA    | 2.16                     | 0.45              |
| 1:ZZ:63:ASP:OD2   | 1:ZZ:79:GLN:N     | 2.50                     | 0.45              |
| 1:Zd:93:PHE:HB2   | 1:Zd:114:MET:HE1  | 1.98                     | 0.45              |
| 1:Ze:383:GLN:O    | 1:Ze:387:GLN:HG2  | 2.16                     | 0.45              |
| 2:5:245:LYS:HE2   | 2:5:245:LYS:HB2   | 1.52                     | 0.45              |
| 2:7:128:LEU:HD23  | 2:7:128:LEU:HA    | 1.82                     | 0.45              |
| 1:ZF:117:THR:HA   | 1:ZF:136:PRO:HA   | 1.97                     | 0.45              |
| 1:ZG:71:ARG:O     | 1:ZG:359:GLY:HA2  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZG:154:MET:HB3  | 1:ZG:154:MET:HE2  | 1.73                     | 0.45              |
| 1:ZK:393:ASP:OD1  | 2:ZE:238:ARG:NE   | 2.49                     | 0.45              |
| 1:ZM:139:ILE:HA   | 1:ZM:312:LEU:HD13 | 1.97                     | 0.45              |
| 1:ZX:144:MET:HE3  | 1:ZX:284:TYR:CE1  | 2.51                     | 0.45              |
| 1:ZX:230:LEU:HD22 | 1:ZX:238:LEU:HD11 | 1.98                     | 0.45              |
| 1:ZY:17:LEU:CD1   | 1:Zd:395:ILE:HD11 | 2.46                     | 0.45              |
| 1:ZY:210:VAL:O    | 1:ZY:227:SER:N    | 2.49                     | 0.45              |
| 1:ZZ:112:GLN:OE1  | 1:ZZ:112:GLN:N    | 2.50                     | 0.45              |
| 2:2:180:ASN:ND2   | 2:x:122:VAL:O     | 2.49                     | 0.45              |
| 2:6:242:ILE:HD12  | 2:ZC:1:MET:HE1    | 1.96                     | 0.45              |
| 2:ZD:59:GLN:N     | 2:ZD:59:GLN:OE1   | 2.49                     | 0.45              |
| 2:w:44:LEU:HB2    | 2:w:70:THR:HB     | 1.97                     | 0.45              |
| 2:w:176:THR:OG1   | 2:w:203:GLU:OE2   | 2.35                     | 0.45              |
| 2:z:238:ARG:O     | 2:z:242:ILE:HG12  | 2.17                     | 0.45              |
| 1:ZI:322:ASN:ND2  | 2:ZD:122:VAL:O    | 2.48                     | 0.45              |
| 1:ZJ:265:ASN:OD1  | 1:ZJ:265:ASN:O    | 2.35                     | 0.45              |
| 1:ZO:180:LYS:HB3  | 1:ZO:200:PHE:HB2  | 1.98                     | 0.45              |
| 1:ZP:396:LEU:HD23 | 1:ZP:396:LEU:HA   | 1.76                     | 0.45              |
| 1:ZQ:233:ASN:ND2  | 1:ZQ:239:GLU:HB3  | 2.31                     | 0.45              |
| 1:ZR:204:LYS:HG2  | 1:ZR:205:ASP:N    | 2.32                     | 0.45              |
| 1:ZS:10:LEU:HD11  | 1:ZS:382:TYR:CE1  | 2.52                     | 0.45              |
| 1:ZS:27:SER:O     | 1:ZS:364:SER:OG   | 2.34                     | 0.45              |
| 1:Zh:2:SER:OG     | 1:Zh:392:GLN:NE2  | 2.49                     | 0.45              |
| 2:4:1:MET:HE3     | 2:t:226:VAL:HG21  | 1.98                     | 0.45              |
| 2:6:57:SER:HB3    | 2:w:108:PRO:HG3   | 1.97                     | 0.45              |
| 2:ZC:95:VAL:HG11  | 2:ZC:214:LEU:HD23 | 1.98                     | 0.45              |
| 2:ZD:54:ALA:HB1   | 2:x:150:THR:HG21  | 1.98                     | 0.45              |
| 2:s:185:GLU:HG3   | 2:x:67:GLN:HE22   | 1.82                     | 0.45              |
| 2:x:147:LEU:HD11  | 2:x:162:GLN:HB2   | 1.98                     | 0.45              |
| 2:y:120:PHE:CD1   | 2:y:136:VAL:HG21  | 2.52                     | 0.45              |
| 2:z:47:GLN:HG2    | 2:z:68:ILE:HB     | 1.99                     | 0.45              |
| 1:ZG:388:THR:HA   | 2:ZB:233:MET:SD   | 2.56                     | 0.45              |
| 1:ZI:75:VAL:HG11  | 1:ZI:356:LEU:HD13 | 1.98                     | 0.45              |
| 1:ZM:217:ASP:HB3  | 1:ZM:220:ALA:HB2  | 1.98                     | 0.45              |
| 1:Zc:10:LEU:HD12  | 1:Zc:10:LEU:HA    | 1.71                     | 0.45              |
| 1:Zc:210:VAL:HB   | 1:Zc:228:THR:HG22 | 1.99                     | 0.45              |
| 1:Zd:3:PHE:O      | 1:Zd:7:VAL:HG13   | 2.16                     | 0.45              |
| 2:4:45:LEU:HD22   | 2:t:98:LYS:HG2    | 1.98                     | 0.45              |
| 2:7:94:ASP:OD2    | 2:ZC:38:ARG:NH1   | 2.43                     | 0.45              |
| 2:0:129:VAL:HG12  | 2:0:135:GLN:HA    | 1.97                     | 0.45              |
| 2:r:7:ILE:HG12    | 2:r:70:THR:O      | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:t:157:VAL:HB    | 2:t:171:GLY:CA    | 2.42                     | 0.45              |
| 2:x:3:SER:O       | 2:x:4:SER:C       | 2.59                     | 0.45              |
| 1:ZH:162:ASP:O    | 1:ZH:202:LYS:NZ   | 2.33                     | 0.45              |
| 1:ZN:53:LYS:HB2   | 2:ZC:88:GLN:NE2   | 2.30                     | 0.45              |
| 1:ZN:380:ARG:HA   | 1:ZN:380:ARG:HD3  | 1.68                     | 0.45              |
| 1:ZR:179:ASN:N    | 1:ZR:200:PHE:O    | 2.45                     | 0.45              |
| 1:ZR:316:VAL:HG21 | 1:ZR:345:LEU:HD23 | 1.98                     | 0.45              |
| 1:ZT:380:ARG:HD3  | 1:ZT:380:ARG:HA   | 1.76                     | 0.45              |
| 1:ZV:102:LEU:HD21 | 1:ZV:106:ARG:HA   | 1.98                     | 0.45              |
| 1:ZV:119:TYR:HB2  | 1:ZV:314:GLN:HB3  | 1.99                     | 0.45              |
| 1:ZX:188:ASP:HA   | 1:ZX:257:ALA:HB2  | 1.99                     | 0.45              |
| 1:ZY:33:LYS:NZ    | 1:ZY:362:GLU:OE2  | 2.49                     | 0.45              |
| 1:Za:157:ASN:ND2  | 1:Zg:143:LEU:HD13 | 2.31                     | 0.45              |
| 1:Zd:116:LEU:HD12 | 1:Zd:117:THR:H    | 1.80                     | 0.45              |
| 1:Ze:380:ARG:HA   | 1:Ze:380:ARG:HD3  | 1.64                     | 0.45              |
| 2:3:10:THR:OG1    | 2:3:71:GLY:HA3    | 2.17                     | 0.45              |
| 2:4:50:ARG:HH21   | 2:z:73:ARG:HH22   | 1.63                     | 0.45              |
| 2:7:1:MET:HE1     | 2:1:239:ALA:HB2   | 1.98                     | 0.45              |
| 2:7:106:MET:HE3   | 2:7:110:GLY:HA2   | 1.98                     | 0.45              |
| 2:9:35:LYS:NZ     | 2:9:220:GLU:OE2   | 2.48                     | 0.45              |
| 2:w:237:GLN:O     | 2:w:241:GLU:HG3   | 2.17                     | 0.45              |
| 1:ZK:210:VAL:HB   | 1:ZK:228:THR:HG22 | 1.98                     | 0.45              |
| 1:ZL:269:GLN:HG2  | 1:ZR:286:PRO:HG2  | 1.98                     | 0.45              |
| 1:ZN:202:LYS:HB2  | 1:ZN:208:TRP:CZ3  | 2.52                     | 0.45              |
| 1:ZO:139:ILE:HA   | 1:ZO:312:LEU:HD22 | 1.98                     | 0.45              |
| 1:ZQ:288:ASP:O    | 1:ZQ:305:SER:N    | 2.50                     | 0.45              |
| 1:ZV:373:VAL:HG11 | 1:Zb:7:VAL:HG22   | 1.98                     | 0.45              |
| 1:Za:352:ASN:O    | 1:Za:352:ASN:OD1  | 2.35                     | 0.45              |
| 1:Zf:378:ALA:O    | 1:Zf:379:GLN:C    | 2.59                     | 0.45              |
| 2:2:196:GLN:HE22  | 2:7:55:GLN:HE21   | 1.63                     | 0.45              |
| 2:3:98:LYS:HB3    | 2:3:213:LEU:HB2   | 1.98                     | 0.45              |
| 2:3:189:GLU:HA    | 2:8:42:GLU:CD     | 2.42                     | 0.45              |
| 2:4:9:LYS:HE3     | 2:y:228:GLU:HG3   | 1.99                     | 0.45              |
| 2:8:70:THR:HG22   | 2:8:71:GLY:N      | 2.30                     | 0.45              |
| 2:ZB:8:ALA:HB1    | 2:ZB:247:VAL:HG23 | 1.99                     | 0.45              |
| 2:ZC:88:GLN:NE2   | 2:ZC:218:TYR:OH   | 2.50                     | 0.45              |
| 2:0:21:VAL:HG21   | 2:0:39:ALA:HB2    | 1.99                     | 0.45              |
| 2:0:112:SER:HB3   | 2:0:137:GLN:NE2   | 2.31                     | 0.45              |
| 2:r:122:VAL:O     | 2:w:180:ASN:ND2   | 2.50                     | 0.45              |
| 2:s:16:GLN:HE21   | 2:s:16:GLN:HB2    | 1.48                     | 0.45              |
| 2:t:147:LEU:HB2   | 2:t:160:THR:HG23  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:x:187:ILE:HD11  | 2:x:193:ILE:HG13  | 1.99                     | 0.45              |
| 2:z:198:SER:O     | 2:z:198:SER:OG    | 2.31                     | 0.45              |
| 1:ZI:352:ASN:OD1  | 1:ZI:352:ASN:N    | 2.49                     | 0.45              |
| 1:ZL:160:SER:HA   | 1:ZL:268:GLN:HE21 | 1.82                     | 0.45              |
| 1:ZM:246:ILE:HD13 | 1:ZM:246:ILE:HA   | 1.88                     | 0.45              |
| 1:ZP:73:LEU:HD21  | 1:ZP:292:TYR:CE1  | 2.52                     | 0.45              |
| 1:ZT:146:ALA:HB2  | 1:ZT:286:PRO:HD3  | 1.99                     | 0.45              |
| 1:ZY:146:ALA:HB2  | 1:ZY:286:PRO:HD3  | 1.98                     | 0.45              |
| 1:Zf:101:LYS:HD3  | 1:Zf:102:LEU:N    | 2.31                     | 0.45              |
| 2:2:28:ASN:ND2    | 2:7:43:ASP:OD1    | 2.49                     | 0.45              |
| 2:2:36:ARG:HE     | 2:2:80:LEU:HD22   | 1.82                     | 0.45              |
| 2:3:123:ASP:OD1   | 2:3:127:GLN:N     | 2.49                     | 0.45              |
| 2:6:1:MET:HE3     | 2:v:29:VAL:HG11   | 1.99                     | 0.45              |
| 2:6:26:LEU:HD11   | 2:6:233:MET:HE2   | 1.98                     | 0.45              |
| 2:ZC:95:VAL:O     | 2:ZC:118:GLY:HA3  | 2.17                     | 0.45              |
| 2:0:184:LEU:HB3   | 2:0:192:TYR:HB3   | 1.98                     | 0.45              |
| 2:1:238:ARG:O     | 2:1:242:ILE:HG12  | 2.17                     | 0.45              |
| 2:r:106:MET:HE2   | 2:r:106:MET:HB2   | 1.86                     | 0.45              |
| 2:y:25:ASN:HD21   | 2:y:37:GLN:H      | 1.64                     | 0.45              |
| 1:ZL:270:ASN:HB2  | 1:ZR:190:GLN:O    | 2.17                     | 0.45              |
| 1:ZQ:265:ASN:C    | 1:ZQ:267:MET:HE2  | 2.42                     | 0.45              |
| 1:ZS:86:VAL:HG23  | 1:ZS:117:THR:HG21 | 1.98                     | 0.45              |
| 1:ZS:128:ILE:HD13 | 1:ZS:128:ILE:HA   | 1.87                     | 0.45              |
| 1:ZT:128:ILE:HD13 | 1:ZT:128:ILE:HA   | 1.83                     | 0.45              |
| 1:ZW:122:THR:OG1  | 1:ZW:129:GLN:NE2  | 2.50                     | 0.45              |
| 1:ZY:212:THR:HG21 | 1:ZY:246:ILE:HD12 | 1.99                     | 0.45              |
| 1:ZY:337:THR:HG23 | 1:ZY:339:ALA:H    | 1.82                     | 0.45              |
| 1:ZY:392:GLN:HA   | 1:ZY:395:ILE:HD12 | 1.99                     | 0.45              |
| 2:2:10:THR:OG1    | 2:2:71:GLY:HA3    | 2.17                     | 0.45              |
| 2:3:35:LYS:NZ     | 2:3:220:GLU:OE2   | 2.48                     | 0.45              |
| 2:4:17:THR:HG23   | 2:9:68:ILE:HD11   | 1.99                     | 0.45              |
| 2:4:238:ARG:NH2   | 2:ZA:251:ASP:OD2  | 2.47                     | 0.45              |
| 2:ZB:184:LEU:HB3  | 2:ZB:192:TYR:HB3  | 1.99                     | 0.45              |
| 2:s:147:LEU:HB2   | 2:s:160:THR:HG23  | 1.98                     | 0.45              |
| 2:u:97:ILE:HD12   | 2:u:116:ARG:HG2   | 1.98                     | 0.45              |
| 2:v:234:ILE:O     | 2:v:238:ARG:HG2   | 2.17                     | 0.45              |
| 1:ZF:71:ARG:HB2   | 1:ZF:74:ASP:OD2   | 2.17                     | 0.44              |
| 1:ZG:39:PHE:CB    | 2:ZB:31:THR:HG22  | 2.46                     | 0.44              |
| 1:ZL:338:GLN:HB3  | 2:ZA:167:PRO:HD3  | 1.99                     | 0.44              |
| 1:ZQ:42:MET:HE2   | 1:ZQ:50:LEU:HD22  | 1.98                     | 0.44              |
| 1:ZQ:373:VAL:O    | 1:ZQ:377:VAL:HG23 | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZT:71:ARG:NH2   | 1:ZT:100:PHE:O    | 2.45                     | 0.44              |
| 1:ZZ:281:GLN:OE1  | 1:ZZ:281:GLN:N    | 2.50                     | 0.44              |
| 1:Za:269:GLN:OE1  | 1:Zg:286:PRO:HG3  | 2.17                     | 0.44              |
| 1:Zc:69:THR:HG21  | 1:Zc:361:LEU:HD12 | 1.99                     | 0.44              |
| 1:Zc:125:PRO:HA   | 1:Zc:126:PRO:HD3  | 1.88                     | 0.44              |
| 1:Zf:196:MET:HE1  | 1:Zf:259:PHE:CZ   | 2.52                     | 0.44              |
| 1:Zh:154:MET:HG2  | 1:Zh:279:THR:HG22 | 1.98                     | 0.44              |
| 2:5:100:GLN:HE21  | 2:5:177:THR:HG21  | 1.82                     | 0.44              |
| 2:9:36:ARG:HH21   | 2:9:80:LEU:HD22   | 1.82                     | 0.44              |
| 2:1:100:GLN:HE22  | 2:w:147:LEU:HD23  | 1.82                     | 0.44              |
| 2:u:178:PHE:HE1   | 2:u:201:PRO:HB3   | 1.82                     | 0.44              |
| 2:w:102:PHE:HB3   | 2:w:114:TYR:HB3   | 1.99                     | 0.44              |
| 1:ZG:384:SER:OG   | 2:ZB:26:LEU:HD22  | 2.17                     | 0.44              |
| 1:ZH:93:PHE:HB3   | 1:ZH:333:VAL:HG13 | 1.99                     | 0.44              |
| 1:ZI:399:LEU:HD13 | 2:7:227:ALA:CB    | 2.46                     | 0.44              |
| 1:ZJ:45:GLY:O     | 2:ZE:186:SER:O    | 2.34                     | 0.44              |
| 1:ZJ:93:PHE:HB3   | 1:ZJ:333:VAL:HG13 | 1.99                     | 0.44              |
| 1:ZJ:350:SER:OG   | 1:ZJ:351:GLY:N    | 2.48                     | 0.44              |
| 1:ZL:47:LYS:HE3   | 1:ZL:47:LYS:HB2   | 1.81                     | 0.44              |
| 1:ZL:322:ASN:OD1  | 1:ZL:325:GLY:N    | 2.50                     | 0.44              |
| 1:ZN:99:GLN:HG2   | 1:ZN:361:LEU:HD11 | 1.98                     | 0.44              |
| 1:ZZ:74:ASP:O     | 1:ZZ:359:GLY:N    | 2.50                     | 0.44              |
| 2:5:55:GLN:HA     | 2:5:55:GLN:HE21   | 1.82                     | 0.44              |
| 2:6:189:GLU:HA    | 2:ZB:42:GLU:HB2   | 1.98                     | 0.44              |
| 2:ZE:70:THR:HG22  | 2:ZE:71:GLY:H     | 1.82                     | 0.44              |
| 2:ZE:255:GLN:O    | 2:ZE:259:GLN:HG2  | 2.17                     | 0.44              |
| 1:ZH:233:ASN:HD21 | 1:ZH:237:ILE:HB   | 1.82                     | 0.44              |
| 1:ZI:95:SER:OG    | 1:ZI:332:ASN:O    | 2.23                     | 0.44              |
| 1:ZJ:396:LEU:HD23 | 1:ZJ:396:LEU:HA   | 1.84                     | 0.44              |
| 1:ZN:44:ALA:CB    | 2:ZC:98:LYS:HE2   | 2.48                     | 0.44              |
| 1:ZP:103:ASP:OD1  | 1:ZP:107:ASN:N    | 2.50                     | 0.44              |
| 1:Ze:80:ASN:OD1   | 1:Ze:81:GLY:N     | 2.50                     | 0.44              |
| 2:4:33:GLY:N      | 2:4:220:GLU:O     | 2.49                     | 0.44              |
| 2:5:257:LEU:O     | 2:5:260:LEU:HB2   | 2.16                     | 0.44              |
| 2:9:37:GLN:HE21   | 2:9:79:ARG:NH1    | 2.08                     | 0.44              |
| 2:ZD:175:LEU:HD12 | 2:ZD:206:PRO:HB3  | 1.99                     | 0.44              |
| 2:1:178:PHE:CE1   | 2:1:201:PRO:HB3   | 2.50                     | 0.44              |
| 2:s:47:GLN:O      | 2:s:67:GLN:HA     | 2.17                     | 0.44              |
| 1:ZI:87:ASP:OD1   | 1:ZI:87:ASP:N     | 2.37                     | 0.44              |
| 1:ZJ:39:PHE:CB    | 2:ZE:31:THR:HG22  | 2.48                     | 0.44              |
| 1:ZJ:146:ALA:HB2  | 1:ZJ:286:PRO:HD3  | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZM:102:LEU:HD12 | 1:ZM:102:LEU:HA   | 1.88                     | 0.44              |
| 1:ZS:53:LYS:HE3   | 1:ZS:53:LYS:HB2   | 1.79                     | 0.44              |
| 1:ZX:382:TYR:CE1  | 1:Zc:395:ILE:HG23 | 2.53                     | 0.44              |
| 1:ZY:74:ASP:OD2   | 1:ZY:361:LEU:HD11 | 2.18                     | 0.44              |
| 1:Zd:184:VAL:HG13 | 1:Zd:196:MET:HB2  | 1.98                     | 0.44              |
| 2:4:185:GLU:OE1   | 2:9:51:GLN:NE2    | 2.50                     | 0.44              |
| 2:8:7:ILE:O       | 2:8:10:THR:OG1    | 2.34                     | 0.44              |
| 2:ZB:164:GLN:C    | 2:ZB:166:ALA:H    | 2.26                     | 0.44              |
| 2:ZD:49:ILE:HB    | 2:ZD:66:LEU:HB3   | 1.99                     | 0.44              |
| 2:ZD:91:ASN:HB2   | 2:ZD:94:ASP:OD2   | 2.17                     | 0.44              |
| 2:1:35:LYS:HD2    | 2:1:81:HIS:HA     | 1.99                     | 0.44              |
| 2:y:43:ASP:HA     | 2:y:72:VAL:HA     | 1.99                     | 0.44              |
| 1:ZF:65:THR:HA    | 1:ZQ:50:LEU:HD11  | 1.99                     | 0.44              |
| 1:ZI:8:SER:HB3    | 1:ZI:52:VAL:H     | 1.81                     | 0.44              |
| 1:ZI:324:GLU:O    | 1:ZI:326:LEU:N    | 2.50                     | 0.44              |
| 1:ZK:126:PRO:HG2  | 1:ZK:310:GLN:HG3  | 2.00                     | 0.44              |
| 1:ZR:182:GLY:O    | 1:ZR:197:ASN:HA   | 2.17                     | 0.44              |
| 1:ZS:331:ASP:HA   | 1:ZX:40:ALA:HB1   | 1.99                     | 0.44              |
| 1:ZT:14:ALA:HB2   | 1:ZT:382:TYR:HE2  | 1.82                     | 0.44              |
| 1:ZV:368:LEU:HD23 | 1:ZV:368:LEU:HA   | 1.84                     | 0.44              |
| 1:ZZ:233:ASN:HD21 | 1:ZZ:237:ILE:HB   | 1.83                     | 0.44              |
| 1:Zf:103:ASP:OD2  | 1:Zf:104:GLU:N    | 2.48                     | 0.44              |
| 2:2:141:THR:C     | 2:2:142:ILE:HD13  | 2.41                     | 0.44              |
| 2:6:123:ASP:OD1   | 2:6:127:GLN:N     | 2.50                     | 0.44              |
| 2:9:70:THR:HG22   | 2:9:71:GLY:N      | 2.30                     | 0.44              |
| 2:0:49:ILE:HB     | 2:0:66:LEU:HG     | 1.98                     | 0.44              |
| 2:1:197:SER:HA    | 2:w:124:GLN:HB3   | 1.99                     | 0.44              |
| 2:r:24:ASN:ND2    | 2:w:69:GLY:HA3    | 2.32                     | 0.44              |
| 2:y:123:ASP:OD2   | 2:y:127:GLN:NE2   | 2.51                     | 0.44              |
| 1:ZF:65:THR:HG21  | 1:ZQ:4:SER:HB2    | 1.99                     | 0.44              |
| 1:ZI:233:ASN:OD1  | 1:ZI:237:ILE:N    | 2.47                     | 0.44              |
| 1:ZJ:178:TYR:HA   | 1:ZJ:201:VAL:HG22 | 2.00                     | 0.44              |
| 1:ZN:269:GLN:HE22 | 1:ZT:146:ALA:H    | 1.65                     | 0.44              |
| 1:ZP:71:ARG:NH1   | 1:ZP:74:ASP:OD1   | 2.51                     | 0.44              |
| 1:ZP:346:GLY:HA3  | 1:ZP:353:PHE:CE2  | 2.53                     | 0.44              |
| 1:ZR:178:TYR:HA   | 1:ZR:201:VAL:HG22 | 1.98                     | 0.44              |
| 1:ZS:170:PHE:CE2  | 1:ZS:223:PRO:HG2  | 2.52                     | 0.44              |
| 1:ZT:99:GLN:NE2   | 1:ZY:38:SER:OG    | 2.47                     | 0.44              |
| 1:ZV:16:ASN:HB2   | 1:ZV:39:PHE:HZ    | 1.83                     | 0.44              |
| 1:ZV:156:ILE:HG22 | 1:ZV:276:ILE:HG12 | 2.00                     | 0.44              |
| 1:ZW:390:LYS:O    | 1:ZW:394:GLN:HG3  | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Ze:117:THR:HA   | 1:Ze:136:PRO:HA   | 2.00                     | 0.44              |
| 1:Zg:71:ARG:NH1   | 1:Zg:74:ASP:OD1   | 2.51                     | 0.44              |
| 1:Zh:5:GLN:H      | 1:Zh:5:GLN:HG2    | 1.62                     | 0.44              |
| 2:3:76:ALA:HB1    | 2:8:64:SER:O      | 2.18                     | 0.44              |
| 2:4:74:PRO:HB2    | 2:9:66:LEU:HD11   | 1.99                     | 0.44              |
| 2:7:58:GLU:OE2    | 2:7:58:GLU:N      | 2.42                     | 0.44              |
| 2:8:137:GLN:HA    | 2:8:138:PRO:C     | 2.43                     | 0.44              |
| 2:ZE:255:GLN:O    | 2:ZE:256:LYS:C    | 2.59                     | 0.44              |
| 2:1:38:ARG:NH1    | 2:w:94:ASP:OD2    | 2.46                     | 0.44              |
| 2:1:254:LEU:O     | 2:1:258:THR:HG23  | 2.17                     | 0.44              |
| 1:ZL:368:LEU:HD12 | 1:ZL:368:LEU:HA   | 1.68                     | 0.44              |
| 1:ZS:233:ASN:OD1  | 1:ZS:237:ILE:N    | 2.49                     | 0.44              |
| 1:ZU:3:PHE:HE2    | 1:ZU:396:LEU:HD12 | 1.81                     | 0.44              |
| 1:ZV:41:ASP:OD2   | 1:ZV:41:ASP:N     | 2.46                     | 0.44              |
| 1:ZV:309:GLU:OE1  | 1:Zg:338:GLN:NE2  | 2.50                     | 0.44              |
| 1:ZY:24:ILE:HD11  | 1:Zd:384:SER:OG   | 2.18                     | 0.44              |
| 1:ZZ:10:LEU:HD21  | 1:Ze:399:LEU:HD21 | 1.99                     | 0.44              |
| 1:ZZ:307:GLU:O    | 1:ZZ:307:GLU:HG2  | 2.17                     | 0.44              |
| 1:Zb:80:ASN:OD1   | 1:Zb:80:ASN:C     | 2.61                     | 0.44              |
| 1:Zf:210:VAL:HB   | 1:Zf:228:THR:HG22 | 2.00                     | 0.44              |
| 2:2:86:LEU:HG     | 2:ZD:45:LEU:HD12  | 1.98                     | 0.44              |
| 2:6:184:LEU:HB3   | 2:6:192:TYR:HB3   | 1.99                     | 0.44              |
| 2:8:180:ASN:OD1   | 2:8:183:GLY:N     | 2.44                     | 0.44              |
| 2:ZB:215:TYR:HB3  | 2:ZB:218:TYR:CD2  | 2.53                     | 0.44              |
| 2:s:20:ASP:OD1    | 2:x:4:SER:OG      | 2.35                     | 0.44              |
| 2:s:189:GLU:O     | 2:s:191:LEU:HG    | 2.18                     | 0.44              |
| 1:ZJ:139:ILE:HG12 | 1:ZJ:312:LEU:HD13 | 1.99                     | 0.44              |
| 1:ZL:373:VAL:O    | 1:ZL:374:ASN:C    | 2.60                     | 0.44              |
| 1:ZM:307:GLU:OE1  | 1:ZM:307:GLU:O    | 2.35                     | 0.44              |
| 1:ZP:373:VAL:O    | 1:ZP:375:MET:N    | 2.50                     | 0.44              |
| 1:ZR:111:MET:N    | 1:ZR:111:MET:SD   | 2.90                     | 0.44              |
| 1:ZR:295:ASN:HB2  | 1:ZR:297:ASP:OD2  | 2.18                     | 0.44              |
| 1:ZZ:144:MET:HE2  | 1:ZZ:144:MET:HB3  | 1.83                     | 0.44              |
| 1:Zg:73:LEU:HB3   | 1:Zg:100:PHE:HB2  | 2.00                     | 0.44              |
| 2:5:3:SER:OG      | 2:0:20:ASP:OD1    | 2.36                     | 0.44              |
| 2:5:49:ILE:HG21   | 2:5:66:LEU:HD23   | 2.00                     | 0.44              |
| 2:ZA:208:LEU:C    | 2:ZA:210:GLY:H    | 2.26                     | 0.44              |
| 2:0:143:PRO:HG2   | 2:0:159:VAL:HG11  | 1.99                     | 0.44              |
| 2:x:6:TRP:O       | 2:x:10:THR:HG23   | 2.18                     | 0.44              |
| 1:ZF:47:LYS:HD3   | 2:ZA:76:ALA:HA    | 2.00                     | 0.44              |
| 1:ZL:380:ARG:HD3  | 1:ZL:380:ARG:HA   | 1.66                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZS:382:TYR:CE1  | 1:ZX:395:ILE:HG23 | 2.52                     | 0.44              |
| 1:ZV:14:ALA:HB2   | 1:ZV:382:TYR:HE2  | 1.83                     | 0.44              |
| 1:ZX:388:THR:O    | 1:ZX:392:GLN:HG2  | 2.18                     | 0.44              |
| 1:ZY:396:LEU:HD23 | 1:ZY:396:LEU:HA   | 1.77                     | 0.44              |
| 1:ZZ:2:SER:OG     | 1:ZZ:3:PHE:N      | 2.48                     | 0.44              |
| 1:Za:112:GLN:N    | 1:Za:112:GLN:OE1  | 2.51                     | 0.44              |
| 1:Zg:42:MET:SD    | 1:Zg:53:LYS:HB3   | 2.58                     | 0.44              |
| 2:5:244:SER:HB2   | 2:ZA:260:LEU:HD11 | 1.99                     | 0.44              |
| 2:6:45:LEU:HD21   | 2:v:215:TYR:HE2   | 1.83                     | 0.44              |
| 2:ZE:44:LEU:HD23  | 2:ZE:44:LEU:HA    | 1.82                     | 0.44              |
| 2:1:114:TYR:CD2   | 2:1:178:PHE:HZ    | 2.36                     | 0.44              |
| 2:w:137:GLN:HA    | 2:w:138:PRO:C     | 2.42                     | 0.44              |
| 2:y:22:ILE:HG21   | 2:y:233:MET:HG3   | 2.00                     | 0.44              |
| 2:y:95:VAL:O      | 2:y:118:GLY:HA3   | 2.18                     | 0.44              |
| 2:z:85:ASN:O      | 2:z:221:THR:OG1   | 2.33                     | 0.44              |
| 1:ZF:47:LYS:CD    | 2:ZA:76:ALA:HA    | 2.48                     | 0.43              |
| 1:ZH:352:ASN:ND2  | 2:ZC:145:ASN:HA   | 2.33                     | 0.43              |
| 1:ZL:84:ARG:HG3   | 1:ZL:84:ARG:HH11  | 1.83                     | 0.43              |
| 1:ZL:93:PHE:HE1   | 1:ZL:329:GLN:HG3  | 1.83                     | 0.43              |
| 1:ZM:6:ALA:HB1    | 1:ZM:389:ILE:HG13 | 2.00                     | 0.43              |
| 1:ZN:9:GLY:C      | 1:ZN:385:ASN:HD22 | 2.25                     | 0.43              |
| 1:ZO:95:SER:HB2   | 1:ZO:333:VAL:HG22 | 2.00                     | 0.43              |
| 1:ZO:288:ASP:H    | 1:ZO:305:SER:HG   | 1.62                     | 0.43              |
| 1:ZU:368:LEU:HD23 | 1:ZU:368:LEU:HA   | 1.80                     | 0.43              |
| 1:ZV:331:ASP:HA   | 1:Za:40:ALA:HB1   | 2.01                     | 0.43              |
| 1:Zf:38:SER:O     | 1:Zf:55:ALA:N     | 2.47                     | 0.43              |
| 2:6:128:LEU:HD23  | 2:6:128:LEU:HA    | 1.86                     | 0.43              |
| 2:7:225:ASN:O     | 2:7:229:GLU:HG2   | 2.18                     | 0.43              |
| 2:ZC:46:TYR:HA    | 2:ZC:69:GLY:HA2   | 2.00                     | 0.43              |
| 2:ZD:42:GLU:HG2   | 2:ZD:75:VAL:HG23  | 2.00                     | 0.43              |
| 2:r:22:ILE:HG21   | 2:r:233:MET:HG2   | 1.99                     | 0.43              |
| 2:x:107:LEU:HB2   | 2:x:111:THR:O     | 2.17                     | 0.43              |
| 2:y:154:ASP:OD1   | 2:y:154:ASP:O     | 2.35                     | 0.43              |
| 1:ZI:154:MET:HE2  | 1:ZI:276:ILE:HD13 | 1.99                     | 0.43              |
| 1:ZI:324:GLU:C    | 1:ZI:326:LEU:H    | 2.25                     | 0.43              |
| 1:ZN:267:MET:HE2  | 1:ZN:267:MET:HB3  | 1.78                     | 0.43              |
| 1:ZR:86:VAL:HG13  | 1:ZR:117:THR:HG21 | 2.00                     | 0.43              |
| 1:ZV:44:ALA:HB3   | 1:ZV:50:LEU:HD22  | 2.01                     | 0.43              |
| 1:ZV:208:TRP:NE1  | 1:ZV:268:GLN:OE1  | 2.50                     | 0.43              |
| 1:ZX:210:VAL:O    | 1:ZX:227:SER:HB2  | 2.18                     | 0.43              |
| 1:ZY:156:ILE:HD11 | 1:ZY:180:LYS:HG2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZY:382:TYR:CE1  | 1:Zd:395:ILE:HG23 | 2.52                     | 0.43              |
| 2:3:238:ARG:NH2   | 2:9:255:GLN:HB2   | 2.33                     | 0.43              |
| 2:4:253:MET:HE2   | 2:z:240:TYR:CD1   | 2.53                     | 0.43              |
| 2:5:208:LEU:C     | 2:5:210:GLY:H     | 2.25                     | 0.43              |
| 2:6:7:ILE:HG23    | 2:6:71:GLY:HA2    | 1.99                     | 0.43              |
| 2:0:257:LEU:HD22  | 2:v:240:TYR:OH    | 2.18                     | 0.43              |
| 2:t:5:LEU:HD23    | 2:t:5:LEU:HA      | 1.90                     | 0.43              |
| 2:t:147:LEU:HD11  | 2:y:210:GLY:HA2   | 1.99                     | 0.43              |
| 2:t:153:ARG:NH2   | 2:z:108:PRO:HG2   | 2.33                     | 0.43              |
| 2:t:188:GLY:O     | 2:t:190:ASN:N     | 2.51                     | 0.43              |
| 2:x:2:ILE:O       | 2:x:3:SER:HB3     | 2.18                     | 0.43              |
| 1:ZJ:78:SER:O     | 1:ZJ:354:GLY:HA3  | 2.18                     | 0.43              |
| 1:ZL:267:MET:HE3  | 1:ZL:267:MET:HB3  | 1.85                     | 0.43              |
| 1:ZM:14:ALA:HB2   | 1:ZM:382:TYR:HE2  | 1.82                     | 0.43              |
| 1:ZM:129:GLN:NE2  | 1:ZM:132:ALA:HB2  | 2.32                     | 0.43              |
| 1:ZR:382:TYR:CE1  | 1:ZW:395:ILE:HG23 | 2.53                     | 0.43              |
| 1:ZU:367:ASP:O    | 1:ZU:371:GLU:HG2  | 2.18                     | 0.43              |
| 1:ZV:144:MET:HB3  | 1:ZV:304:TYR:CE2  | 2.54                     | 0.43              |
| 1:ZX:37:ALA:HA    | 1:ZX:57:ILE:HD13  | 2.00                     | 0.43              |
| 1:ZX:74:ASP:OD1   | 1:ZX:74:ASP:N     | 2.51                     | 0.43              |
| 1:Ze:10:LEU:HD11  | 1:Ze:382:TYR:CE1  | 2.53                     | 0.43              |
| 1:Ze:381:ASN:O    | 1:Ze:382:TYR:C    | 2.61                     | 0.43              |
| 1:Zg:322:ASN:HB3  | 1:Zg:340:SER:HA   | 2.01                     | 0.43              |
| 2:2:95:VAL:O      | 2:2:118:GLY:HA3   | 2.18                     | 0.43              |
| 2:2:231:VAL:HG11  | 2:8:9:LYS:HG3     | 2.00                     | 0.43              |
| 2:2:255:GLN:HE21  | 2:2:259:GLN:NE2   | 2.16                     | 0.43              |
| 2:3:107:LEU:HD21  | 2:3:191:LEU:HD13  | 2.00                     | 0.43              |
| 2:0:85:ASN:O      | 2:0:221:THR:OG1   | 2.34                     | 0.43              |
| 2:0:89:THR:HG21   | 2:0:94:ASP:HB2    | 2.01                     | 0.43              |
| 2:s:95:VAL:O      | 2:s:118:GLY:HA3   | 2.18                     | 0.43              |
| 1:ZF:380:ARG:HH21 | 1:ZL:397:ASN:HB2  | 1.83                     | 0.43              |
| 1:ZJ:74:ASP:O     | 1:ZJ:359:GLY:N    | 2.36                     | 0.43              |
| 1:ZK:380:ARG:HD3  | 1:ZK:380:ARG:HA   | 1.53                     | 0.43              |
| 1:ZM:228:THR:HB   | 1:ZM:244:VAL:HG11 | 2.00                     | 0.43              |
| 1:ZO:159:ASN:ND2  | 1:ZO:162:ASP:OD2  | 2.43                     | 0.43              |
| 1:ZP:73:LEU:HD21  | 1:ZP:292:TYR:HE1  | 1.83                     | 0.43              |
| 1:ZP:107:ASN:ND2  | 1:ZP:138:THR:HG22 | 2.33                     | 0.43              |
| 1:ZU:180:LYS:HB3  | 1:ZU:200:PHE:HD1  | 1.84                     | 0.43              |
| 1:Zc:379:GLN:HE22 | 1:Zh:394:GLN:NE2  | 2.13                     | 0.43              |
| 1:Zd:269:GLN:HG2  | 1:Zd:270:ASN:H    | 1.82                     | 0.43              |
| 2:4:257:LEU:HD23  | 2:4:257:LEU:HA    | 1.81                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:8:154:ASP:O     | 2:8:172:GLN:NE2   | 2.52                     | 0.43              |
| 2:8:249:THR:O     | 2:8:253:MET:HG3   | 2.18                     | 0.43              |
| 2:ZC:128:LEU:HD12 | 2:ZC:140:ILE:HB   | 1.99                     | 0.43              |
| 2:ZE:70:THR:HG22  | 2:ZE:71:GLY:N     | 2.33                     | 0.43              |
| 2:1:188:GLY:O     | 2:1:190:ASN:N     | 2.47                     | 0.43              |
| 2:r:79:ARG:NH1    | 2:r:184:LEU:O     | 2.47                     | 0.43              |
| 2:y:102:PHE:HB3   | 2:y:114:TYR:HB3   | 2.00                     | 0.43              |
| 2:z:254:LEU:O     | 2:z:258:THR:HG23  | 2.19                     | 0.43              |
| 1:ZK:133:ASN:N    | 1:ZK:133:ASN:OD1  | 2.50                     | 0.43              |
| 1:ZK:394:GLN:O    | 1:ZK:398:THR:HG22 | 2.19                     | 0.43              |
| 1:ZN:202:LYS:HZ3  | 1:ZN:203:THR:C    | 2.26                     | 0.43              |
| 1:ZN:373:VAL:O    | 1:ZN:377:VAL:HG23 | 2.19                     | 0.43              |
| 1:ZP:188:ASP:OD2  | 1:ZP:192:ASN:N    | 2.51                     | 0.43              |
| 1:ZQ:34:SER:HB3   | 1:ZQ:366:VAL:HG12 | 2.01                     | 0.43              |
| 1:ZQ:128:ILE:HD13 | 1:ZQ:314:GLN:HB2  | 2.01                     | 0.43              |
| 1:ZQ:373:VAL:HG11 | 1:ZW:7:VAL:HG22   | 2.00                     | 0.43              |
| 1:ZV:42:MET:SD    | 1:ZV:53:LYS:HB3   | 2.58                     | 0.43              |
| 1:ZV:330:GLY:N    | 1:Za:43:PHE:HB2   | 2.33                     | 0.43              |
| 1:ZZ:56:GLY:C     | 1:ZZ:57:ILE:HD12  | 2.43                     | 0.43              |
| 1:Za:149:THR:HG23 | 1:Za:259:PHE:HB3  | 2.01                     | 0.43              |
| 1:Zb:17:LEU:CD1   | 1:Zg:395:ILE:HD11 | 2.47                     | 0.43              |
| 1:Ze:156:ILE:HD11 | 1:Ze:180:LYS:HE2  | 1.99                     | 0.43              |
| 1:Zf:114:MET:HE3  | 1:Zf:333:VAL:HG21 | 2.00                     | 0.43              |
| 2:2:42:GLU:HG3    | 2:2:43:ASP:O      | 2.18                     | 0.43              |
| 2:2:79:ARG:HG3    | 2:2:79:ARG:NH1    | 2.34                     | 0.43              |
| 2:4:47:GLN:N      | 2:4:68:ILE:O      | 2.50                     | 0.43              |
| 2:6:44:LEU:HA     | 2:6:44:LEU:HD23   | 1.83                     | 0.43              |
| 2:ZD:44:LEU:HD23  | 2:ZD:44:LEU:HA    | 1.88                     | 0.43              |
| 2:ZE:121:GLN:NE2  | 2:ZE:131:ALA:HA   | 2.33                     | 0.43              |
| 2:x:2:ILE:CG1     | 2:x:254:LEU:HD11  | 2.48                     | 0.43              |
| 1:ZG:210:VAL:O    | 1:ZG:227:SER:N    | 2.52                     | 0.43              |
| 1:ZG:288:ASP:N    | 1:ZG:288:ASP:OD1  | 2.51                     | 0.43              |
| 1:ZR:122:THR:OG1  | 1:ZR:129:GLN:OE1  | 2.26                     | 0.43              |
| 1:ZS:6:ALA:C      | 1:ZS:8:SER:N      | 2.77                     | 0.43              |
| 1:Zc:381:ASN:O    | 1:Zc:385:ASN:ND2  | 2.51                     | 0.43              |
| 1:Ze:107:ASN:HD22 | 1:Ze:138:THR:HG22 | 1.82                     | 0.43              |
| 2:5:95:VAL:O      | 2:5:118:GLY:HA3   | 2.18                     | 0.43              |
| 2:5:249:THR:O     | 2:5:253:MET:HG3   | 2.19                     | 0.43              |
| 2:6:238:ARG:HD3   | 2:6:238:ARG:HA    | 1.79                     | 0.43              |
| 2:ZE:19:MET:HE2   | 2:ZE:19:MET:HB2   | 1.92                     | 0.43              |
| 2:u:187:ILE:HG23  | 2:u:193:ILE:HG12  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZF:47:LYS:HD3   | 2:ZA:76:ALA:CB    | 2.49                     | 0.43              |
| 1:ZJ:248:THR:HG23 | 1:ZJ:257:ALA:O    | 2.19                     | 0.43              |
| 1:ZK:58:THR:OG1   | 1:ZK:324:GLU:OE2  | 2.30                     | 0.43              |
| 1:ZK:102:LEU:HD21 | 1:ZK:106:ARG:HA   | 1.99                     | 0.43              |
| 1:ZM:30:TYR:HD1   | 1:ZM:363:ALA:HA   | 1.83                     | 0.43              |
| 1:ZP:50:LEU:HD22  | 2:ZE:85:ASN:ND2   | 2.33                     | 0.43              |
| 1:ZV:188:ASP:OD2  | 1:ZV:194:HIS:NE2  | 2.51                     | 0.43              |
| 1:ZV:380:ARG:NE   | 1:Zb:393:ASP:OD2  | 2.46                     | 0.43              |
| 1:Za:108:LEU:HD23 | 1:Za:108:LEU:HA   | 1.83                     | 0.43              |
| 1:Zg:269:GLN:HG2  | 1:Zg:270:ASN:H    | 1.83                     | 0.43              |
| 2:5:67:GLN:O      | 2:0:37:GLN:NE2    | 2.49                     | 0.43              |
| 2:7:44:LEU:HD23   | 2:7:44:LEU:HA     | 1.84                     | 0.43              |
| 2:8:185:GLU:HG3   | 2:ZD:67:GLN:HE22  | 1.83                     | 0.43              |
| 2:ZE:89:THR:HG23  | 2:ZE:91:ASN:HB2   | 1.99                     | 0.43              |
| 2:y:87:SER:OG     | 2:y:219:VAL:HG23  | 2.19                     | 0.43              |
| 1:ZF:158:LEU:HD22 | 1:ZF:208:TRP:CZ3  | 2.54                     | 0.43              |
| 1:ZG:399:LEU:CD2  | 2:ZB:244:SER:HB2  | 2.49                     | 0.43              |
| 1:ZI:396:LEU:HD23 | 1:ZI:396:LEU:HA   | 1.91                     | 0.43              |
| 1:ZJ:121:ALA:HB1  | 1:ZJ:126:PRO:HB2  | 2.00                     | 0.43              |
| 1:ZP:77:ILE:HD13  | 1:ZP:356:LEU:HG   | 2.00                     | 0.43              |
| 1:ZP:352:ASN:O    | 1:ZP:352:ASN:OD1  | 2.37                     | 0.43              |
| 1:ZQ:75:VAL:O     | 1:ZQ:98:GLY:HA3   | 2.18                     | 0.43              |
| 1:ZQ:352:ASN:OD1  | 1:ZQ:352:ASN:O    | 2.37                     | 0.43              |
| 1:ZS:202:LYS:HG3  | 1:ZS:208:TRP:CE2  | 2.53                     | 0.43              |
| 1:ZT:185:THR:HG22 | 1:ZT:187:TYR:HE1  | 1.84                     | 0.43              |
| 1:ZT:186:VAL:C    | 1:ZT:187:TYR:HD1  | 2.26                     | 0.43              |
| 1:ZU:159:ASN:HA   | 1:ZU:269:GLN:O    | 2.19                     | 0.43              |
| 1:ZX:307:GLU:O    | 1:ZX:308:GLN:HG2  | 2.18                     | 0.43              |
| 1:ZX:396:LEU:HD23 | 1:ZX:396:LEU:HA   | 1.78                     | 0.43              |
| 1:Zb:194:HIS:CE1  | 1:Zb:251:ILE:HD12 | 2.53                     | 0.43              |
| 1:Zd:83:PHE:HB2   | 1:Zd:95:SER:O     | 2.19                     | 0.43              |
| 1:Zh:185:THR:OG1  | 1:Zh:195:ASP:OD1  | 2.22                     | 0.43              |
| 2:6:175:LEU:HG    | 2:6:206:PRO:HG3   | 2.00                     | 0.43              |
| 2:8:42:GLU:N      | 2:8:73:ARG:O      | 2.52                     | 0.43              |
| 2:s:225:ASN:OD1   | 2:s:226:VAL:N     | 2.51                     | 0.43              |
| 2:u:195:THR:HG22  | 2:u:197:SER:H     | 1.84                     | 0.43              |
| 2:v:35:LYS:HA     | 2:v:35:LYS:HD3    | 1.92                     | 0.43              |
| 2:z:7:ILE:HG12    | 2:z:70:THR:O      | 2.19                     | 0.43              |
| 1:ZG:296:ASN:O    | 1:ZG:296:ASN:ND2  | 2.52                     | 0.43              |
| 1:ZJ:367:ASP:CG   | 1:ZJ:370:LYS:HB2  | 2.44                     | 0.43              |
| 1:ZL:65:THR:HA    | 1:ZW:50:LEU:HD13  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZP:159:ASN:N    | 1:ZP:274:ASN:OD1  | 2.47                     | 0.43              |
| 1:ZQ:27:SER:OG    | 1:ZV:381:ASN:ND2  | 2.52                     | 0.43              |
| 1:ZR:229:THR:O    | 1:ZR:241:GLY:HA3  | 2.19                     | 0.43              |
| 1:ZS:103:ASP:OD2  | 1:ZS:103:ASP:C    | 2.62                     | 0.43              |
| 1:ZY:5:GLN:HG2    | 1:ZY:50:LEU:O     | 2.19                     | 0.43              |
| 1:Zc:60:ASP:O     | 1:Zc:365:ASN:ND2  | 2.52                     | 0.43              |
| 1:Zf:71:ARG:HB2   | 1:Zf:74:ASP:OD2   | 2.19                     | 0.43              |
| 2:ZD:77:THR:O     | 2:ZD:77:THR:OG1   | 2.32                     | 0.43              |
| 2:ZE:137:GLN:HA   | 2:ZE:138:PRO:C    | 2.43                     | 0.43              |
| 2:w:95:VAL:O      | 2:w:118:GLY:HA3   | 2.18                     | 0.43              |
| 2:y:195:THR:HG22  | 2:y:197:SER:H     | 1.83                     | 0.43              |
| 1:ZJ:199:TYR:O    | 1:ZJ:210:VAL:HA   | 2.19                     | 0.43              |
| 1:ZL:78:SER:O     | 1:ZL:354:GLY:HA3  | 2.19                     | 0.43              |
| 1:ZO:212:THR:O    | 1:ZO:223:PRO:HG3  | 2.19                     | 0.43              |
| 1:ZR:211:TYR:CE1  | 1:ZR:226:ALA:HA   | 2.53                     | 0.43              |
| 1:ZW:111:MET:HE2  | 1:ZW:111:MET:HA   | 2.00                     | 0.43              |
| 1:ZX:99:GLN:HB3   | 1:ZX:111:MET:HE3  | 2.01                     | 0.43              |
| 1:ZZ:119:TYR:HB2  | 1:ZZ:128:ILE:HD11 | 2.01                     | 0.43              |
| 1:Ze:397:ASN:O    | 1:Ze:400:VAL:N    | 2.52                     | 0.43              |
| 2:2:237:GLN:O     | 2:2:241:GLU:HG3   | 2.19                     | 0.43              |
| 2:3:36:ARG:HE     | 2:3:80:LEU:HD22   | 1.84                     | 0.43              |
| 2:5:153:ARG:HH22  | 2:ZB:108:PRO:HG2  | 1.82                     | 0.43              |
| 2:8:179:MET:HE2   | 2:8:179:MET:HA    | 2.01                     | 0.43              |
| 2:9:95:VAL:O      | 2:9:118:GLY:HA3   | 2.19                     | 0.43              |
| 2:ZA:35:LYS:O     | 2:ZA:79:ARG:NH1   | 2.46                     | 0.43              |
| 2:0:95:VAL:O      | 2:0:118:GLY:HA3   | 2.18                     | 0.43              |
| 2:t:77:THR:HG23   | 2:y:66:LEU:HB2    | 2.01                     | 0.43              |
| 1:ZG:107:ASN:ND2  | 1:ZG:138:THR:HG22 | 2.33                     | 0.42              |
| 1:ZM:71:ARG:NH1   | 1:ZM:74:ASP:OD1   | 2.52                     | 0.42              |
| 1:ZN:165:PRO:HB3  | 1:ZN:176:ASP:O    | 2.19                     | 0.42              |
| 1:ZN:230:LEU:HD12 | 1:ZN:230:LEU:HA   | 1.85                     | 0.42              |
| 1:ZQ:382:TYR:CE1  | 1:ZV:395:ILE:HG23 | 2.53                     | 0.42              |
| 1:ZR:204:LYS:HG2  | 1:ZR:205:ASP:H    | 1.84                     | 0.42              |
| 1:ZU:396:LEU:HD23 | 1:ZU:396:LEU:HA   | 1.80                     | 0.42              |
| 1:ZY:137:ILE:HG21 | 1:ZY:300:VAL:HG21 | 2.00                     | 0.42              |
| 1:ZZ:319:ASN:HB2  | 1:ZZ:353:PHE:CE1  | 2.54                     | 0.42              |
| 1:Ze:100:PHE:CE2  | 1:Ze:116:LEU:HD13 | 2.53                     | 0.42              |
| 1:Zf:99:GLN:HE21  | 1:Zf:361:LEU:HD11 | 1.84                     | 0.42              |
| 1:Zf:107:ASN:ND2  | 1:Zf:138:THR:HG22 | 2.34                     | 0.42              |
| 1:Zg:117:THR:HA   | 1:Zg:136:PRO:HA   | 2.01                     | 0.42              |
| 1:Zh:392:GLN:HA   | 1:Zh:395:ILE:CG2  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4:34:PHE:HB3    | 2:4:222:SER:HB3   | 2.01                     | 0.42              |
| 2:5:3:SER:HB2     | 2:u:85:ASN:ND2    | 2.34                     | 0.42              |
| 2:7:49:ILE:HB     | 2:7:66:LEU:HB3    | 2.01                     | 0.42              |
| 2:7:142:ILE:HD13  | 2:7:170:VAL:HG21  | 2.00                     | 0.42              |
| 2:9:257:LEU:O     | 2:9:258:THR:C     | 2.61                     | 0.42              |
| 2:ZA:103:PHE:HE1  | 2:ZA:214:LEU:HD21 | 1.83                     | 0.42              |
| 2:ZB:44:LEU:HD23  | 2:ZB:44:LEU:HA    | 1.87                     | 0.42              |
| 2:ZD:138:PRO:O    | 2:ZD:140:ILE:HG13 | 2.18                     | 0.42              |
| 2:ZE:19:MET:HE2   | 2:ZE:236:VAL:HG12 | 2.01                     | 0.42              |
| 2:t:80:LEU:HD22   | 2:t:82:SER:HB3    | 2.00                     | 0.42              |
| 2:y:189:GLU:O     | 2:y:191:LEU:HG    | 2.19                     | 0.42              |
| 1:ZG:396:LEU:HD23 | 1:ZG:396:LEU:HA   | 1.80                     | 0.42              |
| 1:ZH:398:THR:HG21 | 2:ZC:241:GLU:HG2  | 2.00                     | 0.42              |
| 1:ZK:112:GLN:HG2  | 1:ZK:331:ASP:HB3  | 1.99                     | 0.42              |
| 1:ZL:280:ASN:OD1  | 1:ZL:281:GLN:N    | 2.52                     | 0.42              |
| 1:ZS:41:ASP:OD2   | 1:ZS:41:ASP:N     | 2.45                     | 0.42              |
| 1:ZS:288:ASP:O    | 1:ZS:305:SER:N    | 2.52                     | 0.42              |
| 1:ZT:262:SER:OG   | 1:ZT:264:LEU:HG   | 2.18                     | 0.42              |
| 1:ZX:361:LEU:HD12 | 1:ZX:361:LEU:HA   | 1.89                     | 0.42              |
| 1:Zc:5:GLN:HG2    | 1:Zc:50:LEU:O     | 2.19                     | 0.42              |
| 1:Zh:320:PHE:CD2  | 1:Zh:340:SER:HB2  | 2.54                     | 0.42              |
| 2:3:173:LEU:HD23  | 2:3:214:LEU:HD13  | 1.99                     | 0.42              |
| 2:3:218:TYR:CE1   | 2:ZE:73:ARG:HD2   | 2.53                     | 0.42              |
| 2:ZA:86:LEU:HD22  | 2:ZA:96:ALA:HB1   | 2.01                     | 0.42              |
| 2:ZD:123:ASP:OD1  | 2:ZD:123:ASP:N    | 2.46                     | 0.42              |
| 2:1:7:ILE:HG12    | 2:1:70:THR:O      | 2.18                     | 0.42              |
| 1:ZG:393:ASP:OD1  | 2:ZA:238:ARG:NE   | 2.40                     | 0.42              |
| 1:ZH:281:GLN:OE1  | 1:ZH:281:GLN:C    | 2.63                     | 0.42              |
| 1:ZI:49:GLY:CA    | 2:ZD:24:ASN:ND2   | 2.74                     | 0.42              |
| 1:ZI:105:ASN:OD1  | 1:ZI:105:ASN:N    | 2.53                     | 0.42              |
| 1:ZL:3:PHE:HE1    | 1:ZL:396:LEU:HD12 | 1.85                     | 0.42              |
| 1:ZL:159:ASN:HD21 | 1:ZL:161:THR:HG23 | 1.84                     | 0.42              |
| 1:ZQ:319:ASN:OD1  | 1:ZQ:344:LEU:HB2  | 2.20                     | 0.42              |
| 1:ZS:180:LYS:NZ   | 1:ZS:274:ASN:O    | 2.52                     | 0.42              |
| 1:ZS:245:ASN:OD1  | 1:ZS:245:ASN:N    | 2.53                     | 0.42              |
| 1:ZS:319:ASN:C    | 1:ZS:319:ASN:OD1  | 2.62                     | 0.42              |
| 1:ZV:346:GLY:HA3  | 1:ZV:353:PHE:CE2  | 2.54                     | 0.42              |
| 1:Za:125:PRO:HA   | 1:Za:126:PRO:HD2  | 1.85                     | 0.42              |
| 1:Za:375:MET:HE2  | 1:Za:375:MET:HB2  | 1.82                     | 0.42              |
| 1:Zf:27:SER:O     | 1:Zf:364:SER:OG   | 2.36                     | 0.42              |
| 1:Zf:187:TYR:HB3  | 1:Zf:191:GLY:HA2  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Zg:96:ARG:H     | 1:Zg:334:TRP:HZ3  | 1.67                     | 0.42              |
| 2:4:67:GLN:NE2    | 2:z:185:GLU:OE2   | 2.52                     | 0.42              |
| 2:4:122:VAL:HG13  | 2:4:126:GLY:HA2   | 2.02                     | 0.42              |
| 2:ZA:59:GLN:HG2   | 2:ZA:60:THR:HG23  | 2.01                     | 0.42              |
| 2:ZE:70:THR:CG2   | 2:ZE:71:GLY:H     | 2.32                     | 0.42              |
| 2:1:100:GLN:NE2   | 2:1:210:GLY:O     | 2.51                     | 0.42              |
| 2:t:151:ILE:HG12  | 2:t:157:VAL:HG22  | 2.01                     | 0.42              |
| 1:ZF:93:PHE:HB3   | 1:ZF:333:VAL:HG13 | 2.00                     | 0.42              |
| 1:ZF:104:GLU:CD   | 1:ZK:341:GLY:HA2  | 2.45                     | 0.42              |
| 1:ZK:153:SER:HB2  | 1:ZK:280:ASN:OD1  | 2.19                     | 0.42              |
| 1:ZK:317:LEU:HD11 | 1:ZK:356:LEU:HD11 | 2.00                     | 0.42              |
| 1:ZP:175:ALA:HA   | 1:ZP:178:TYR:CZ   | 2.55                     | 0.42              |
| 1:ZR:10:LEU:HG    | 1:ZR:382:TYR:CE2  | 2.55                     | 0.42              |
| 1:ZS:109:VAL:HG12 | 1:ZS:115:GLN:HA   | 2.01                     | 0.42              |
| 1:ZS:373:VAL:O    | 1:ZS:377:VAL:HG23 | 2.20                     | 0.42              |
| 1:ZU:322:ASN:HB3  | 1:ZU:340:SER:HA   | 2.01                     | 0.42              |
| 1:ZU:386:ALA:O    | 1:ZU:389:ILE:HG22 | 2.20                     | 0.42              |
| 1:ZZ:95:SER:OG    | 1:ZZ:332:ASN:O    | 2.34                     | 0.42              |
| 1:ZZ:97:ASN:HD22  | 1:ZZ:332:ASN:ND2  | 2.17                     | 0.42              |
| 1:Za:368:LEU:O    | 1:Za:372:LEU:N    | 2.47                     | 0.42              |
| 1:Zb:379:GLN:OE1  | 1:Zg:391:THR:HG23 | 2.19                     | 0.42              |
| 1:Zd:296:ASN:OD1  | 1:Zd:355:LYS:HD2  | 2.20                     | 0.42              |
| 2:4:196:GLN:NE2   | 2:9:53:GLY:O      | 2.52                     | 0.42              |
| 2:9:124:GLN:HB2   | 2:ZE:199:GLY:HA2  | 2.01                     | 0.42              |
| 2:ZA:55:GLN:HG3   | 2:ZA:57:SER:O     | 2.19                     | 0.42              |
| 2:ZB:225:ASN:O    | 2:ZB:229:GLU:HG2  | 2.19                     | 0.42              |
| 2:1:1:MET:HE3     | 2:1:1:MET:HB3     | 1.80                     | 0.42              |
| 2:u:175:LEU:HD12  | 2:u:206:PRO:HB3   | 2.00                     | 0.42              |
| 2:x:98:LYS:O      | 2:x:98:LYS:HG2    | 2.19                     | 0.42              |
| 2:y:120:PHE:CE1   | 2:y:136:VAL:HG21  | 2.54                     | 0.42              |
| 1:ZK:27:SER:HA    | 1:ZK:366:VAL:CG2  | 2.48                     | 0.42              |
| 1:ZN:390:LYS:O    | 1:ZN:394:GLN:HG3  | 2.19                     | 0.42              |
| 1:ZR:18:ASP:HB3   | 1:ZW:5:GLN:HE22   | 1.85                     | 0.42              |
| 1:Zb:111:MET:N    | 1:Zb:111:MET:SD   | 2.92                     | 0.42              |
| 1:Zb:326:LEU:HD12 | 1:Zb:340:SER:HB2  | 2.01                     | 0.42              |
| 1:Zb:373:VAL:HG11 | 1:Zh:7:VAL:HG22   | 2.02                     | 0.42              |
| 1:Zc:213:HIS:HB2  | 1:Zc:223:PRO:HG3  | 2.01                     | 0.42              |
| 2:2:256:LYS:HG2   | 2:x:241:GLU:HG2   | 2.01                     | 0.42              |
| 2:6:42:GLU:HB3    | 2:6:75:VAL:HG22   | 2.01                     | 0.42              |
| 2:6:43:ASP:OD1    | 2:1:28:ASN:ND2    | 2.53                     | 0.42              |
| 2:7:76:ALA:HB1    | 2:ZC:64:SER:O     | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZD:58:GLU:HB3   | 2:ZD:59:GLN:OE1   | 2.20                     | 0.42              |
| 2:0:9:LYS:HG3     | 2:u:231:VAL:HG21  | 2.01                     | 0.42              |
| 2:r:107:LEU:HD11  | 2:r:191:LEU:HD13  | 2.01                     | 0.42              |
| 2:t:189:GLU:HG2   | 2:y:42:GLU:CD     | 2.45                     | 0.42              |
| 2:z:185:GLU:HB3   | 2:z:193:ILE:HG13  | 2.02                     | 0.42              |
| 1:ZF:374:ASN:HA   | 1:ZF:377:VAL:HG22 | 2.00                     | 0.42              |
| 1:ZG:214:ASP:OD2  | 1:ZG:249:GLY:N    | 2.46                     | 0.42              |
| 1:ZL:22:ASN:OD1   | 1:ZL:26:ASN:ND2   | 2.53                     | 0.42              |
| 1:ZM:381:ASN:O    | 1:ZM:385:ASN:ND2  | 2.53                     | 0.42              |
| 1:ZN:6:ALA:HB1    | 1:ZN:389:ILE:HG12 | 2.02                     | 0.42              |
| 1:ZN:269:GLN:HG2  | 1:ZT:190:GLN:O    | 2.20                     | 0.42              |
| 1:ZR:38:SER:O     | 1:ZR:55:ALA:N     | 2.51                     | 0.42              |
| 1:ZS:373:VAL:HG11 | 1:ZY:7:VAL:HG22   | 2.02                     | 0.42              |
| 1:ZS:396:LEU:HD23 | 1:ZS:396:LEU:HA   | 1.88                     | 0.42              |
| 1:ZT:93:PHE:HB3   | 1:ZT:333:VAL:HG13 | 2.01                     | 0.42              |
| 2:8:98:LYS:NZ     | 2:ZE:187:ILE:O    | 2.51                     | 0.42              |
| 2:0:35:LYS:HD2    | 2:0:81:HIS:HA     | 2.01                     | 0.42              |
| 2:t:95:VAL:O      | 2:t:118:GLY:HA3   | 2.20                     | 0.42              |
| 2:x:180:ASN:O     | 2:x:198:SER:HB2   | 2.19                     | 0.42              |
| 1:ZN:95:SER:OG    | 1:ZN:332:ASN:O    | 2.30                     | 0.42              |
| 1:ZR:380:ARG:HD3  | 1:ZR:380:ARG:HA   | 1.75                     | 0.42              |
| 1:ZR:387:GLN:O    | 1:ZR:391:THR:HG23 | 2.19                     | 0.42              |
| 1:ZT:331:ASP:HA   | 1:ZY:40:ALA:HB1   | 2.01                     | 0.42              |
| 1:ZU:78:SER:O     | 1:ZU:354:GLY:HA3  | 2.20                     | 0.42              |
| 1:ZV:24:ILE:O     | 1:ZV:27:SER:OG    | 2.28                     | 0.42              |
| 1:ZV:212:THR:HG21 | 1:ZV:246:ILE:HD11 | 2.01                     | 0.42              |
| 1:ZV:401:ASN:O    | 1:ZV:402:LEU:C    | 2.62                     | 0.42              |
| 1:ZW:331:ASP:O    | 1:ZW:333:VAL:HG23 | 2.20                     | 0.42              |
| 1:ZY:60:ASP:OD2   | 1:ZY:365:ASN:ND2  | 2.53                     | 0.42              |
| 1:ZY:298:GLY:HA3  | 1:ZY:315:ILE:HG22 | 2.01                     | 0.42              |
| 1:Za:83:PHE:HB2   | 1:Za:95:SER:O     | 2.19                     | 0.42              |
| 1:Zb:380:ARG:HA   | 1:Zb:380:ARG:HD3  | 1.68                     | 0.42              |
| 1:Zg:103:ASP:HB3  | 1:Zg:109:VAL:HG21 | 2.01                     | 0.42              |
| 2:4:1:MET:HE2     | 2:4:254:LEU:HD22  | 2.02                     | 0.42              |
| 2:7:145:ASN:HB2   | 2:ZC:209:ASN:O    | 2.19                     | 0.42              |
| 2:8:44:LEU:HD23   | 2:8:44:LEU:HA     | 1.82                     | 0.42              |
| 2:8:55:GLN:HG3    | 2:s:169:GLN:HE22  | 1.85                     | 0.42              |
| 2:9:43:ASP:OD1    | 2:9:44:LEU:N      | 2.53                     | 0.42              |
| 2:ZC:184:LEU:HB3  | 2:ZC:192:TYR:HB3  | 2.00                     | 0.42              |
| 2:s:238:ARG:NH2   | 2:y:251:ASP:OD1   | 2.27                     | 0.42              |
| 2:x:127:GLN:HA    | 2:x:140:ILE:O     | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZG:7:VAL:HG22   | 2:ZA:231:VAL:HG11 | 2.02                     | 0.42              |
| 1:ZG:93:PHE:HB3   | 1:ZG:333:VAL:HG13 | 2.01                     | 0.42              |
| 1:ZI:63:ASP:OD2   | 1:ZI:96:ARG:NH2   | 2.52                     | 0.42              |
| 1:ZK:138:THR:HG22 | 1:ZK:140:PRO:HD3  | 2.00                     | 0.42              |
| 1:ZN:269:GLN:HB3  | 1:ZT:286:PRO:HG2  | 2.02                     | 0.42              |
| 1:ZP:71:ARG:O     | 1:ZP:359:GLY:HA2  | 2.19                     | 0.42              |
| 1:ZR:246:ILE:HD13 | 1:ZR:246:ILE:HA   | 1.88                     | 0.42              |
| 1:ZU:380:ARG:HH21 | 1:ZU:383:GLN:NE2  | 2.18                     | 0.42              |
| 1:ZX:16:ASN:HB2   | 1:ZX:39:PHE:HZ    | 1.85                     | 0.42              |
| 1:Zd:210:VAL:HG11 | 1:Zd:263:PHE:CZ   | 2.55                     | 0.42              |
| 1:Zf:94:TYR:CG    | 1:Zf:320:PHE:HZ   | 2.37                     | 0.42              |
| 1:Zg:396:LEU:HD23 | 1:Zg:396:LEU:HA   | 1.78                     | 0.42              |
| 2:6:142:ILE:HD13  | 2:6:149:ILE:HD13  | 2.01                     | 0.42              |
| 2:9:116:ARG:HG3   | 2:9:116:ARG:O     | 2.20                     | 0.42              |
| 2:x:19:MET:HE1    | 2:x:233:MET:HG2   | 2.02                     | 0.42              |
| 1:ZF:380:ARG:HD3  | 1:ZF:380:ARG:HA   | 1.69                     | 0.42              |
| 1:ZI:24:ILE:HG22  | 1:ZN:385:ASN:OD1  | 2.18                     | 0.42              |
| 1:ZK:399:LEU:CD1  | 2:9:227:ALA:HB1   | 2.50                     | 0.42              |
| 1:ZN:397:ASN:O    | 1:ZN:398:THR:C    | 2.60                     | 0.42              |
| 1:ZO:380:ARG:HD3  | 1:ZO:380:ARG:HA   | 1.81                     | 0.42              |
| 1:ZQ:10:LEU:HD23  | 1:ZQ:10:LEU:HA    | 1.78                     | 0.42              |
| 1:ZS:232:PHE:HB3  | 1:ZS:236:GLY:HA2  | 2.01                     | 0.42              |
| 1:ZT:34:SER:HB3   | 1:ZT:366:VAL:HG22 | 2.01                     | 0.42              |
| 1:ZT:71:ARG:O     | 1:ZT:359:GLY:HA2  | 2.20                     | 0.42              |
| 1:ZW:69:THR:HG21  | 1:ZW:361:LEU:HD12 | 2.02                     | 0.42              |
| 1:ZY:269:GLN:OE1  | 1:Ze:286:PRO:HB3  | 2.20                     | 0.42              |
| 1:Ze:150:THR:OG1  | 1:Ze:282:ASN:ND2  | 2.51                     | 0.42              |
| 1:Zg:367:ASP:O    | 1:Zg:371:GLU:HG2  | 2.20                     | 0.42              |
| 2:5:10:THR:OG1    | 2:5:71:GLY:HA3    | 2.20                     | 0.42              |
| 2:5:175:LEU:HG    | 2:5:206:PRO:HG3   | 2.02                     | 0.42              |
| 2:6:76:ALA:HB1    | 2:ZB:64:SER:O     | 2.20                     | 0.42              |
| 2:9:245:LYS:HB2   | 2:9:245:LYS:HE2   | 1.78                     | 0.42              |
| 2:s:43:ASP:N      | 2:s:43:ASP:OD1    | 2.53                     | 0.42              |
| 2:t:185:GLU:HB3   | 2:t:193:ILE:HG22  | 2.02                     | 0.42              |
| 2:x:5:LEU:HD23    | 2:x:5:LEU:HA      | 1.87                     | 0.42              |
| 1:ZF:47:LYS:HZ2   | 2:ZA:76:ALA:HA    | 1.85                     | 0.42              |
| 1:ZG:144:MET:HE2  | 1:ZG:310:GLN:HE21 | 1.85                     | 0.42              |
| 1:ZG:399:LEU:HD11 | 2:ZB:240:TYR:HH   | 1.78                     | 0.42              |
| 1:ZH:373:VAL:HG11 | 1:ZN:7:VAL:HG22   | 2.02                     | 0.42              |
| 1:ZK:14:ALA:HB2   | 1:ZK:382:TYR:HE2  | 1.85                     | 0.42              |
| 1:ZO:148:SER:HB3  | 1:ZO:188:ASP:C    | 2.45                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZQ:337:THR:HG22 | 1:ZQ:339:ALA:H    | 1.84                     | 0.42              |
| 1:ZS:17:LEU:CD1   | 1:ZX:395:ILE:HD11 | 2.50                     | 0.42              |
| 1:ZS:380:ARG:NH2  | 1:ZY:397:ASN:OD1  | 2.53                     | 0.42              |
| 1:ZU:78:SER:HB3   | 1:ZU:79:GLN:OE1   | 2.19                     | 0.42              |
| 1:ZY:126:PRO:HG2  | 1:ZY:310:GLN:NE2  | 2.35                     | 0.42              |
| 1:Za:284:TYR:HB3  | 1:Za:308:GLN:HE22 | 1.85                     | 0.42              |
| 1:Zb:233:ASN:OD1  | 1:Zb:237:ILE:N    | 2.51                     | 0.42              |
| 1:Zd:397:ASN:C    | 1:Zd:399:LEU:H    | 2.28                     | 0.42              |
| 2:2:241:GLU:HG2   | 2:7:256:LYS:HG2   | 2.01                     | 0.42              |
| 2:3:230:LEU:HD13  | 2:ZE:257:LEU:HB3  | 2.01                     | 0.42              |
| 2:ZC:80:LEU:HD23  | 2:ZC:80:LEU:HA    | 1.75                     | 0.42              |
| 2:t:228:GLU:HG3   | 2:z:9:LYS:HE3     | 2.02                     | 0.42              |
| 2:v:188:GLY:O     | 2:v:190:ASN:N     | 2.45                     | 0.42              |
| 2:x:193:ILE:HG22  | 2:x:194:GLU:O     | 2.20                     | 0.42              |
| 2:y:88:GLN:HB2    | 2:y:218:TYR:CE1   | 2.55                     | 0.42              |
| 1:ZF:106:ARG:HB3  | 1:ZF:139:ILE:O    | 2.19                     | 0.41              |
| 1:ZH:352:ASN:O    | 1:ZH:352:ASN:CG   | 2.63                     | 0.41              |
| 1:ZI:42:MET:O     | 1:ZI:50:LEU:HB2   | 2.20                     | 0.41              |
| 1:ZM:281:GLN:NE2  | 1:ZM:283:GLY:O    | 2.47                     | 0.41              |
| 1:ZO:248:THR:HG1  | 1:ZO:257:ALA:N    | 2.18                     | 0.41              |
| 1:ZO:396:LEU:HD23 | 1:ZO:396:LEU:HA   | 1.82                     | 0.41              |
| 1:ZW:326:LEU:HD22 | 1:ZW:334:TRP:HB3  | 2.01                     | 0.41              |
| 1:ZY:375:MET:SD   | 1:Zd:388:THR:HA   | 2.60                     | 0.41              |
| 1:ZZ:112:GLN:HG2  | 1:ZZ:331:ASP:HB3  | 2.02                     | 0.41              |
| 1:Za:83:PHE:O     | 1:Za:94:TYR:HA    | 2.19                     | 0.41              |
| 1:Zd:399:LEU:HD23 | 1:Zd:399:LEU:HA   | 1.85                     | 0.41              |
| 1:Zg:33:LYS:NZ    | 1:Zg:362:GLU:OE2  | 2.52                     | 0.41              |
| 1:Zh:380:ARG:HD3  | 1:Zh:380:ARG:HA   | 1.76                     | 0.41              |
| 2:6:256:LYS:HE3   | 2:1:241:GLU:HG3   | 2.01                     | 0.41              |
| 2:7:45:LEU:HG     | 2:w:86:LEU:HD11   | 2.02                     | 0.41              |
| 2:ZD:89:THR:OG1   | 2:ZD:94:ASP:OD2   | 2.37                     | 0.41              |
| 2:t:238:ARG:NH2   | 2:z:255:GLN:HB2   | 2.35                     | 0.41              |
| 2:w:223:ASN:O     | 2:w:223:ASN:OD1   | 2.38                     | 0.41              |
| 1:ZF:85:LEU:HD13  | 1:ZF:114:MET:HB2  | 2.02                     | 0.41              |
| 1:ZF:197:ASN:HD22 | 1:ZF:197:ASN:N    | 2.17                     | 0.41              |
| 1:ZH:280:ASN:OD1  | 1:ZH:281:GLN:N    | 2.53                     | 0.41              |
| 1:ZI:143:LEU:HD12 | 1:ZI:287:GLY:O    | 2.20                     | 0.41              |
| 1:ZI:196:MET:HE3  | 1:ZI:196:MET:HB3  | 1.98                     | 0.41              |
| 1:ZO:160:SER:HA   | 1:ZO:268:GLN:HE21 | 1.85                     | 0.41              |
| 1:ZQ:112:GLN:HE21 | 1:ZQ:331:ASP:HB3  | 1.82                     | 0.41              |
| 1:ZS:233:ASN:HD21 | 1:ZS:237:ILE:HB   | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZS:314:GLN:NE2  | 1:ZS:347:THR:OG1  | 2.47                     | 0.41              |
| 1:ZU:3:PHE:O      | 1:ZU:7:VAL:HG23   | 2.20                     | 0.41              |
| 1:ZU:102:LEU:HD21 | 1:ZU:106:ARG:HA   | 2.02                     | 0.41              |
| 1:Zc:71:ARG:O     | 1:Zc:359:GLY:HA2  | 2.20                     | 0.41              |
| 1:Zd:16:ASN:HB2   | 1:Zd:39:PHE:HZ    | 1.85                     | 0.41              |
| 1:Ze:30:TYR:HD1   | 1:Ze:363:ALA:HA   | 1.85                     | 0.41              |
| 1:Zg:5:GLN:H      | 1:Zg:5:GLN:HG3    | 1.59                     | 0.41              |
| 1:Zg:75:VAL:HG21  | 1:Zg:294:ILE:HG21 | 2.02                     | 0.41              |
| 1:Zg:385:ASN:O    | 1:Zg:386:ALA:C    | 2.63                     | 0.41              |
| 1:Zh:396:LEU:HA   | 1:Zh:396:LEU:HD23 | 1.83                     | 0.41              |
| 2:5:185:GLU:HB3   | 2:5:193:ILE:HG12  | 2.02                     | 0.41              |
| 2:7:194:GLU:OE2   | 2:7:201:PRO:HD3   | 2.20                     | 0.41              |
| 2:8:28:ASN:ND2    | 2:ZD:43:ASP:OD1   | 2.54                     | 0.41              |
| 2:ZC:42:GLU:OE2   | 2:ZC:73:ARG:NH2   | 2.47                     | 0.41              |
| 2:ZC:56:SER:O     | 2:w:153:ARG:N     | 2.52                     | 0.41              |
| 2:ZD:95:VAL:O     | 2:ZD:118:GLY:HA3  | 2.20                     | 0.41              |
| 2:r:17:THR:HG23   | 2:w:68:ILE:HD11   | 2.02                     | 0.41              |
| 2:t:193:ILE:HD12  | 2:t:193:ILE:HA    | 1.92                     | 0.41              |
| 2:v:178:PHE:CE1   | 2:v:201:PRO:HB3   | 2.55                     | 0.41              |
| 1:ZF:198:VAL:HG22 | 1:ZF:212:THR:HG22 | 2.02                     | 0.41              |
| 1:ZG:52:VAL:CG2   | 2:ZB:28:ASN:ND2   | 2.83                     | 0.41              |
| 1:ZG:267:MET:HE3  | 1:ZG:267:MET:HB3  | 1.89                     | 0.41              |
| 1:ZI:53:LYS:NZ    | 2:ZD:189:GLU:OE1  | 2.52                     | 0.41              |
| 1:ZJ:397:ASN:ND2  | 2:ZD:238:ARG:NH1  | 2.67                     | 0.41              |
| 1:ZK:18:ASP:HB3   | 1:ZP:5:GLN:HE22   | 1.85                     | 0.41              |
| 1:ZN:161:THR:O    | 1:ZN:161:THR:OG1  | 2.29                     | 0.41              |
| 1:ZN:373:VAL:HG11 | 1:ZT:7:VAL:HG22   | 2.02                     | 0.41              |
| 1:ZP:50:LEU:HD22  | 2:ZE:85:ASN:CG    | 2.46                     | 0.41              |
| 1:ZQ:125:PRO:HA   | 1:ZQ:126:PRO:HD3  | 1.92                     | 0.41              |
| 1:ZR:396:LEU:HD23 | 1:ZR:396:LEU:HA   | 1.76                     | 0.41              |
| 1:ZS:158:LEU:HD13 | 1:ZS:208:TRP:CD2  | 2.56                     | 0.41              |
| 1:ZV:181:LYS:HD3  | 1:Zg:129:GLN:HE21 | 1.83                     | 0.41              |
| 1:ZW:83:PHE:HB2   | 1:ZW:95:SER:O     | 2.19                     | 0.41              |
| 1:ZX:188:ASP:OD1  | 1:ZX:188:ASP:N    | 2.40                     | 0.41              |
| 1:Zd:144:MET:HE3  | 1:Zd:145:ALA:H    | 1.85                     | 0.41              |
| 1:Zf:78:SER:OG    | 1:Zf:355:LYS:O    | 2.29                     | 0.41              |
| 2:5:64:SER:O      | 2:0:76:ALA:HB1    | 2.21                     | 0.41              |
| 2:6:225:ASN:O     | 2:6:229:GLU:HG2   | 2.20                     | 0.41              |
| 2:8:45:LEU:HD21   | 2:x:98:LYS:CG     | 2.48                     | 0.41              |
| 2:9:41:PHE:HA     | 2:9:74:PRO:HA     | 2.01                     | 0.41              |
| 2:ZA:3:SER:HA     | 2:z:85:ASN:ND2    | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZA:137:GLN:HA   | 2:ZA:139:ALA:N    | 2.31                     | 0.41              |
| 2:ZE:208:LEU:HB3  | 2:ZE:209:ASN:H    | 1.61                     | 0.41              |
| 2:1:3:SER:C       | 2:1:5:LEU:H       | 2.28                     | 0.41              |
| 2:t:98:LYS:HD3    | 2:t:213:LEU:HB2   | 2.01                     | 0.41              |
| 2:u:95:VAL:O      | 2:u:118:GLY:HA3   | 2.20                     | 0.41              |
| 2:u:98:LYS:HD3    | 2:u:213:LEU:HD12  | 2.03                     | 0.41              |
| 2:u:154:ASP:O     | 2:u:154:ASP:OD2   | 2.39                     | 0.41              |
| 2:w:113:ALA:HB1   | 2:w:191:LEU:HB3   | 2.03                     | 0.41              |
| 2:z:173:LEU:HD23  | 2:z:173:LEU:HA    | 1.84                     | 0.41              |
| 1:ZF:154:MET:HE3  | 1:ZF:184:VAL:HB   | 2.03                     | 0.41              |
| 1:ZH:306:ASN:C    | 1:ZH:307:GLU:HG2  | 2.45                     | 0.41              |
| 1:ZI:204:LYS:O    | 1:ZI:207:GLU:N    | 2.53                     | 0.41              |
| 1:ZL:367:ASP:HB3  | 1:ZL:370:LYS:CG   | 2.47                     | 0.41              |
| 1:ZO:235:ASN:O    | 1:ZO:237:ILE:N    | 2.51                     | 0.41              |
| 1:ZS:146:ALA:HB2  | 1:ZS:286:PRO:HD3  | 2.02                     | 0.41              |
| 1:ZW:104:GLU:OE2  | 1:ZW:104:GLU:N    | 2.35                     | 0.41              |
| 1:ZW:285:LYS:HB2  | 1:ZW:285:LYS:HE3  | 1.91                     | 0.41              |
| 1:ZX:290:VAL:HG12 | 1:ZX:303:ASN:O    | 2.20                     | 0.41              |
| 1:Zd:183:THR:HG23 | 1:Zd:195:ASP:OD2  | 2.21                     | 0.41              |
| 2:2:241:GLU:OE1   | 2:8:258:THR:HG21  | 2.20                     | 0.41              |
| 2:3:3:SER:HB3     | 2:y:20:ASP:OD1    | 2.19                     | 0.41              |
| 2:0:138:PRO:O     | 2:0:140:ILE:HG13  | 2.19                     | 0.41              |
| 2:s:233:MET:HE1   | 2:x:245:LYS:HG3   | 2.02                     | 0.41              |
| 1:ZH:78:SER:HG    | 1:ZH:355:LYS:H    | 1.62                     | 0.41              |
| 1:ZH:128:ILE:HD13 | 1:ZH:314:GLN:OE1  | 2.21                     | 0.41              |
| 1:ZI:323:ASN:H    | 1:ZI:323:ASN:HD22 | 1.69                     | 0.41              |
| 1:ZL:53:LYS:HB2   | 2:ZA:218:TYR:OH   | 2.20                     | 0.41              |
| 1:ZM:59:GLN:NE2   | 1:ZM:334:TRP:HE1  | 2.18                     | 0.41              |
| 1:ZO:71:ARG:HH11  | 1:ZO:71:ARG:HB3   | 1.84                     | 0.41              |
| 1:ZP:170:PHE:HE2  | 1:ZP:223:PRO:HG2  | 1.85                     | 0.41              |
| 1:ZT:121:ALA:HB2  | 1:ZT:128:ILE:HD13 | 2.03                     | 0.41              |
| 1:ZT:200:PHE:HZ   | 1:ZT:263:PHE:HE2  | 1.69                     | 0.41              |
| 1:ZT:297:ASP:OD2  | 1:ZT:297:ASP:N    | 2.53                     | 0.41              |
| 1:ZT:367:ASP:HB3  | 1:ZT:370:LYS:HG3  | 2.03                     | 0.41              |
| 1:ZU:151:THR:OG1  | 1:ZU:282:ASN:OD1  | 2.23                     | 0.41              |
| 1:ZV:103:ASP:OD1  | 1:ZV:107:ASN:N    | 2.41                     | 0.41              |
| 1:ZW:184:VAL:HG13 | 1:ZW:196:MET:HB2  | 2.02                     | 0.41              |
| 1:ZW:330:GLY:N    | 1:Zb:43:PHE:HB2   | 2.36                     | 0.41              |
| 1:Za:34:SER:HB3   | 1:Za:366:VAL:HG22 | 2.01                     | 0.41              |
| 2:4:28:ASN:ND2    | 2:9:43:ASP:HB2    | 2.36                     | 0.41              |
| 2:4:258:THR:HG21  | 2:y:241:GLU:OE1   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:5:102:PHE:HE2   | 2:5:181:ASP:OD1   | 2.03                     | 0.41              |
| 2:ZE:140:ILE:HD13 | 2:ZE:157:VAL:HG21 | 2.03                     | 0.41              |
| 2:1:95:VAL:O      | 2:1:118:GLY:HA3   | 2.20                     | 0.41              |
| 2:r:161:GLN:HA    | 2:r:161:GLN:OE1   | 2.21                     | 0.41              |
| 2:y:6:TRP:O       | 2:y:10:THR:HG23   | 2.21                     | 0.41              |
| 2:z:178:PHE:CE1   | 2:z:201:PRO:HB3   | 2.56                     | 0.41              |
| 1:ZF:319:ASN:OD1  | 1:ZF:320:PHE:N    | 2.54                     | 0.41              |
| 1:ZG:60:ASP:OD1   | 1:ZG:62:THR:HG23  | 2.21                     | 0.41              |
| 1:ZJ:66:THR:OG1   | 1:ZU:42:MET:SD    | 2.77                     | 0.41              |
| 1:ZL:16:ASN:HB2   | 1:ZL:39:PHE:HZ    | 1.85                     | 0.41              |
| 1:ZO:167:LYS:HE2  | 1:ZO:174:ASP:OD2  | 2.21                     | 0.41              |
| 1:ZO:288:ASP:N    | 1:ZO:305:SER:OG   | 2.43                     | 0.41              |
| 1:ZP:269:GLN:NE2  | 1:ZV:146:ALA:HB3  | 2.35                     | 0.41              |
| 1:ZQ:99:GLN:HG2   | 1:ZQ:111:MET:HE3  | 2.02                     | 0.41              |
| 1:ZU:230:LEU:HD22 | 1:ZU:238:LEU:HD11 | 2.03                     | 0.41              |
| 1:ZU:232:PHE:HE2  | 1:ZU:267:MET:HA   | 1.86                     | 0.41              |
| 1:ZW:2:SER:O      | 1:ZW:2:SER:OG     | 2.36                     | 0.41              |
| 1:ZW:212:THR:HG21 | 1:ZW:246:ILE:HG21 | 2.03                     | 0.41              |
| 1:ZY:349:GLY:O    | 1:Ze:89:ASN:ND2   | 2.53                     | 0.41              |
| 1:ZY:380:ARG:HB3  | 1:Ze:396:LEU:HD23 | 2.02                     | 0.41              |
| 1:Zb:361:LEU:HD23 | 1:Zb:361:LEU:HA   | 1.86                     | 0.41              |
| 1:Zd:33:LYS:O     | 1:Zd:59:GLN:NE2   | 2.54                     | 0.41              |
| 1:Ze:78:SER:O     | 1:Ze:354:GLY:HA3  | 2.20                     | 0.41              |
| 1:Zf:58:THR:HG23  | 1:Zf:324:GLU:HG2  | 2.02                     | 0.41              |
| 2:2:208:LEU:HB3   | 2:2:209:ASN:H     | 1.71                     | 0.41              |
| 2:3:47:GLN:N      | 2:3:68:ILE:O      | 2.53                     | 0.41              |
| 2:3:109:ASP:OD2   | 2:3:111:THR:HG22  | 2.20                     | 0.41              |
| 2:8:100:GLN:HG3   | 2:8:210:GLY:O     | 2.20                     | 0.41              |
| 2:ZB:164:GLN:C    | 2:ZB:166:ALA:N    | 2.78                     | 0.41              |
| 2:ZB:256:LYS:HA   | 2:ZB:256:LYS:HD3  | 1.90                     | 0.41              |
| 1:ZI:324:GLU:C    | 1:ZI:326:LEU:N    | 2.78                     | 0.41              |
| 1:ZL:128:ILE:HD12 | 1:ZL:314:GLN:HB2  | 2.03                     | 0.41              |
| 1:ZO:49:GLY:O     | 1:ZO:50:LEU:C     | 2.63                     | 0.41              |
| 1:ZP:50:LEU:HD21  | 2:ZE:85:ASN:OD1   | 2.20                     | 0.41              |
| 1:ZS:381:ASN:O    | 1:ZS:385:ASN:ND2  | 2.54                     | 0.41              |
| 1:ZU:108:LEU:HD12 | 1:ZU:137:ILE:HG21 | 2.02                     | 0.41              |
| 1:ZU:139:ILE:HA   | 1:ZU:312:LEU:HD22 | 2.02                     | 0.41              |
| 1:ZU:187:TYR:CE1  | 1:ZU:285:LYS:HE2  | 2.56                     | 0.41              |
| 1:ZV:93:PHE:HB3   | 1:ZV:333:VAL:HG22 | 2.03                     | 0.41              |
| 1:ZV:213:HIS:HB2  | 1:ZV:223:PRO:HG3  | 2.02                     | 0.41              |
| 1:ZY:116:LEU:HD11 | 1:ZY:315:ILE:HD11 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZY:171:SER:O    | 1:ZY:177:SER:OG   | 2.39                     | 0.41              |
| 1:ZY:399:LEU:HA   | 1:ZY:399:LEU:HD23 | 1.84                     | 0.41              |
| 1:ZZ:77:ILE:HD11  | 1:ZZ:83:PHE:CD1   | 2.56                     | 0.41              |
| 1:Zf:73:LEU:HD22  | 1:Zf:108:LEU:HD11 | 2.03                     | 0.41              |
| 1:Zf:228:THR:HB   | 1:Zf:244:VAL:HG21 | 2.01                     | 0.41              |
| 1:Zf:298:GLY:O    | 1:Zf:315:ILE:HG13 | 2.20                     | 0.41              |
| 2:3:143:PRO:HG2   | 2:3:159:VAL:HG21  | 2.02                     | 0.41              |
| 2:6:245:LYS:HD3   | 2:6:245:LYS:HA    | 1.85                     | 0.41              |
| 2:7:175:LEU:HG    | 2:7:206:PRO:HG3   | 2.02                     | 0.41              |
| 2:9:92:SER:O      | 2:9:216:GLN:NE2   | 2.45                     | 0.41              |
| 2:s:2:ILE:HG23    | 2:s:5:LEU:HB2     | 2.03                     | 0.41              |
| 2:s:35:LYS:HD2    | 2:s:81:HIS:HA     | 2.02                     | 0.41              |
| 1:ZF:355:LYS:H    | 1:ZF:355:LYS:HG2  | 1.66                     | 0.41              |
| 1:ZI:374:ASN:C    | 1:ZI:376:ILE:N    | 2.79                     | 0.41              |
| 1:ZJ:399:LEU:HD22 | 2:8:227:ALA:HB1   | 1.97                     | 0.41              |
| 1:ZM:27:SER:HB2   | 1:ZR:381:ASN:ND2  | 2.36                     | 0.41              |
| 1:ZM:380:ARG:HB3  | 1:ZS:396:LEU:HD13 | 2.02                     | 0.41              |
| 1:ZR:380:ARG:HD2  | 1:ZX:396:LEU:HB3  | 2.03                     | 0.41              |
| 1:ZU:197:ASN:HD21 | 1:ZU:215:SER:HB2  | 1.85                     | 0.41              |
| 1:ZV:198:VAL:HG12 | 1:ZV:212:THR:HG22 | 2.03                     | 0.41              |
| 1:ZY:148:SER:HB3  | 1:ZY:189:SER:HA   | 2.03                     | 0.41              |
| 1:Zb:159:ASN:ND2  | 1:Zb:161:THR:OG1  | 2.49                     | 0.41              |
| 1:Zc:388:THR:O    | 1:Zc:392:GLN:HG2  | 2.20                     | 0.41              |
| 1:Zh:20:ILE:HG23  | 1:Zh:371:GLU:OE2  | 2.20                     | 0.41              |
| 2:3:46:TYR:HA     | 2:3:69:GLY:HA2    | 2.02                     | 0.41              |
| 2:5:208:LEU:HA    | 2:5:208:LEU:HD13  | 1.83                     | 0.41              |
| 2:ZE:35:LYS:NZ    | 2:ZE:220:GLU:OE1  | 2.54                     | 0.41              |
| 2:1:73:ARG:HG3    | 2:1:75:VAL:HG13   | 2.03                     | 0.41              |
| 2:r:151:ILE:HB    | 2:r:216:GLN:HG3   | 2.02                     | 0.41              |
| 2:t:233:MET:HE1   | 2:y:246:ALA:HA    | 2.01                     | 0.41              |
| 1:ZF:401:ASN:HD22 | 1:ZF:401:ASN:HA   | 1.74                     | 0.41              |
| 1:ZH:157:ASN:ND2  | 1:ZN:143:LEU:HD13 | 2.36                     | 0.41              |
| 1:ZL:77:ILE:HD11  | 1:ZL:96:ARG:CZ    | 2.51                     | 0.41              |
| 1:ZL:233:ASN:OD1  | 1:ZL:237:ILE:N    | 2.48                     | 0.41              |
| 1:ZM:111:MET:HE3  | 1:ZM:111:MET:HB3  | 1.92                     | 0.41              |
| 1:ZM:320:PHE:CE1  | 1:ZM:343:ALA:HB2  | 2.55                     | 0.41              |
| 1:ZN:73:LEU:HD21  | 1:ZN:292:TYR:HE2  | 1.85                     | 0.41              |
| 1:ZN:167:LYS:NZ   | 1:ZN:168:THR:O    | 2.54                     | 0.41              |
| 1:ZO:112:GLN:HG2  | 1:ZO:331:ASP:HB3  | 2.02                     | 0.41              |
| 1:ZR:18:ASP:CB    | 1:ZW:5:GLN:HE22   | 2.33                     | 0.41              |
| 1:ZS:118:GLY:HA3  | 1:ZS:314:GLN:O    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZS:186:VAL:HG23 | 1:ZS:194:HIS:HB2  | 2.02                     | 0.41              |
| 1:ZT:380:ARG:NH2  | 1:ZZ:397:ASN:OD1  | 2.53                     | 0.41              |
| 1:ZU:172:VAL:HG11 | 1:ZU:223:PRO:HD2  | 2.03                     | 0.41              |
| 1:ZV:217:ASP:HA   | 1:ZV:251:ILE:HD11 | 2.01                     | 0.41              |
| 1:ZW:75:VAL:O     | 1:ZW:98:GLY:HA3   | 2.21                     | 0.41              |
| 1:ZX:242:GLY:HA2  | 1:ZX:263:PHE:HB2  | 2.03                     | 0.41              |
| 1:ZX:285:LYS:HE2  | 1:ZX:285:LYS:HB3  | 1.76                     | 0.41              |
| 1:ZZ:107:ASN:ND2  | 1:ZZ:138:THR:HG22 | 2.35                     | 0.41              |
| 1:Zb:110:ASN:OD1  | 1:Zb:114:MET:N    | 2.50                     | 0.41              |
| 1:Zc:304:TYR:HE1  | 1:Zc:310:GLN:HB3  | 1.86                     | 0.41              |
| 1:Zc:348:ALA:HB2  | 1:Zc:356:LEU:HG   | 2.02                     | 0.41              |
| 1:Ze:85:LEU:HD23  | 1:Ze:114:MET:HB3  | 2.02                     | 0.41              |
| 1:Ze:86:VAL:HG23  | 1:Ze:117:THR:HG21 | 2.03                     | 0.41              |
| 1:Zf:380:ARG:HA   | 1:Zf:380:ARG:HD3  | 1.77                     | 0.41              |
| 1:Zg:370:LYS:HB2  | 1:Zg:370:LYS:HE2  | 1.90                     | 0.41              |
| 1:Zh:33:LYS:O     | 1:Zh:59:GLN:NE2   | 2.54                     | 0.41              |
| 1:Zh:71:ARG:HD3   | 1:Zh:73:LEU:HB2   | 2.03                     | 0.41              |
| 1:Zh:285:LYS:HG2  | 1:Zh:286:PRO:HD2  | 2.02                     | 0.41              |
| 2:2:100:GLN:NE2   | 2:2:210:GLY:O     | 2.43                     | 0.41              |
| 2:3:95:VAL:O      | 2:3:118:GLY:HA3   | 2.20                     | 0.41              |
| 2:7:70:THR:HG23   | 2:w:85:ASN:OD1    | 2.21                     | 0.41              |
| 2:7:109:ASP:OD2   | 2:7:109:ASP:C     | 2.63                     | 0.41              |
| 2:ZB:116:ARG:HH21 | 2:ZB:220:GLU:CD   | 2.28                     | 0.41              |
| 2:ZC:10:THR:OG1   | 2:ZC:72:VAL:O     | 2.39                     | 0.41              |
| 2:ZC:45:LEU:HD12  | 2:1:83:GLN:HE21   | 1.86                     | 0.41              |
| 2:r:44:LEU:HD13   | 2:r:70:THR:HG22   | 2.02                     | 0.41              |
| 2:r:138:PRO:HG3   | 2:r:174:ASN:ND2   | 2.36                     | 0.41              |
| 2:r:140:ILE:HG21  | 2:r:157:VAL:HG11  | 2.02                     | 0.41              |
| 2:r:189:GLU:HB2   | 2:w:42:GLU:CD     | 2.46                     | 0.41              |
| 2:t:3:SER:O       | 2:t:7:ILE:HD12    | 2.21                     | 0.41              |
| 2:u:42:GLU:OE1    | 2:u:73:ARG:NH2    | 2.54                     | 0.41              |
| 2:u:114:TYR:CE2   | 2:u:178:PHE:HZ    | 2.39                     | 0.41              |
| 2:x:248:SER:O     | 2:x:252:GLN:HG3   | 2.20                     | 0.41              |
| 2:z:129:VAL:HG12  | 2:z:135:GLN:HA    | 2.02                     | 0.41              |
| 1:ZF:174:ASP:HB3  | 1:ZF:176:ASP:OD1  | 2.21                     | 0.41              |
| 1:ZJ:39:PHE:HB2   | 2:ZE:31:THR:HG22  | 2.03                     | 0.41              |
| 1:ZJ:156:ILE:HG13 | 1:ZJ:276:ILE:HA   | 2.03                     | 0.41              |
| 1:ZJ:174:ASP:HB3  | 1:ZJ:176:ASP:OD1  | 2.21                     | 0.41              |
| 1:ZJ:208:TRP:HE1  | 1:ZJ:268:GLN:CD   | 2.29                     | 0.41              |
| 1:ZM:237:ILE:H    | 1:ZM:237:ILE:HD12 | 1.85                     | 0.41              |
| 1:ZN:184:VAL:HG13 | 1:ZN:196:MET:HB2  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZN:233:ASN:ND2  | 1:ZN:237:ILE:HB   | 2.35                     | 0.41              |
| 1:ZO:195:ASP:OD2  | 1:ZO:216:SER:OG   | 2.37                     | 0.41              |
| 1:ZP:42:MET:SD    | 1:ZP:53:LYS:HB3   | 2.61                     | 0.41              |
| 1:ZP:75:VAL:O     | 1:ZP:98:GLY:HA3   | 2.21                     | 0.41              |
| 1:ZT:33:LYS:NZ    | 1:ZT:362:GLU:OE1  | 2.36                     | 0.41              |
| 1:ZT:373:VAL:HG11 | 1:ZZ:7:VAL:HG22   | 2.02                     | 0.41              |
| 1:Za:190:GLN:HG3  | 1:Za:254:ALA:HB2  | 2.03                     | 0.41              |
| 1:Zf:267:MET:HG3  | 1:Zf:268:GLN:N    | 2.35                     | 0.41              |
| 2:4:10:THR:OG1    | 2:4:71:GLY:HA3    | 2.21                     | 0.41              |
| 2:5:79:ARG:NH2    | 2:5:184:LEU:O     | 2.50                     | 0.41              |
| 2:5:144:ALA:HA    | 2:ZA:179:MET:SD   | 2.61                     | 0.41              |
| 2:7:119:SER:OG    | 2:ZC:38:ARG:NH2   | 2.54                     | 0.41              |
| 2:ZA:7:ILE:HG23   | 2:ZA:71:GLY:HA2   | 2.03                     | 0.41              |
| 2:1:22:ILE:HD11   | 2:1:232:ASN:HB3   | 2.02                     | 0.41              |
| 2:s:155:GLY:HA2   | 2:s:214:LEU:HD12  | 2.03                     | 0.41              |
| 2:t:2:ILE:O       | 2:t:3:SER:HB3     | 2.21                     | 0.41              |
| 2:z:225:ASN:O     | 2:z:229:GLU:HG2   | 2.20                     | 0.41              |
| 1:ZF:47:LYS:HD3   | 2:ZA:76:ALA:HB1   | 2.04                     | 0.40              |
| 1:ZI:147:LYS:HE2  | 1:ZI:282:ASN:ND2  | 2.36                     | 0.40              |
| 1:ZJ:351:GLY:C    | 1:ZJ:353:PHE:H    | 2.29                     | 0.40              |
| 1:ZK:71:ARG:O     | 1:ZK:359:GLY:HA2  | 2.20                     | 0.40              |
| 1:ZM:149:THR:O    | 1:ZM:259:PHE:HB3  | 2.21                     | 0.40              |
| 1:ZN:174:ASP:OD2  | 1:ZN:174:ASP:N    | 2.52                     | 0.40              |
| 1:ZO:374:ASN:O    | 1:ZO:375:MET:C    | 2.65                     | 0.40              |
| 1:ZR:79:GLN:HB3   | 1:ZR:80:ASN:H     | 1.75                     | 0.40              |
| 1:ZS:42:MET:HE2   | 1:ZS:42:MET:HB2   | 1.96                     | 0.40              |
| 1:ZU:299:THR:HG22 | 1:ZU:314:GLN:OE1  | 2.21                     | 0.40              |
| 1:ZV:46:SER:HB3   | 1:ZV:48:VAL:HG22  | 2.03                     | 0.40              |
| 1:Zb:399:LEU:HD23 | 1:Zb:399:LEU:HA   | 1.78                     | 0.40              |
| 2:8:45:LEU:HD23   | 2:8:45:LEU:HA     | 1.81                     | 0.40              |
| 2:ZC:44:LEU:HD23  | 2:ZC:44:LEU:HA    | 1.82                     | 0.40              |
| 2:ZD:208:LEU:C    | 2:ZD:210:GLY:H    | 2.29                     | 0.40              |
| 2:x:130:THR:OG1   | 2:x:131:ALA:N     | 2.54                     | 0.40              |
| 2:z:83:GLN:NE2    | 2:z:97:ILE:O      | 2.36                     | 0.40              |
| 1:ZF:393:ASP:C    | 1:ZF:395:ILE:N    | 2.76                     | 0.40              |
| 1:ZH:111:MET:N    | 1:ZH:111:MET:SD   | 2.94                     | 0.40              |
| 1:ZM:396:LEU:HD23 | 1:ZM:396:LEU:HA   | 1.85                     | 0.40              |
| 1:ZR:183:THR:HG22 | 1:ZR:197:ASN:HD22 | 1.86                     | 0.40              |
| 1:ZS:71:ARG:NH1   | 1:ZS:74:ASP:OD1   | 2.54                     | 0.40              |
| 1:ZS:399:LEU:HD23 | 1:ZS:399:LEU:HA   | 1.92                     | 0.40              |
| 1:ZT:139:ILE:HA   | 1:ZT:312:LEU:HD13 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZZ:74:ASP:HB3   | 1:ZZ:361:LEU:HG   | 2.03                     | 0.40              |
| 1:Zb:308:GLN:NE2  | 1:Zb:309:GLU:OE1  | 2.55                     | 0.40              |
| 1:Ze:71:ARG:NH2   | 1:Ze:74:ASP:OD1   | 2.54                     | 0.40              |
| 1:Zh:78:SER:OG    | 1:Zh:355:LYS:O    | 2.36                     | 0.40              |
| 2:4:117:ASP:OD1   | 2:4:117:ASP:C     | 2.64                     | 0.40              |
| 2:5:1:MET:HE3     | 2:5:1:MET:HB2     | 1.88                     | 0.40              |
| 2:6:22:ILE:HD11   | 2:6:232:ASN:HB3   | 2.03                     | 0.40              |
| 2:8:127:GLN:NE2   | 2:8:139:ALA:HB1   | 2.35                     | 0.40              |
| 2:0:11:GLY:O      | 2:0:15:GLN:HG2    | 2.21                     | 0.40              |
| 2:1:107:LEU:HD11  | 2:1:113:ALA:HB2   | 2.03                     | 0.40              |
| 2:v:175:LEU:HD23  | 2:v:175:LEU:HA    | 1.97                     | 0.40              |
| 1:ZG:14:ALA:HB2   | 1:ZG:382:TYR:HE2  | 1.86                     | 0.40              |
| 1:ZG:147:LYS:HB2  | 1:ZG:147:LYS:HE2  | 1.66                     | 0.40              |
| 1:ZG:352:ASN:OD1  | 2:ZB:147:LEU:CD2  | 2.70                     | 0.40              |
| 1:ZG:380:ARG:NH1  | 1:ZG:383:GLN:OE1  | 2.54                     | 0.40              |
| 1:ZH:144:MET:SD   | 1:ZH:310:GLN:NE2  | 2.95                     | 0.40              |
| 1:ZI:45:GLY:O     | 2:ZD:186:SER:O    | 2.39                     | 0.40              |
| 1:ZJ:75:VAL:O     | 1:ZJ:98:GLY:HA3   | 2.21                     | 0.40              |
| 1:ZL:122:THR:OG1  | 1:ZL:129:GLN:OE1  | 2.38                     | 0.40              |
| 1:ZO:262:SER:OG   | 1:ZO:264:LEU:HD23 | 2.22                     | 0.40              |
| 1:ZP:185:THR:HG22 | 1:ZP:187:TYR:HE1  | 1.87                     | 0.40              |
| 1:ZQ:97:ASN:HD22  | 1:ZQ:332:ASN:HD21 | 1.70                     | 0.40              |
| 1:ZU:188:ASP:OD1  | 1:ZU:192:ASN:N    | 2.54                     | 0.40              |
| 1:ZX:171:SER:O    | 1:ZX:177:SER:OG   | 2.39                     | 0.40              |
| 1:ZZ:106:ARG:HA   | 1:ZZ:106:ARG:HD2  | 1.79                     | 0.40              |
| 1:Zh:38:SER:O     | 1:Zh:55:ALA:N     | 2.52                     | 0.40              |
| 2:2:50:ARG:HD3    | 2:2:66:LEU:HB2    | 2.03                     | 0.40              |
| 2:9:76:ALA:HB1    | 2:ZE:64:SER:O     | 2.22                     | 0.40              |
| 2:ZD:104:GLN:O    | 2:ZD:137:GLN:N    | 2.54                     | 0.40              |
| 2:ZD:160:THR:HG22 | 2:ZD:167:PRO:HB3  | 2.04                     | 0.40              |
| 2:ZE:40:VAL:O     | 2:ZE:75:VAL:N     | 2.51                     | 0.40              |
| 2:ZE:225:ASN:O    | 2:ZE:229:GLU:HG2  | 2.21                     | 0.40              |
| 2:0:35:LYS:HA     | 2:0:35:LYS:HD3    | 1.96                     | 0.40              |
| 2:0:67:GLN:HE22   | 2:v:185:GLU:HA    | 1.87                     | 0.40              |
| 2:x:179:MET:HE2   | 2:x:200:ALA:HB3   | 2.03                     | 0.40              |
| 2:y:49:ILE:O      | 2:y:65:GLY:HA3    | 2.21                     | 0.40              |
| 1:ZF:157:ASN:ND2  | 1:ZL:143:LEU:HD13 | 2.36                     | 0.40              |
| 1:ZH:3:PHE:CG     | 2:ZB:235:GLN:NE2  | 2.67                     | 0.40              |
| 1:ZJ:2:SER:HB3    | 1:ZJ:392:GLN:CG   | 2.49                     | 0.40              |
| 1:ZJ:180:LYS:HE3  | 1:ZJ:276:ILE:HG13 | 2.03                     | 0.40              |
| 1:ZL:93:PHE:HB3   | 1:ZL:333:VAL:HG13 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ZL:125:PRO:HA   | 1:ZL:126:PRO:HD3  | 1.98                     | 0.40              |
| 1:ZN:170:PHE:CD2  | 1:ZN:170:PHE:C    | 2.99                     | 0.40              |
| 1:ZO:104:GLU:OE2  | 1:ZO:104:GLU:N    | 2.35                     | 0.40              |
| 1:ZP:16:ASN:O     | 1:ZP:20:ILE:HG13  | 2.22                     | 0.40              |
| 1:ZP:104:GLU:CD   | 1:ZP:104:GLU:H    | 2.29                     | 0.40              |
| 1:ZP:248:THR:HG1  | 1:ZP:257:ALA:H    | 1.65                     | 0.40              |
| 1:ZQ:199:TYR:O    | 1:ZQ:210:VAL:HA   | 2.21                     | 0.40              |
| 1:ZU:281:GLN:NE2  | 1:ZU:283:GLY:O    | 2.53                     | 0.40              |
| 1:ZW:78:SER:O     | 1:ZW:354:GLY:HA3  | 2.22                     | 0.40              |
| 1:ZX:56:GLY:HA2   | 1:Zc:47:LYS:NZ    | 2.36                     | 0.40              |
| 1:ZX:230:LEU:HD11 | 1:ZX:263:PHE:HD2  | 1.87                     | 0.40              |
| 1:ZY:75:VAL:HG21  | 1:ZY:356:LEU:HD23 | 2.04                     | 0.40              |
| 1:Zb:42:MET:HG2   | 1:Zb:53:LYS:HE3   | 2.04                     | 0.40              |
| 1:Zc:110:ASN:OD1  | 1:Zc:114:MET:N    | 2.40                     | 0.40              |
| 1:Ze:84:ARG:C     | 1:Ze:85:LEU:HD12  | 2.46                     | 0.40              |
| 1:Ze:367:ASP:O    | 1:Ze:371:GLU:HG2  | 2.21                     | 0.40              |
| 2:5:42:GLU:OE1    | 2:0:189:GLU:HB2   | 2.21                     | 0.40              |
| 2:6:153:ARG:NH1   | 2:6:213:LEU:HD22  | 2.37                     | 0.40              |
| 2:0:137:GLN:HA    | 2:0:138:PRO:C     | 2.45                     | 0.40              |
| 2:r:44:LEU:H      | 2:r:44:LEU:HD12   | 1.86                     | 0.40              |
| 2:t:123:ASP:OD1   | 2:t:127:GLN:HB3   | 2.22                     | 0.40              |
| 1:ZG:111:MET:N    | 1:ZG:111:MET:SD   | 2.95                     | 0.40              |
| 1:ZH:399:LEU:O    | 1:ZH:402:LEU:HG   | 2.21                     | 0.40              |
| 1:ZI:2:SER:O      | 1:ZI:2:SER:OG     | 2.31                     | 0.40              |
| 1:ZI:49:GLY:CA    | 2:ZD:24:ASN:HD21  | 2.33                     | 0.40              |
| 1:ZK:104:GLU:HG2  | 1:ZP:338:GLN:O    | 2.21                     | 0.40              |
| 1:ZM:180:LYS:HG3  | 1:ZM:181:LYS:N    | 2.37                     | 0.40              |
| 1:ZN:74:ASP:O     | 1:ZN:359:GLY:N    | 2.52                     | 0.40              |
| 1:ZN:109:VAL:HG12 | 1:ZN:115:GLN:HA   | 2.02                     | 0.40              |
| 1:ZP:85:LEU:HD23  | 1:ZP:116:LEU:HA   | 2.04                     | 0.40              |
| 1:ZS:81:GLY:O     | 1:ZS:82:PHE:HD1   | 2.05                     | 0.40              |
| 1:ZT:103:ASP:OD1  | 1:ZT:105:ASN:N    | 2.54                     | 0.40              |
| 1:ZY:53:LYS:HE3   | 1:ZY:53:LYS:HB2   | 1.86                     | 0.40              |
| 1:ZZ:17:LEU:CD1   | 1:Ze:395:ILE:HD11 | 2.51                     | 0.40              |
| 1:Zd:4:SER:HA     | 1:Zd:7:VAL:HG22   | 2.03                     | 0.40              |
| 2:5:42:GLU:HG2    | 2:5:73:ARG:HG2    | 2.04                     | 0.40              |
| 2:6:17:THR:HG23   | 2:ZB:68:ILE:HD11  | 2.04                     | 0.40              |
| 2:8:205:THR:HA    | 2:8:206:PRO:HD3   | 1.91                     | 0.40              |
| 2:8:255:GLN:HA    | 2:8:258:THR:HG22  | 2.03                     | 0.40              |
| 2:ZB:34:PHE:HB3   | 2:ZB:222:SER:HB3  | 2.04                     | 0.40              |
| 2:1:42:GLU:OE2    | 2:1:75:VAL:HG11   | 2.22                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:r:75:VAL:HG23 | 2:r:76:ALA:H     | 1.87                     | 0.40              |
| 2:s:51:GLN:H    | 2:s:51:GLN:HG2   | 1.71                     | 0.40              |
| 2:s:153:ARG:NE  | 2:s:213:LEU:HD13 | 2.36                     | 0.40              |
| 2:t:155:GLY:HA2 | 2:t:214:LEU:HD12 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | ZF    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | ZG    | 399/403 (99%) | 392 (98%) | 6 (2%)  | 1 (0%)   | 36          | 65  |
| 1   | ZH    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | ZI    | 399/403 (99%) | 387 (97%) | 10 (2%) | 2 (0%)   | 24          | 55  |
| 1   | ZJ    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |
| 1   | ZK    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 1   | ZL    | 399/403 (99%) | 389 (98%) | 9 (2%)  | 1 (0%)   | 36          | 65  |
| 1   | ZM    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | ZN    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | ZO    | 399/403 (99%) | 381 (96%) | 15 (4%) | 3 (1%)   | 16          | 45  |
| 1   | ZP    | 399/403 (99%) | 385 (96%) | 13 (3%) | 1 (0%)   | 36          | 65  |
| 1   | ZQ    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | ZR    | 399/403 (99%) | 390 (98%) | 8 (2%)  | 1 (0%)   | 36          | 65  |
| 1   | ZS    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 1   | ZT    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | ZU    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | ZV    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 1   | ZW    | 399/403 (99%) | 385 (96%) | 14 (4%) | 0        | 100         | 100 |
| 1   | ZX    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | ZY    | 399/403 (99%) | 386 (97%) | 13 (3%) | 0        | 100         | 100 |
| 1   | ZZ    | 399/403 (99%) | 389 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | Za    | 399/403 (99%) | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | Zb    | 399/403 (99%) | 392 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | Zc    | 399/403 (99%) | 390 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 1   | Zd    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |
| 1   | Ze    | 399/403 (99%) | 385 (96%) | 14 (4%) | 0        | 100         | 100 |
| 1   | Zf    | 399/403 (99%) | 386 (97%) | 13 (3%) | 0        | 100         | 100 |
| 1   | Zg    | 399/403 (99%) | 387 (97%) | 12 (3%) | 0        | 100         | 100 |
| 1   | Zh    | 399/403 (99%) | 392 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 2   | 0     | 244/260 (94%) | 236 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60  |
| 2   | 1     | 248/260 (95%) | 238 (96%) | 9 (4%)  | 1 (0%)   | 30          | 60  |
| 2   | 2     | 258/260 (99%) | 247 (96%) | 9 (4%)  | 2 (1%)   | 16          | 45  |
| 2   | 3     | 258/260 (99%) | 248 (96%) | 8 (3%)  | 2 (1%)   | 16          | 45  |
| 2   | 4     | 258/260 (99%) | 248 (96%) | 7 (3%)  | 3 (1%)   | 10          | 37  |
| 2   | 5     | 258/260 (99%) | 242 (94%) | 14 (5%) | 2 (1%)   | 16          | 45  |
| 2   | 6     | 258/260 (99%) | 244 (95%) | 12 (5%) | 2 (1%)   | 16          | 45  |
| 2   | 7     | 258/260 (99%) | 245 (95%) | 10 (4%) | 3 (1%)   | 10          | 37  |
| 2   | 8     | 258/260 (99%) | 247 (96%) | 9 (4%)  | 2 (1%)   | 16          | 45  |
| 2   | 9     | 258/260 (99%) | 245 (95%) | 11 (4%) | 2 (1%)   | 16          | 45  |
| 2   | ZA    | 258/260 (99%) | 242 (94%) | 13 (5%) | 3 (1%)   | 10          | 37  |
| 2   | ZB    | 258/260 (99%) | 244 (95%) | 11 (4%) | 3 (1%)   | 10          | 37  |
| 2   | ZC    | 258/260 (99%) | 243 (94%) | 12 (5%) | 3 (1%)   | 10          | 37  |
| 2   | ZD    | 258/260 (99%) | 244 (95%) | 12 (5%) | 2 (1%)   | 16          | 45  |
| 2   | ZE    | 258/260 (99%) | 245 (95%) | 12 (5%) | 1 (0%)   | 30          | 60  |
| 2   | r     | 250/260 (96%) | 237 (95%) | 12 (5%) | 1 (0%)   | 30          | 60  |
| 2   | s     | 251/260 (96%) | 237 (94%) | 13 (5%) | 1 (0%)   | 30          | 60  |
| 2   | t     | 252/260 (97%) | 241 (96%) | 10 (4%) | 1 (0%)   | 30          | 60  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|----------|-------------|----|
| 2   | u     | 250/260 (96%)     | 242 (97%)   | 6 (2%)   | 2 (1%)   | 16          | 45 |
| 2   | v     | 251/260 (96%)     | 241 (96%)   | 9 (4%)   | 1 (0%)   | 30          | 60 |
| 2   | w     | 239/260 (92%)     | 232 (97%)   | 6 (2%)   | 1 (0%)   | 30          | 60 |
| 2   | x     | 244/260 (94%)     | 237 (97%)   | 4 (2%)   | 3 (1%)   | 10          | 37 |
| 2   | y     | 244/260 (94%)     | 237 (97%)   | 6 (2%)   | 1 (0%)   | 30          | 60 |
| 2   | z     | 244/260 (94%)     | 240 (98%)   | 3 (1%)   | 1 (0%)   | 30          | 60 |
| All | All   | 17642/17927 (98%) | 17056 (97%) | 533 (3%) | 53 (0%)  | 37          | 65 |

All (53) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZG    | 46  | SER  |
| 2   | 2     | 209 | ASN  |
| 2   | 5     | 209 | ASN  |
| 2   | 8     | 209 | ASN  |
| 2   | ZA    | 209 | ASN  |
| 2   | ZB    | 164 | GLN  |
| 2   | ZC    | 139 | ALA  |
| 1   | ZI    | 375 | MET  |
| 1   | ZO    | 237 | ILE  |
| 1   | ZR    | 87  | ASP  |
| 2   | 9     | 139 | ALA  |
| 2   | ZB    | 165 | ALA  |
| 2   | ZB    | 209 | ASN  |
| 2   | ZC    | 209 | ASN  |
| 2   | ZD    | 209 | ASN  |
| 2   | ZE    | 209 | ASN  |
| 2   | u     | 165 | ALA  |
| 2   | x     | 4   | SER  |
| 2   | z     | 127 | GLN  |
| 1   | ZL    | 374 | ASN  |
| 2   | 2     | 49  | ILE  |
| 2   | 3     | 49  | ILE  |
| 2   | 4     | 49  | ILE  |
| 2   | 4     | 139 | ALA  |
| 2   | 4     | 140 | ILE  |
| 2   | 5     | 49  | ILE  |
| 2   | 0     | 127 | GLN  |
| 2   | r     | 127 | GLN  |
| 2   | x     | 3   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | y     | 127 | GLN  |
| 1   | ZO    | 142 | THR  |
| 1   | ZP    | 374 | ASN  |
| 2   | 6     | 49  | ILE  |
| 2   | 6     | 58  | GLU  |
| 2   | 7     | 49  | ILE  |
| 2   | 7     | 138 | PRO  |
| 2   | 8     | 49  | ILE  |
| 2   | 9     | 49  | ILE  |
| 2   | ZA    | 49  | ILE  |
| 2   | ZA    | 139 | ALA  |
| 2   | ZD    | 139 | ALA  |
| 2   | s     | 127 | GLN  |
| 2   | u     | 127 | GLN  |
| 2   | w     | 127 | GLN  |
| 2   | x     | 127 | GLN  |
| 2   | 7     | 210 | GLY  |
| 2   | 1     | 127 | GLN  |
| 2   | t     | 127 | GLN  |
| 2   | v     | 127 | GLN  |
| 1   | ZO    | 375 | MET  |
| 2   | 3     | 139 | ALA  |
| 1   | ZI    | 325 | GLY  |
| 2   | ZC    | 138 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 1   | ZF    | 321/323 (99%) | 315 (98%)  | 6 (2%)   | 50          | 68 |
| 1   | ZG    | 321/323 (99%) | 316 (98%)  | 5 (2%)   | 55          | 72 |
| 1   | ZH    | 321/323 (99%) | 316 (98%)  | 5 (2%)   | 55          | 72 |
| 1   | ZI    | 321/323 (99%) | 316 (98%)  | 5 (2%)   | 55          | 72 |
| 1   | ZJ    | 321/323 (99%) | 320 (100%) | 1 (0%)   | 86          | 86 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | ZK    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | ZL    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | ZM    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | ZN    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 81  |
| 1   | ZO    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | ZP    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | ZQ    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | ZR    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | ZS    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | ZT    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | ZU    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | ZV    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 81  |
| 1   | ZW    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | ZX    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | ZY    | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 1   | ZZ    | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 1   | Za    | 321/323 (99%)  | 321 (100%) | 0        | 100         | 100 |
| 1   | Zb    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | Zc    | 321/323 (99%)  | 318 (99%)  | 3 (1%)   | 70          | 78  |
| 1   | Zd    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | Ze    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 81  |
| 1   | Zf    | 321/323 (99%)  | 319 (99%)  | 2 (1%)   | 78          | 81  |
| 1   | Zg    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 1   | Zh    | 321/323 (99%)  | 320 (100%) | 1 (0%)   | 86          | 86  |
| 2   | 0     | 205/215 (95%)  | 200 (98%)  | 5 (2%)   | 43          | 65  |
| 2   | 1     | 209/215 (97%)  | 206 (99%)  | 3 (1%)   | 59          | 73  |
| 2   | 2     | 215/215 (100%) | 214 (100%) | 1 (0%)   | 81          | 83  |
| 2   | 3     | 215/215 (100%) | 213 (99%)  | 2 (1%)   | 70          | 78  |
| 2   | 4     | 215/215 (100%) | 214 (100%) | 1 (0%)   | 81          | 83  |
| 2   | 5     | 215/215 (100%) | 213 (99%)  | 2 (1%)   | 70          | 78  |
| 2   | 6     | 215/215 (100%) | 212 (99%)  | 3 (1%)   | 59          | 73  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 2   | 7     | 215/215 (100%)    | 215 (100%)  | 0        | 100         | 100 |
| 2   | 8     | 215/215 (100%)    | 213 (99%)   | 2 (1%)   | 70          | 78  |
| 2   | 9     | 215/215 (100%)    | 212 (99%)   | 3 (1%)   | 59          | 73  |
| 2   | ZA    | 215/215 (100%)    | 214 (100%)  | 1 (0%)   | 81          | 83  |
| 2   | ZB    | 215/215 (100%)    | 211 (98%)   | 4 (2%)   | 50          | 68  |
| 2   | ZC    | 215/215 (100%)    | 212 (99%)   | 3 (1%)   | 59          | 73  |
| 2   | ZD    | 215/215 (100%)    | 213 (99%)   | 2 (1%)   | 70          | 78  |
| 2   | ZE    | 215/215 (100%)    | 214 (100%)  | 1 (0%)   | 81          | 83  |
| 2   | r     | 209/215 (97%)     | 206 (99%)   | 3 (1%)   | 59          | 73  |
| 2   | s     | 210/215 (98%)     | 203 (97%)   | 7 (3%)   | 33          | 59  |
| 2   | t     | 211/215 (98%)     | 206 (98%)   | 5 (2%)   | 43          | 65  |
| 2   | u     | 209/215 (97%)     | 204 (98%)   | 5 (2%)   | 43          | 65  |
| 2   | v     | 210/215 (98%)     | 207 (99%)   | 3 (1%)   | 59          | 73  |
| 2   | w     | 200/215 (93%)     | 199 (100%)  | 1 (0%)   | 81          | 83  |
| 2   | x     | 205/215 (95%)     | 203 (99%)   | 2 (1%)   | 68          | 76  |
| 2   | y     | 205/215 (95%)     | 200 (98%)   | 5 (2%)   | 43          | 65  |
| 2   | z     | 205/215 (95%)     | 201 (98%)   | 4 (2%)   | 48          | 68  |
| All | All   | 14382/14527 (99%) | 14251 (99%) | 131 (1%) | 68          | 78  |

All (131) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZF    | 60  | ASP  |
| 1   | ZF    | 134 | PRO  |
| 1   | ZF    | 154 | MET  |
| 1   | ZF    | 229 | THR  |
| 1   | ZF    | 352 | ASN  |
| 1   | ZF    | 355 | LYS  |
| 1   | ZG    | 3   | PHE  |
| 1   | ZG    | 234 | GLU  |
| 1   | ZG    | 296 | ASN  |
| 1   | ZG    | 332 | ASN  |
| 1   | ZG    | 397 | ASN  |
| 1   | ZH    | 42  | MET  |
| 1   | ZH    | 128 | ILE  |
| 1   | ZH    | 288 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZH    | 355 | LYS  |
| 1   | ZH    | 399 | LEU  |
| 1   | ZI    | 52  | VAL  |
| 1   | ZI    | 99  | GLN  |
| 1   | ZI    | 105 | ASN  |
| 1   | ZI    | 246 | ILE  |
| 1   | ZI    | 352 | ASN  |
| 1   | ZJ    | 42  | MET  |
| 1   | ZK    | 338 | GLN  |
| 1   | ZL    | 338 | GLN  |
| 1   | ZL    | 368 | LEU  |
| 1   | ZL    | 370 | LYS  |
| 1   | ZM    | 89  | ASN  |
| 1   | ZM    | 156 | ILE  |
| 1   | ZM    | 369 | SER  |
| 1   | ZN    | 396 | LEU  |
| 1   | ZN    | 402 | LEU  |
| 1   | ZO    | 141 | ASN  |
| 1   | ZO    | 235 | ASN  |
| 1   | ZO    | 237 | ILE  |
| 1   | ZP    | 333 | VAL  |
| 1   | ZP    | 369 | SER  |
| 1   | ZP    | 370 | LYS  |
| 1   | ZQ    | 158 | LEU  |
| 1   | ZQ    | 367 | ASP  |
| 1   | ZQ    | 370 | LYS  |
| 1   | ZR    | 255 | THR  |
| 1   | ZR    | 269 | GLN  |
| 1   | ZR    | 331 | ASP  |
| 1   | ZS    | 367 | ASP  |
| 1   | ZT    | 42  | MET  |
| 1   | ZU    | 237 | ILE  |
| 1   | ZV    | 397 | ASN  |
| 1   | ZV    | 399 | LEU  |
| 1   | ZW    | 114 | MET  |
| 1   | ZX    | 63  | ASP  |
| 1   | Zb    | 36  | THR  |
| 1   | Zb    | 331 | ASP  |
| 1   | Zb    | 367 | ASP  |
| 1   | Zc    | 369 | SER  |
| 1   | Zc    | 370 | LYS  |
| 1   | Zc    | 399 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Zd    | 397 | ASN  |
| 1   | Ze    | 58  | THR  |
| 1   | Ze    | 395 | ILE  |
| 1   | Zf    | 395 | ILE  |
| 1   | Zf    | 396 | LEU  |
| 1   | Zg    | 375 | MET  |
| 1   | Zh    | 54  | VAL  |
| 2   | 2     | 238 | ARG  |
| 2   | 3     | 43  | ASP  |
| 2   | 3     | 153 | ARG  |
| 2   | 4     | 209 | ASN  |
| 2   | 5     | 137 | GLN  |
| 2   | 5     | 245 | LYS  |
| 2   | 6     | 59  | GLN  |
| 2   | 6     | 78  | GLU  |
| 2   | 6     | 203 | GLU  |
| 2   | 8     | 58  | GLU  |
| 2   | 8     | 100 | GLN  |
| 2   | 9     | 66  | LEU  |
| 2   | 9     | 137 | GLN  |
| 2   | 9     | 226 | VAL  |
| 2   | ZA    | 136 | VAL  |
| 2   | ZB    | 58  | GLU  |
| 2   | ZB    | 95  | VAL  |
| 2   | ZB    | 100 | GLN  |
| 2   | ZB    | 137 | GLN  |
| 2   | ZC    | 1   | MET  |
| 2   | ZC    | 43  | ASP  |
| 2   | ZC    | 136 | VAL  |
| 2   | ZD    | 136 | VAL  |
| 2   | ZD    | 196 | GLN  |
| 2   | ZE    | 141 | THR  |
| 2   | 0     | 1   | MET  |
| 2   | 0     | 36  | ARG  |
| 2   | 0     | 50  | ARG  |
| 2   | 0     | 52  | PRO  |
| 2   | 0     | 73  | ARG  |
| 2   | 1     | 1   | MET  |
| 2   | 1     | 42  | GLU  |
| 2   | 1     | 241 | GLU  |
| 2   | r     | 36  | ARG  |
| 2   | r     | 106 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | r     | 256 | LYS  |
| 2   | s     | 16  | GLN  |
| 2   | s     | 17  | THR  |
| 2   | s     | 137 | GLN  |
| 2   | s     | 169 | GLN  |
| 2   | s     | 170 | VAL  |
| 2   | s     | 251 | ASP  |
| 2   | s     | 257 | LEU  |
| 2   | t     | 1   | MET  |
| 2   | t     | 66  | LEU  |
| 2   | t     | 75  | VAL  |
| 2   | t     | 100 | GLN  |
| 2   | t     | 135 | GLN  |
| 2   | u     | 4   | SER  |
| 2   | u     | 179 | MET  |
| 2   | u     | 181 | ASP  |
| 2   | u     | 194 | GLU  |
| 2   | u     | 208 | LEU  |
| 2   | v     | 73  | ARG  |
| 2   | v     | 127 | GLN  |
| 2   | v     | 150 | THR  |
| 2   | w     | 4   | SER  |
| 2   | x     | 1   | MET  |
| 2   | x     | 137 | GLN  |
| 2   | y     | 1   | MET  |
| 2   | y     | 36  | ARG  |
| 2   | y     | 50  | ARG  |
| 2   | y     | 208 | LEU  |
| 2   | y     | 209 | ASN  |
| 2   | z     | 1   | MET  |
| 2   | z     | 3   | SER  |
| 2   | z     | 179 | MET  |
| 2   | z     | 252 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (526) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZF    | 5   | GLN  |
| 1   | ZF    | 107 | ASN  |
| 1   | ZF    | 155 | GLN  |
| 1   | ZF    | 194 | HIS  |
| 1   | ZF    | 197 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZF    | 265 | ASN  |
| 1   | ZF    | 270 | ASN  |
| 1   | ZF    | 280 | ASN  |
| 1   | ZF    | 282 | ASN  |
| 1   | ZF    | 310 | GLN  |
| 1   | ZF    | 358 | ASN  |
| 1   | ZF    | 385 | ASN  |
| 1   | ZF    | 387 | GLN  |
| 1   | ZG    | 22  | ASN  |
| 1   | ZG    | 89  | ASN  |
| 1   | ZG    | 107 | ASN  |
| 1   | ZG    | 115 | GLN  |
| 1   | ZG    | 130 | GLN  |
| 1   | ZG    | 133 | ASN  |
| 1   | ZG    | 233 | ASN  |
| 1   | ZG    | 265 | ASN  |
| 1   | ZG    | 270 | ASN  |
| 1   | ZG    | 293 | GLN  |
| 1   | ZG    | 303 | ASN  |
| 1   | ZG    | 332 | ASN  |
| 1   | ZG    | 385 | ASN  |
| 1   | ZG    | 387 | GLN  |
| 1   | ZG    | 397 | ASN  |
| 1   | ZG    | 401 | ASN  |
| 1   | ZH    | 5   | GLN  |
| 1   | ZH    | 206 | ASN  |
| 1   | ZH    | 252 | ASN  |
| 1   | ZH    | 270 | ASN  |
| 1   | ZH    | 296 | ASN  |
| 1   | ZH    | 303 | ASN  |
| 1   | ZH    | 329 | GLN  |
| 1   | ZH    | 352 | ASN  |
| 1   | ZH    | 365 | ASN  |
| 1   | ZH    | 379 | GLN  |
| 1   | ZH    | 385 | ASN  |
| 1   | ZH    | 392 | GLN  |
| 1   | ZI    | 5   | GLN  |
| 1   | ZI    | 22  | ASN  |
| 1   | ZI    | 130 | GLN  |
| 1   | ZI    | 197 | ASN  |
| 1   | ZI    | 245 | ASN  |
| 1   | ZI    | 252 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZI    | 265 | ASN  |
| 1   | ZI    | 269 | GLN  |
| 1   | ZI    | 322 | ASN  |
| 1   | ZI    | 323 | ASN  |
| 1   | ZI    | 385 | ASN  |
| 1   | ZI    | 387 | GLN  |
| 1   | ZI    | 392 | GLN  |
| 1   | ZI    | 394 | GLN  |
| 1   | ZI    | 401 | ASN  |
| 1   | ZJ    | 22  | ASN  |
| 1   | ZJ    | 133 | ASN  |
| 1   | ZJ    | 159 | ASN  |
| 1   | ZJ    | 197 | ASN  |
| 1   | ZJ    | 265 | ASN  |
| 1   | ZJ    | 270 | ASN  |
| 1   | ZJ    | 274 | ASN  |
| 1   | ZJ    | 282 | ASN  |
| 1   | ZJ    | 293 | GLN  |
| 1   | ZJ    | 310 | GLN  |
| 1   | ZJ    | 379 | GLN  |
| 1   | ZJ    | 392 | GLN  |
| 1   | ZJ    | 397 | ASN  |
| 1   | ZJ    | 401 | ASN  |
| 1   | ZK    | 89  | ASN  |
| 1   | ZK    | 107 | ASN  |
| 1   | ZK    | 197 | ASN  |
| 1   | ZK    | 252 | ASN  |
| 1   | ZK    | 274 | ASN  |
| 1   | ZK    | 303 | ASN  |
| 1   | ZK    | 319 | ASN  |
| 1   | ZK    | 332 | ASN  |
| 1   | ZK    | 392 | GLN  |
| 1   | ZK    | 401 | ASN  |
| 1   | ZL    | 5   | GLN  |
| 1   | ZL    | 89  | ASN  |
| 1   | ZL    | 99  | GLN  |
| 1   | ZL    | 179 | ASN  |
| 1   | ZL    | 190 | GLN  |
| 1   | ZL    | 197 | ASN  |
| 1   | ZL    | 252 | ASN  |
| 1   | ZL    | 282 | ASN  |
| 1   | ZL    | 293 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZL    | 303 | ASN  |
| 1   | ZL    | 306 | ASN  |
| 1   | ZL    | 310 | GLN  |
| 1   | ZL    | 338 | GLN  |
| 1   | ZL    | 385 | ASN  |
| 1   | ZL    | 401 | ASN  |
| 1   | ZM    | 5   | GLN  |
| 1   | ZM    | 22  | ASN  |
| 1   | ZM    | 59  | GLN  |
| 1   | ZM    | 89  | ASN  |
| 1   | ZM    | 197 | ASN  |
| 1   | ZM    | 213 | HIS  |
| 1   | ZM    | 235 | ASN  |
| 1   | ZM    | 252 | ASN  |
| 1   | ZM    | 381 | ASN  |
| 1   | ZM    | 397 | ASN  |
| 1   | ZN    | 22  | ASN  |
| 1   | ZN    | 79  | GLN  |
| 1   | ZN    | 107 | ASN  |
| 1   | ZN    | 129 | GLN  |
| 1   | ZN    | 133 | ASN  |
| 1   | ZN    | 157 | ASN  |
| 1   | ZN    | 190 | GLN  |
| 1   | ZN    | 192 | ASN  |
| 1   | ZN    | 197 | ASN  |
| 1   | ZN    | 213 | HIS  |
| 1   | ZN    | 270 | ASN  |
| 1   | ZN    | 319 | ASN  |
| 1   | ZN    | 332 | ASN  |
| 1   | ZN    | 338 | GLN  |
| 1   | ZN    | 379 | GLN  |
| 1   | ZN    | 385 | ASN  |
| 1   | ZN    | 387 | GLN  |
| 1   | ZN    | 401 | ASN  |
| 1   | ZO    | 5   | GLN  |
| 1   | ZO    | 22  | ASN  |
| 1   | ZO    | 141 | ASN  |
| 1   | ZO    | 192 | ASN  |
| 1   | ZO    | 235 | ASN  |
| 1   | ZO    | 270 | ASN  |
| 1   | ZO    | 296 | ASN  |
| 1   | ZO    | 322 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZO    | 332 | ASN  |
| 1   | ZP    | 11  | ASN  |
| 1   | ZP    | 89  | ASN  |
| 1   | ZP    | 107 | ASN  |
| 1   | ZP    | 129 | GLN  |
| 1   | ZP    | 192 | ASN  |
| 1   | ZP    | 194 | HIS  |
| 1   | ZP    | 213 | HIS  |
| 1   | ZP    | 245 | ASN  |
| 1   | ZP    | 270 | ASN  |
| 1   | ZP    | 314 | GLN  |
| 1   | ZP    | 322 | ASN  |
| 1   | ZP    | 338 | GLN  |
| 1   | ZP    | 381 | ASN  |
| 1   | ZP    | 385 | ASN  |
| 1   | ZP    | 392 | GLN  |
| 1   | ZQ    | 89  | ASN  |
| 1   | ZQ    | 97  | ASN  |
| 1   | ZQ    | 105 | ASN  |
| 1   | ZQ    | 133 | ASN  |
| 1   | ZQ    | 141 | ASN  |
| 1   | ZQ    | 155 | GLN  |
| 1   | ZQ    | 197 | ASN  |
| 1   | ZQ    | 213 | HIS  |
| 1   | ZQ    | 233 | ASN  |
| 1   | ZQ    | 265 | ASN  |
| 1   | ZQ    | 308 | GLN  |
| 1   | ZQ    | 383 | GLN  |
| 1   | ZQ    | 387 | GLN  |
| 1   | ZR    | 107 | ASN  |
| 1   | ZR    | 133 | ASN  |
| 1   | ZR    | 157 | ASN  |
| 1   | ZR    | 197 | ASN  |
| 1   | ZR    | 206 | ASN  |
| 1   | ZR    | 252 | ASN  |
| 1   | ZR    | 268 | GLN  |
| 1   | ZR    | 269 | GLN  |
| 1   | ZR    | 293 | GLN  |
| 1   | ZR    | 295 | ASN  |
| 1   | ZR    | 310 | GLN  |
| 1   | ZR    | 401 | ASN  |
| 1   | ZS    | 22  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZS    | 133 | ASN  |
| 1   | ZS    | 197 | ASN  |
| 1   | ZS    | 206 | ASN  |
| 1   | ZS    | 303 | ASN  |
| 1   | ZS    | 394 | GLN  |
| 1   | ZT    | 5   | GLN  |
| 1   | ZT    | 22  | ASN  |
| 1   | ZT    | 99  | GLN  |
| 1   | ZT    | 129 | GLN  |
| 1   | ZT    | 133 | ASN  |
| 1   | ZT    | 197 | ASN  |
| 1   | ZT    | 213 | HIS  |
| 1   | ZT    | 235 | ASN  |
| 1   | ZT    | 252 | ASN  |
| 1   | ZT    | 270 | ASN  |
| 1   | ZT    | 275 | ASN  |
| 1   | ZT    | 293 | GLN  |
| 1   | ZT    | 303 | ASN  |
| 1   | ZT    | 310 | GLN  |
| 1   | ZT    | 314 | GLN  |
| 1   | ZT    | 352 | ASN  |
| 1   | ZU    | 22  | ASN  |
| 1   | ZU    | 59  | GLN  |
| 1   | ZU    | 99  | GLN  |
| 1   | ZU    | 107 | ASN  |
| 1   | ZU    | 133 | ASN  |
| 1   | ZU    | 159 | ASN  |
| 1   | ZU    | 197 | ASN  |
| 1   | ZU    | 293 | GLN  |
| 1   | ZU    | 310 | GLN  |
| 1   | ZU    | 314 | GLN  |
| 1   | ZU    | 332 | ASN  |
| 1   | ZU    | 379 | GLN  |
| 1   | ZU    | 387 | GLN  |
| 1   | ZU    | 401 | ASN  |
| 1   | ZV    | 89  | ASN  |
| 1   | ZV    | 107 | ASN  |
| 1   | ZV    | 130 | GLN  |
| 1   | ZV    | 133 | ASN  |
| 1   | ZV    | 159 | ASN  |
| 1   | ZV    | 197 | ASN  |
| 1   | ZV    | 213 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZV    | 252 | ASN  |
| 1   | ZV    | 269 | GLN  |
| 1   | ZV    | 280 | ASN  |
| 1   | ZV    | 293 | GLN  |
| 1   | ZV    | 295 | ASN  |
| 1   | ZV    | 303 | ASN  |
| 1   | ZV    | 314 | GLN  |
| 1   | ZV    | 381 | ASN  |
| 1   | ZV    | 394 | GLN  |
| 1   | ZW    | 5   | GLN  |
| 1   | ZW    | 107 | ASN  |
| 1   | ZW    | 129 | GLN  |
| 1   | ZW    | 133 | ASN  |
| 1   | ZW    | 213 | HIS  |
| 1   | ZW    | 252 | ASN  |
| 1   | ZW    | 270 | ASN  |
| 1   | ZW    | 310 | GLN  |
| 1   | ZW    | 314 | GLN  |
| 1   | ZW    | 332 | ASN  |
| 1   | ZX    | 89  | ASN  |
| 1   | ZX    | 159 | ASN  |
| 1   | ZX    | 270 | ASN  |
| 1   | ZX    | 314 | GLN  |
| 1   | ZX    | 401 | ASN  |
| 1   | ZY    | 5   | GLN  |
| 1   | ZY    | 59  | GLN  |
| 1   | ZY    | 80  | ASN  |
| 1   | ZY    | 115 | GLN  |
| 1   | ZY    | 159 | ASN  |
| 1   | ZY    | 190 | GLN  |
| 1   | ZY    | 197 | ASN  |
| 1   | ZY    | 265 | ASN  |
| 1   | ZY    | 268 | GLN  |
| 1   | ZY    | 270 | ASN  |
| 1   | ZY    | 314 | GLN  |
| 1   | ZY    | 332 | ASN  |
| 1   | ZY    | 385 | ASN  |
| 1   | ZY    | 392 | GLN  |
| 1   | ZZ    | 99  | GLN  |
| 1   | ZZ    | 107 | ASN  |
| 1   | ZZ    | 133 | ASN  |
| 1   | ZZ    | 194 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | ZZ    | 197 | ASN  |
| 1   | ZZ    | 213 | HIS  |
| 1   | ZZ    | 293 | GLN  |
| 1   | ZZ    | 303 | ASN  |
| 1   | ZZ    | 308 | GLN  |
| 1   | ZZ    | 314 | GLN  |
| 1   | ZZ    | 332 | ASN  |
| 1   | ZZ    | 387 | GLN  |
| 1   | ZZ    | 394 | GLN  |
| 1   | ZZ    | 401 | ASN  |
| 1   | Za    | 22  | ASN  |
| 1   | Za    | 129 | GLN  |
| 1   | Za    | 133 | ASN  |
| 1   | Za    | 157 | ASN  |
| 1   | Za    | 197 | ASN  |
| 1   | Za    | 293 | GLN  |
| 1   | Za    | 332 | ASN  |
| 1   | Za    | 385 | ASN  |
| 1   | Za    | 387 | GLN  |
| 1   | Zb    | 5   | GLN  |
| 1   | Zb    | 79  | GLN  |
| 1   | Zb    | 107 | ASN  |
| 1   | Zb    | 133 | ASN  |
| 1   | Zb    | 159 | ASN  |
| 1   | Zb    | 197 | ASN  |
| 1   | Zb    | 293 | GLN  |
| 1   | Zb    | 308 | GLN  |
| 1   | Zb    | 314 | GLN  |
| 1   | Zb    | 358 | ASN  |
| 1   | Zb    | 385 | ASN  |
| 1   | Zb    | 401 | ASN  |
| 1   | Zc    | 107 | ASN  |
| 1   | Zc    | 115 | GLN  |
| 1   | Zc    | 129 | GLN  |
| 1   | Zc    | 159 | ASN  |
| 1   | Zc    | 190 | GLN  |
| 1   | Zc    | 197 | ASN  |
| 1   | Zc    | 270 | ASN  |
| 1   | Zc    | 293 | GLN  |
| 1   | Zc    | 352 | ASN  |
| 1   | Zc    | 379 | GLN  |
| 1   | Zc    | 387 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Zd    | 5   | GLN  |
| 1   | Zd    | 22  | ASN  |
| 1   | Zd    | 105 | ASN  |
| 1   | Zd    | 129 | GLN  |
| 1   | Zd    | 130 | GLN  |
| 1   | Zd    | 133 | ASN  |
| 1   | Zd    | 293 | GLN  |
| 1   | Zd    | 295 | ASN  |
| 1   | Zd    | 303 | ASN  |
| 1   | Zd    | 322 | ASN  |
| 1   | Zd    | 387 | GLN  |
| 1   | Ze    | 5   | GLN  |
| 1   | Ze    | 22  | ASN  |
| 1   | Ze    | 99  | GLN  |
| 1   | Ze    | 107 | ASN  |
| 1   | Ze    | 133 | ASN  |
| 1   | Ze    | 197 | ASN  |
| 1   | Ze    | 252 | ASN  |
| 1   | Ze    | 303 | ASN  |
| 1   | Ze    | 322 | ASN  |
| 1   | Ze    | 358 | ASN  |
| 1   | Ze    | 394 | GLN  |
| 1   | Zf    | 22  | ASN  |
| 1   | Zf    | 105 | ASN  |
| 1   | Zf    | 107 | ASN  |
| 1   | Zf    | 115 | GLN  |
| 1   | Zf    | 159 | ASN  |
| 1   | Zf    | 197 | ASN  |
| 1   | Zf    | 252 | ASN  |
| 1   | Zf    | 293 | GLN  |
| 1   | Zf    | 303 | ASN  |
| 1   | Zf    | 308 | GLN  |
| 1   | Zf    | 314 | GLN  |
| 1   | Zf    | 332 | ASN  |
| 1   | Zf    | 385 | ASN  |
| 1   | Zg    | 5   | GLN  |
| 1   | Zg    | 107 | ASN  |
| 1   | Zg    | 129 | GLN  |
| 1   | Zg    | 133 | ASN  |
| 1   | Zg    | 159 | ASN  |
| 1   | Zg    | 179 | ASN  |
| 1   | Zg    | 197 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Zg    | 213 | HIS  |
| 1   | Zg    | 310 | GLN  |
| 1   | Zg    | 381 | ASN  |
| 1   | Zh    | 97  | ASN  |
| 1   | Zh    | 99  | GLN  |
| 1   | Zh    | 115 | GLN  |
| 1   | Zh    | 197 | ASN  |
| 1   | Zh    | 303 | ASN  |
| 1   | Zh    | 383 | GLN  |
| 1   | Zh    | 385 | ASN  |
| 1   | Zh    | 392 | GLN  |
| 2   | 2     | 51  | GLN  |
| 2   | 2     | 164 | GLN  |
| 2   | 2     | 180 | ASN  |
| 2   | 2     | 255 | GLN  |
| 2   | 3     | 32  | ASN  |
| 2   | 3     | 37  | GLN  |
| 2   | 3     | 67  | GLN  |
| 2   | 3     | 104 | GLN  |
| 2   | 3     | 137 | GLN  |
| 2   | 3     | 255 | GLN  |
| 2   | 4     | 37  | GLN  |
| 2   | 4     | 81  | HIS  |
| 2   | 4     | 88  | GLN  |
| 2   | 4     | 104 | GLN  |
| 2   | 4     | 125 | ASN  |
| 2   | 4     | 127 | GLN  |
| 2   | 4     | 174 | ASN  |
| 2   | 4     | 216 | GLN  |
| 2   | 4     | 235 | GLN  |
| 2   | 4     | 252 | GLN  |
| 2   | 4     | 255 | GLN  |
| 2   | 5     | 32  | ASN  |
| 2   | 5     | 55  | GLN  |
| 2   | 5     | 85  | ASN  |
| 2   | 5     | 100 | GLN  |
| 2   | 5     | 237 | GLN  |
| 2   | 5     | 252 | GLN  |
| 2   | 6     | 16  | GLN  |
| 2   | 6     | 59  | GLN  |
| 2   | 6     | 91  | ASN  |
| 2   | 6     | 121 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 6     | 127 | GLN  |
| 2   | 6     | 135 | GLN  |
| 2   | 6     | 161 | GLN  |
| 2   | 6     | 209 | ASN  |
| 2   | 6     | 237 | GLN  |
| 2   | 7     | 55  | GLN  |
| 2   | 7     | 81  | HIS  |
| 2   | 7     | 125 | ASN  |
| 2   | 7     | 164 | GLN  |
| 2   | 7     | 190 | ASN  |
| 2   | 7     | 235 | GLN  |
| 2   | 8     | 83  | GLN  |
| 2   | 8     | 85  | ASN  |
| 2   | 8     | 196 | GLN  |
| 2   | 8     | 209 | ASN  |
| 2   | 9     | 37  | GLN  |
| 2   | 9     | 47  | GLN  |
| 2   | 9     | 85  | ASN  |
| 2   | 9     | 88  | GLN  |
| 2   | 9     | 91  | ASN  |
| 2   | 9     | 137 | GLN  |
| 2   | 9     | 259 | GLN  |
| 2   | ZA    | 32  | ASN  |
| 2   | ZA    | 37  | GLN  |
| 2   | ZA    | 83  | GLN  |
| 2   | ZA    | 137 | GLN  |
| 2   | ZA    | 235 | GLN  |
| 2   | ZB    | 24  | ASN  |
| 2   | ZB    | 25  | ASN  |
| 2   | ZB    | 28  | ASN  |
| 2   | ZB    | 37  | GLN  |
| 2   | ZB    | 100 | GLN  |
| 2   | ZB    | 137 | GLN  |
| 2   | ZB    | 235 | GLN  |
| 2   | ZB    | 243 | ASN  |
| 2   | ZC    | 16  | GLN  |
| 2   | ZC    | 24  | ASN  |
| 2   | ZC    | 55  | GLN  |
| 2   | ZC    | 67  | GLN  |
| 2   | ZC    | 83  | GLN  |
| 2   | ZC    | 88  | GLN  |
| 2   | ZC    | 100 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | ZC    | 125 | ASN  |
| 2   | ZC    | 127 | GLN  |
| 2   | ZC    | 137 | GLN  |
| 2   | ZC    | 190 | ASN  |
| 2   | ZC    | 202 | ASN  |
| 2   | ZC    | 259 | GLN  |
| 2   | ZD    | 24  | ASN  |
| 2   | ZD    | 67  | GLN  |
| 2   | ZD    | 88  | GLN  |
| 2   | ZD    | 91  | ASN  |
| 2   | ZD    | 124 | GLN  |
| 2   | ZD    | 135 | GLN  |
| 2   | ZD    | 161 | GLN  |
| 2   | ZE    | 37  | GLN  |
| 2   | ZE    | 67  | GLN  |
| 2   | ZE    | 91  | ASN  |
| 2   | ZE    | 121 | GLN  |
| 2   | ZE    | 252 | GLN  |
| 2   | 0     | 32  | ASN  |
| 2   | 0     | 88  | GLN  |
| 2   | 0     | 100 | GLN  |
| 2   | 0     | 135 | GLN  |
| 2   | 0     | 137 | GLN  |
| 2   | 0     | 180 | ASN  |
| 2   | 0     | 237 | GLN  |
| 2   | 0     | 255 | GLN  |
| 2   | 1     | 67  | GLN  |
| 2   | 1     | 83  | GLN  |
| 2   | 1     | 85  | ASN  |
| 2   | 1     | 135 | GLN  |
| 2   | 1     | 237 | GLN  |
| 2   | 1     | 252 | GLN  |
| 2   | r     | 83  | GLN  |
| 2   | r     | 85  | ASN  |
| 2   | r     | 121 | GLN  |
| 2   | r     | 135 | GLN  |
| 2   | r     | 161 | GLN  |
| 2   | r     | 172 | GLN  |
| 2   | r     | 174 | ASN  |
| 2   | r     | 223 | ASN  |
| 2   | s     | 16  | GLN  |
| 2   | s     | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | s     | 37  | GLN  |
| 2   | s     | 137 | GLN  |
| 2   | s     | 169 | GLN  |
| 2   | s     | 180 | ASN  |
| 2   | s     | 223 | ASN  |
| 2   | s     | 259 | GLN  |
| 2   | t     | 37  | GLN  |
| 2   | t     | 90  | ASN  |
| 2   | t     | 104 | GLN  |
| 2   | t     | 127 | GLN  |
| 2   | t     | 162 | GLN  |
| 2   | t     | 223 | ASN  |
| 2   | t     | 259 | GLN  |
| 2   | u     | 16  | GLN  |
| 2   | u     | 32  | ASN  |
| 2   | u     | 37  | GLN  |
| 2   | u     | 196 | GLN  |
| 2   | u     | 202 | ASN  |
| 2   | v     | 85  | ASN  |
| 2   | v     | 90  | ASN  |
| 2   | v     | 161 | GLN  |
| 2   | v     | 164 | GLN  |
| 2   | v     | 169 | GLN  |
| 2   | v     | 172 | GLN  |
| 2   | v     | 223 | ASN  |
| 2   | v     | 232 | ASN  |
| 2   | w     | 28  | ASN  |
| 2   | w     | 32  | ASN  |
| 2   | w     | 104 | GLN  |
| 2   | w     | 121 | GLN  |
| 2   | w     | 135 | GLN  |
| 2   | w     | 172 | GLN  |
| 2   | w     | 180 | ASN  |
| 2   | w     | 196 | GLN  |
| 2   | w     | 223 | ASN  |
| 2   | w     | 235 | GLN  |
| 2   | x     | 32  | ASN  |
| 2   | x     | 37  | GLN  |
| 2   | x     | 81  | HIS  |
| 2   | x     | 104 | GLN  |
| 2   | x     | 121 | GLN  |
| 2   | x     | 127 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | x     | 145 | ASN  |
| 2   | y     | 25  | ASN  |
| 2   | y     | 37  | GLN  |
| 2   | y     | 51  | GLN  |
| 2   | y     | 67  | GLN  |
| 2   | y     | 91  | ASN  |
| 2   | y     | 125 | ASN  |
| 2   | y     | 127 | GLN  |
| 2   | y     | 209 | ASN  |
| 2   | y     | 223 | ASN  |
| 2   | y     | 252 | GLN  |
| 2   | z     | 37  | GLN  |
| 2   | z     | 67  | GLN  |
| 2   | z     | 125 | ASN  |
| 2   | z     | 137 | GLN  |
| 2   | z     | 161 | GLN  |
| 2   | z     | 235 | 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 ⓘ

There are no chain breaks in this entry.

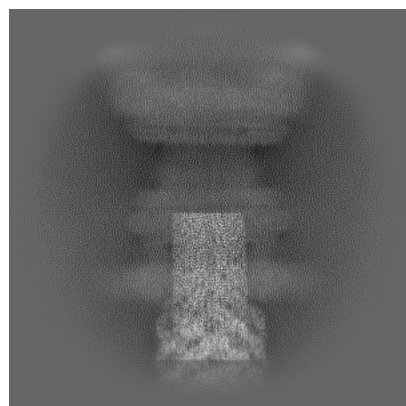
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37600. These allow visual inspection of the internal detail of the map and identification of artifacts.

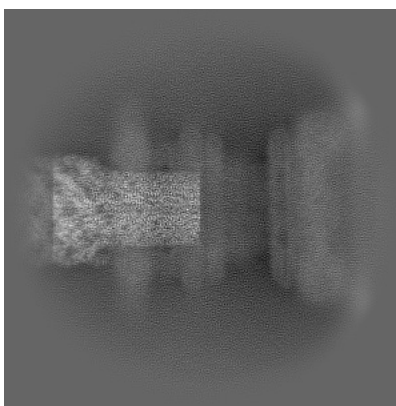
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

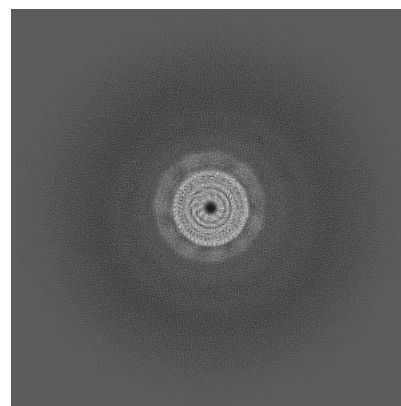
#### 6.1.1 Primary map



X

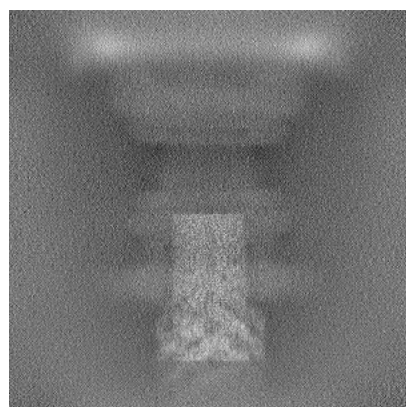


Y

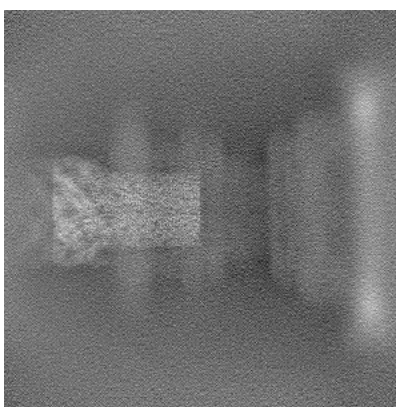


Z

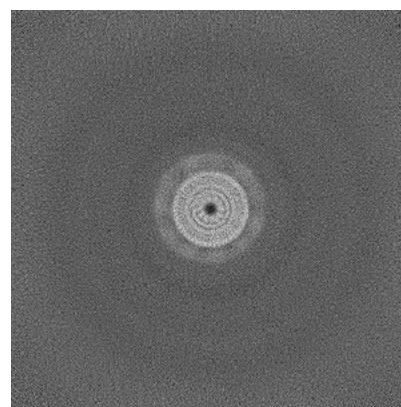
#### 6.1.2 Raw map



X



Y

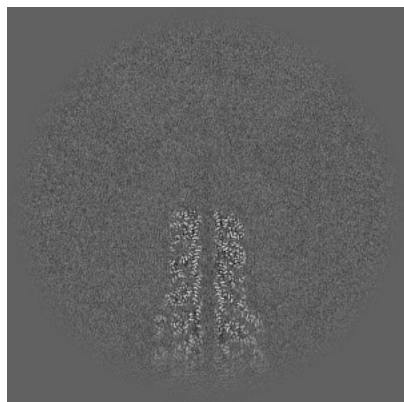


Z

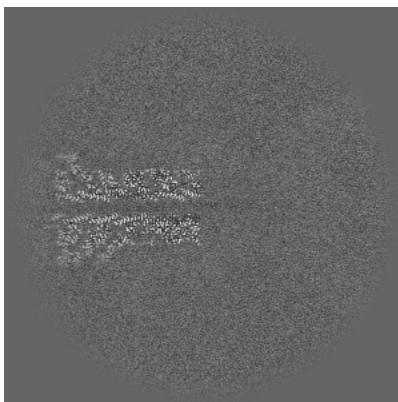
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

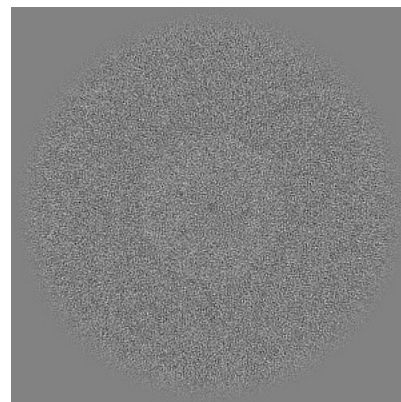
### 6.2.1 Primary map



X Index: 256

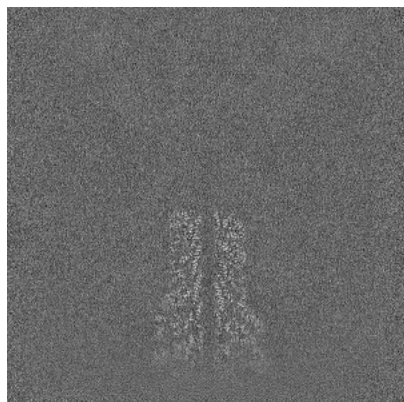


Y Index: 256

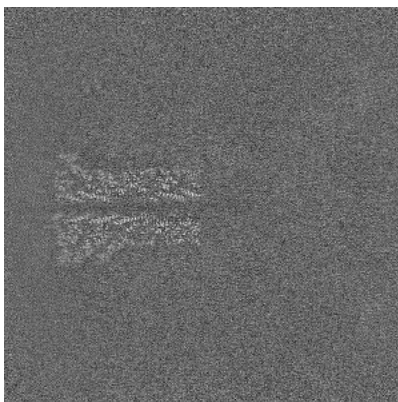


Z Index: 256

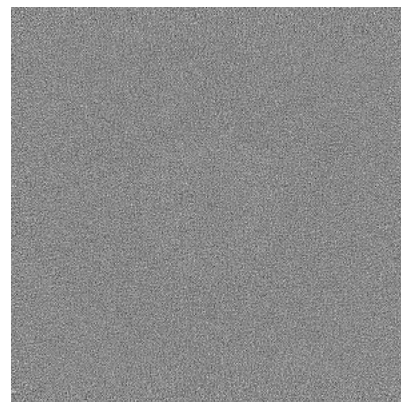
### 6.2.2 Raw map



X Index: 256



Y Index: 256

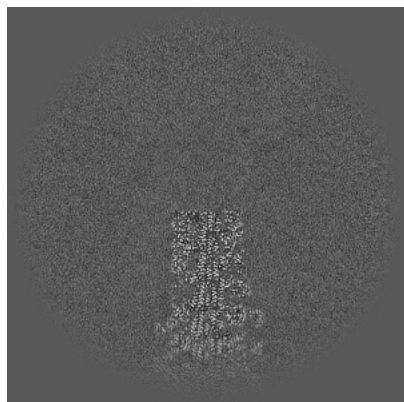


Z Index: 256

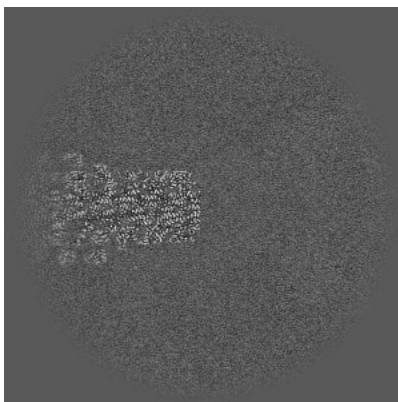
The images above show central slices of the map in three orthogonal directions.

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

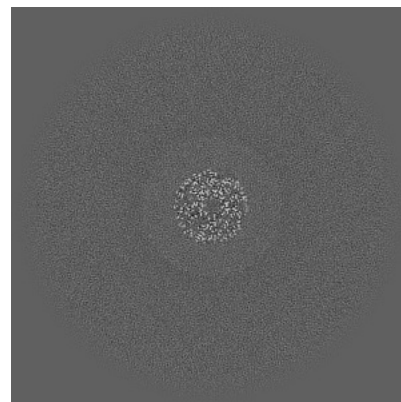
### 6.3.1 Primary map



X Index: 242

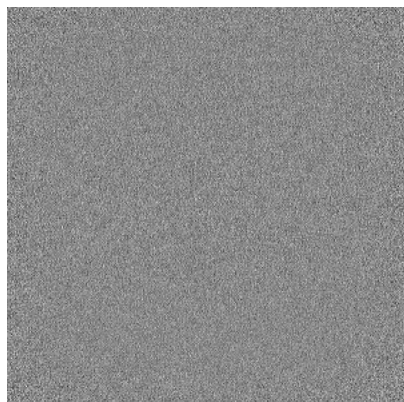


Y Index: 268

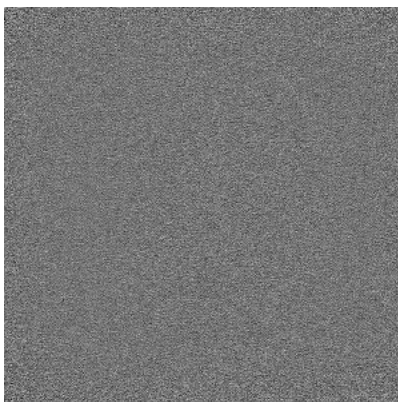


Z Index: 218

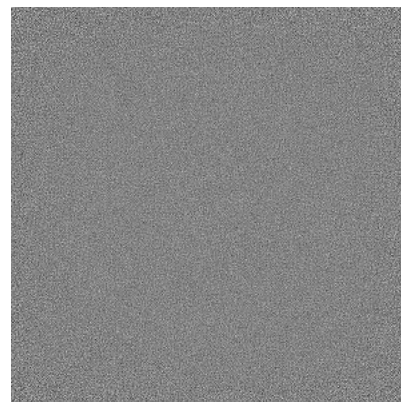
### 6.3.2 Raw map



X Index: 0



Y Index: 0

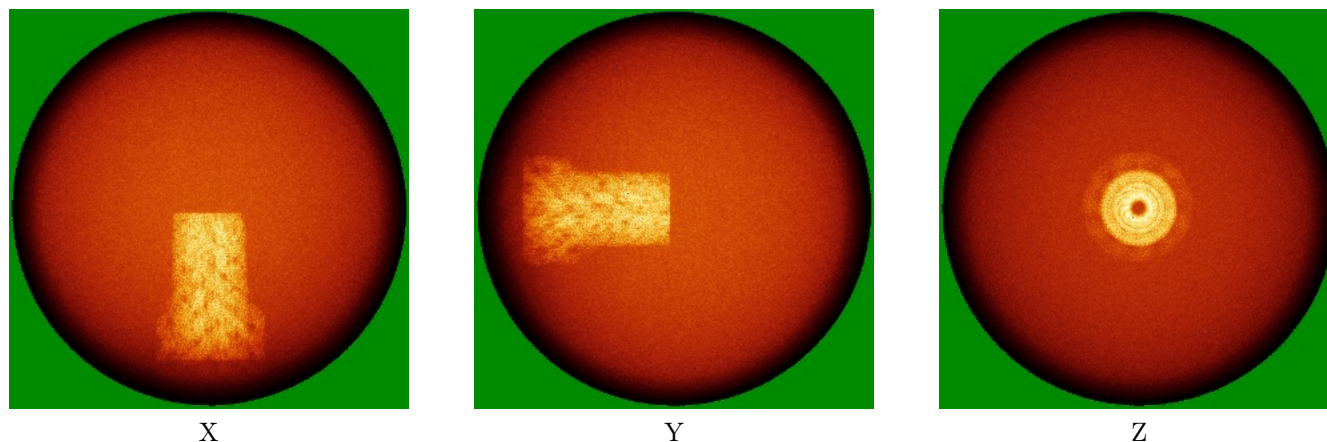


Z Index: 0

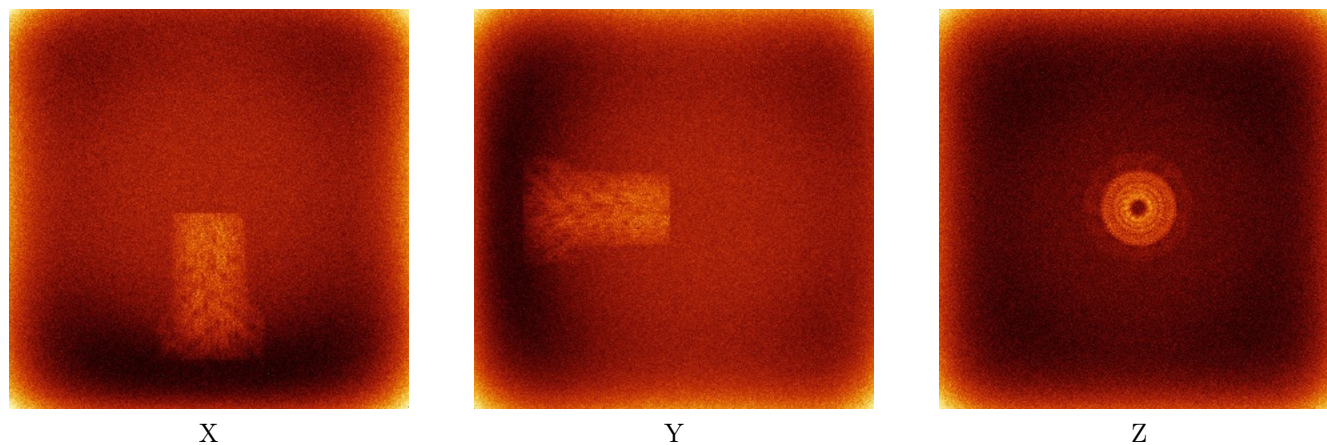
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



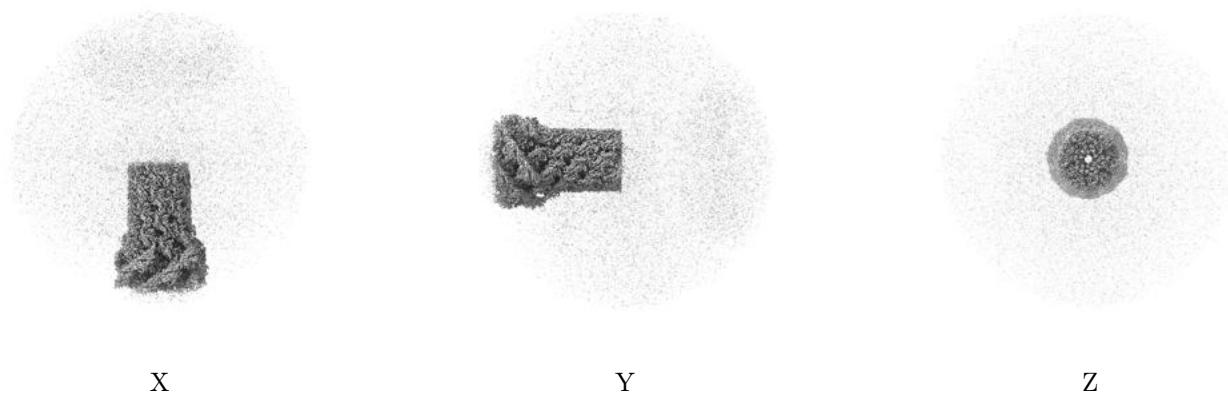
### 6.4.2 Raw map



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

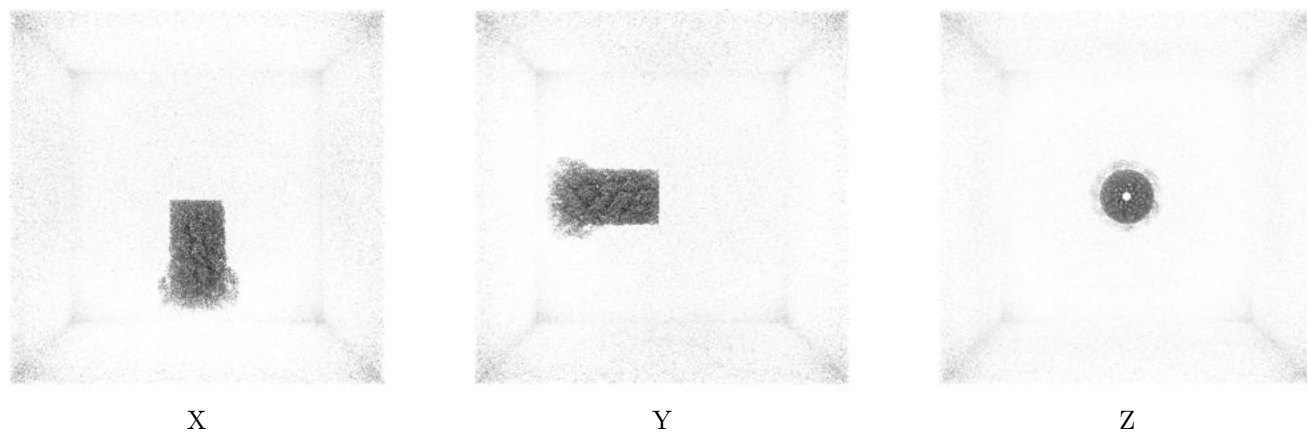
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

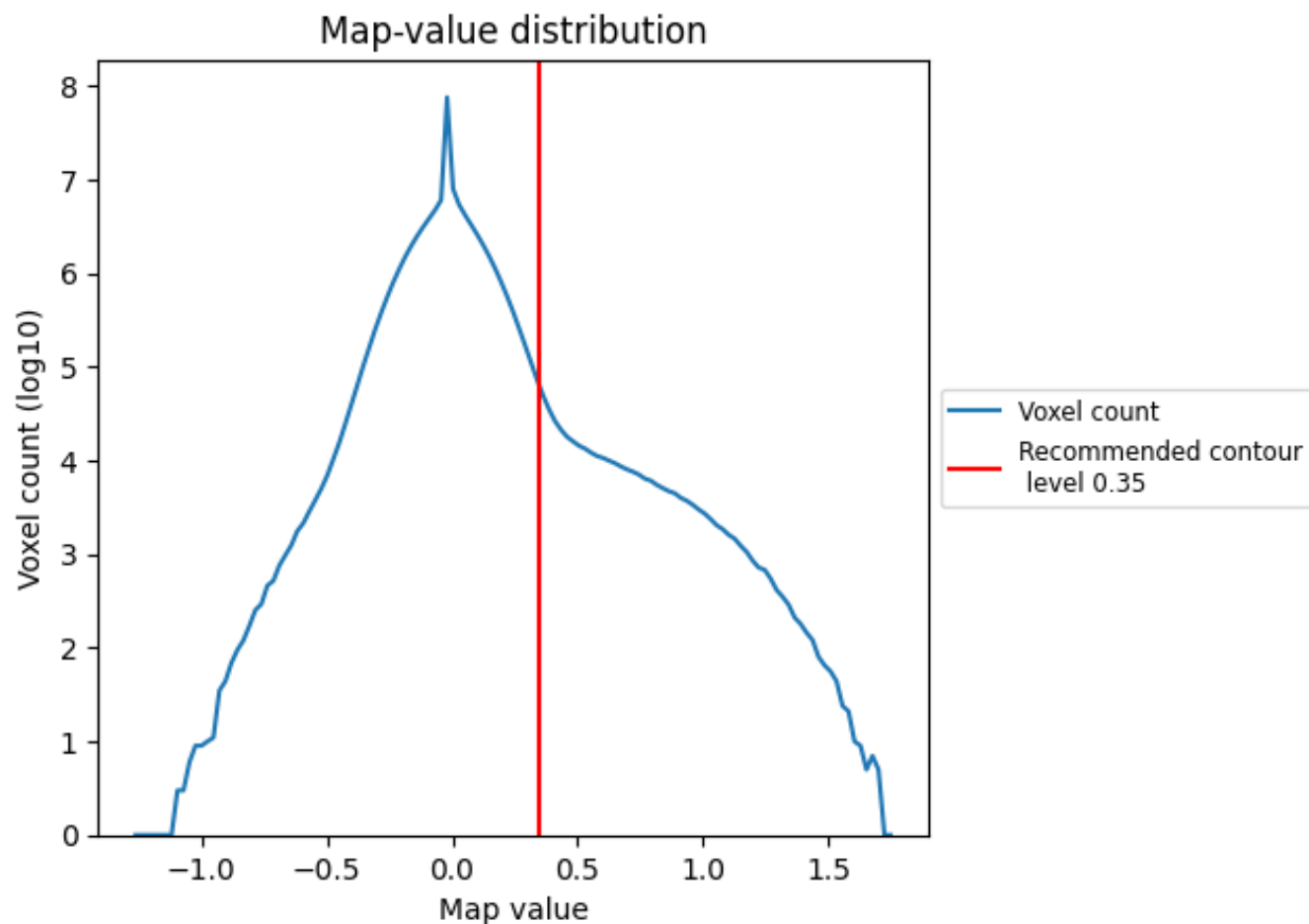
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

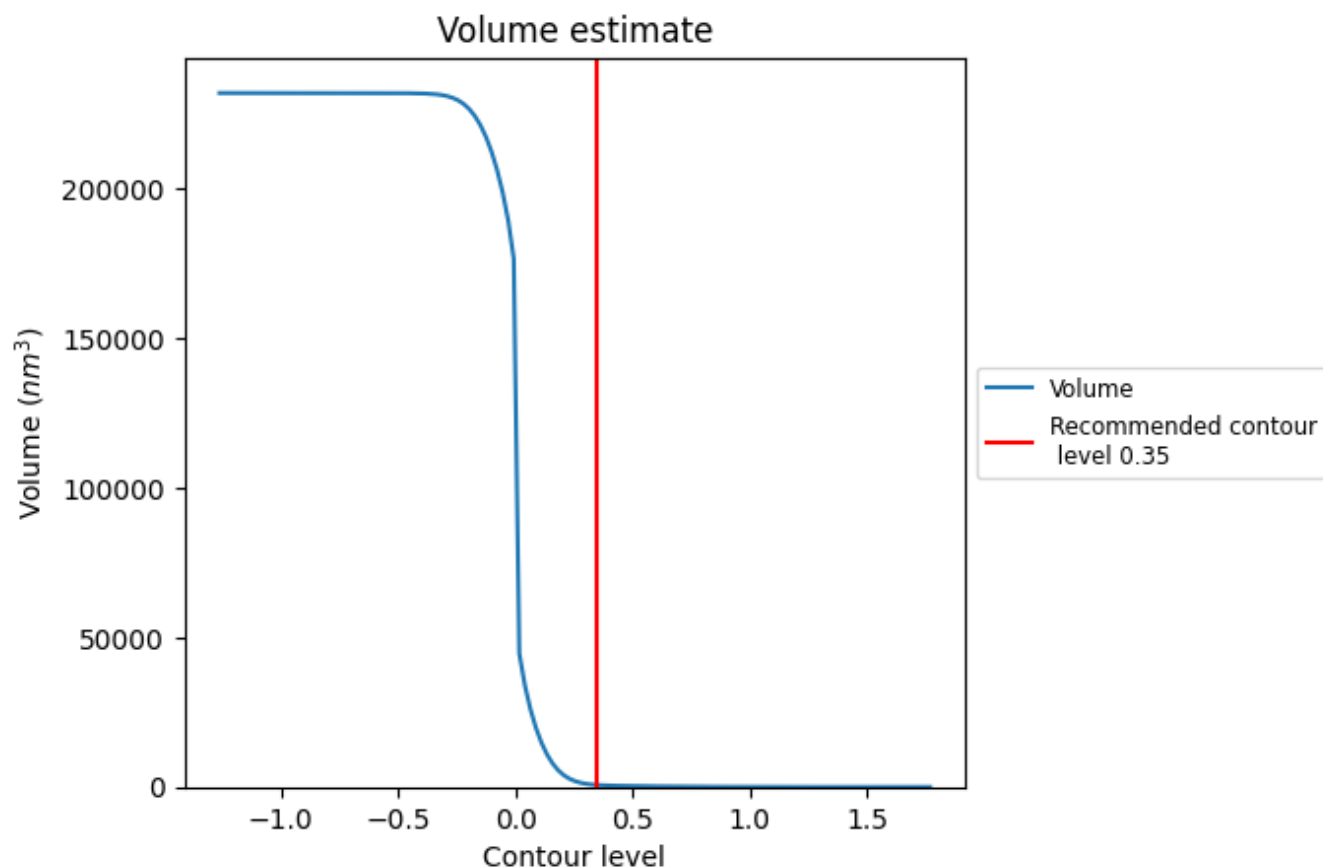
This section contains the results of statistical analysis of the map.

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



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

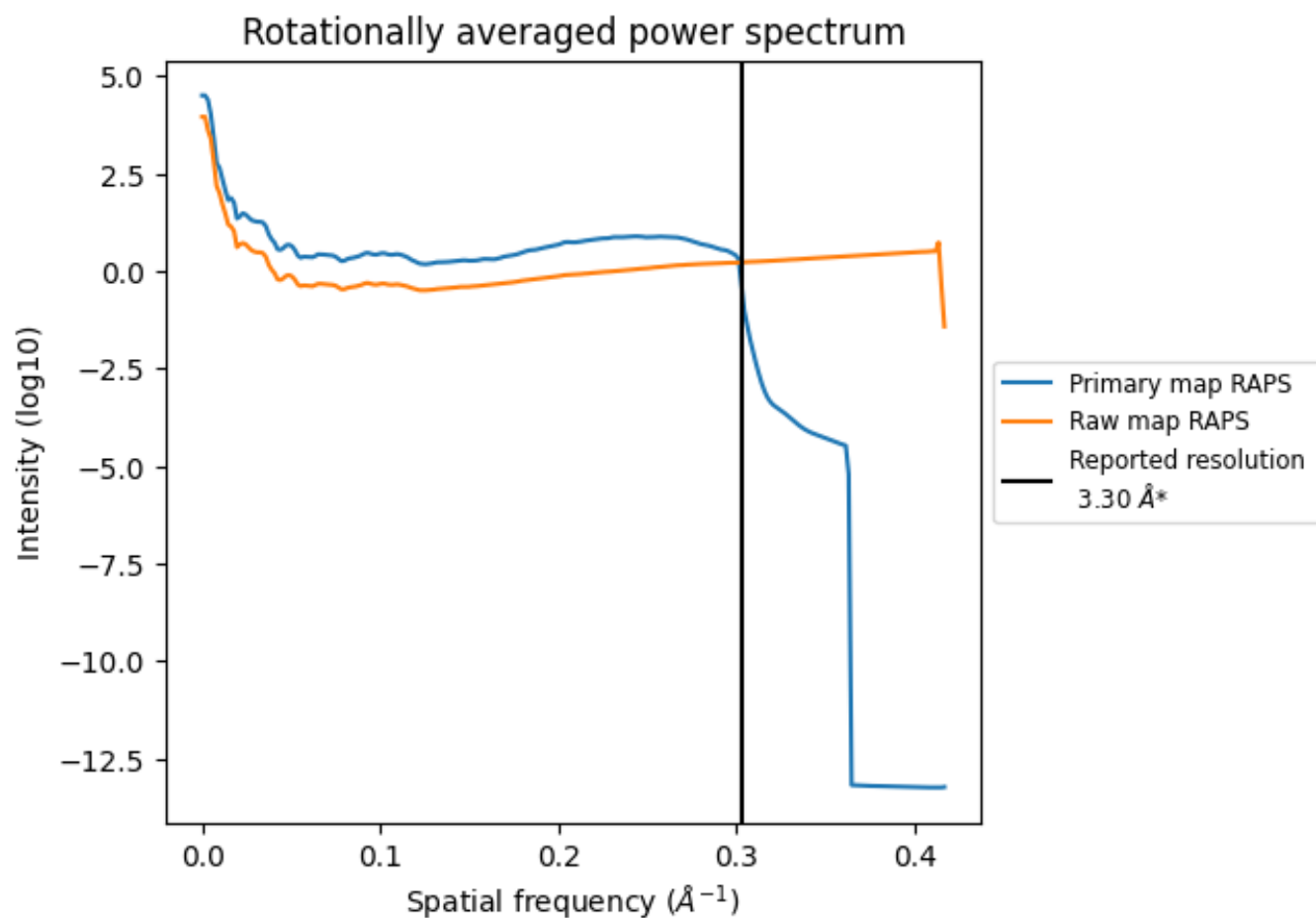
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 652  $\text{nm}^3$ ; this corresponds to an approximate mass of 589 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 ⓘ

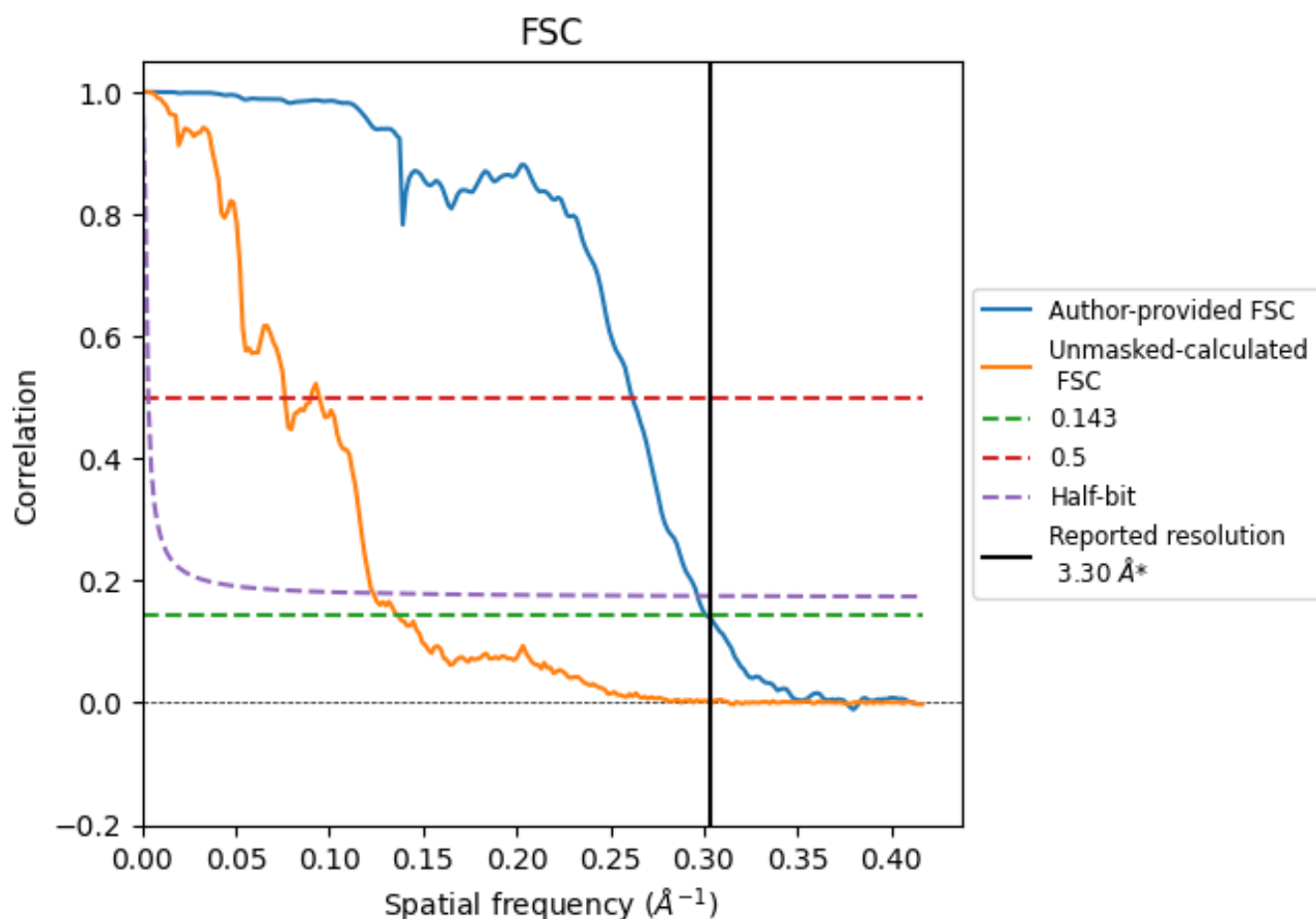


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

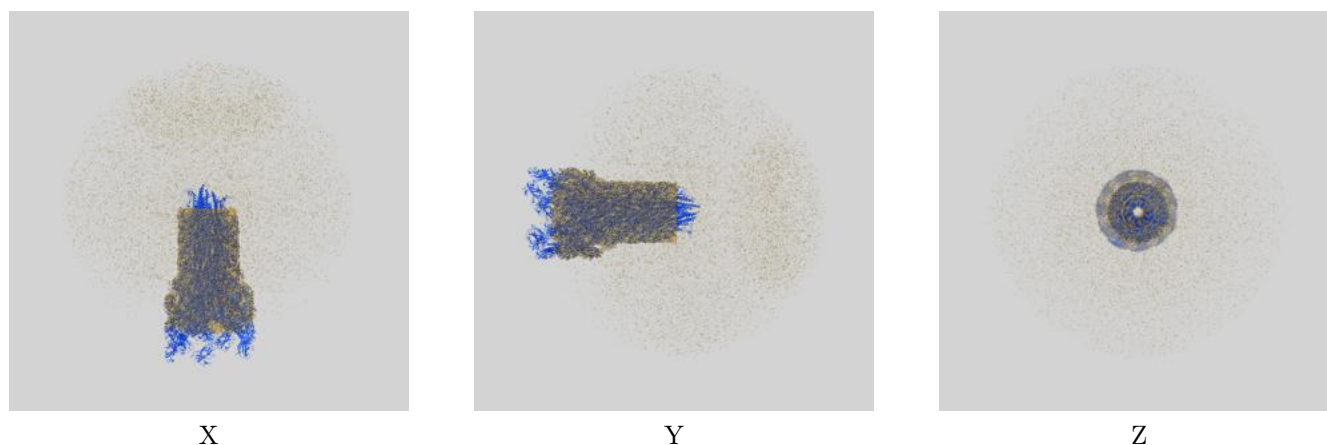
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.30                               | -     | -        |
| Author-provided FSC curve | 3.32                               | 3.82  | 3.37     |
| Unmasked-calculated*      | 7.32                               | 13.12 | 8.10     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.32 differs from the reported value 3.3 by more than 10 %

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

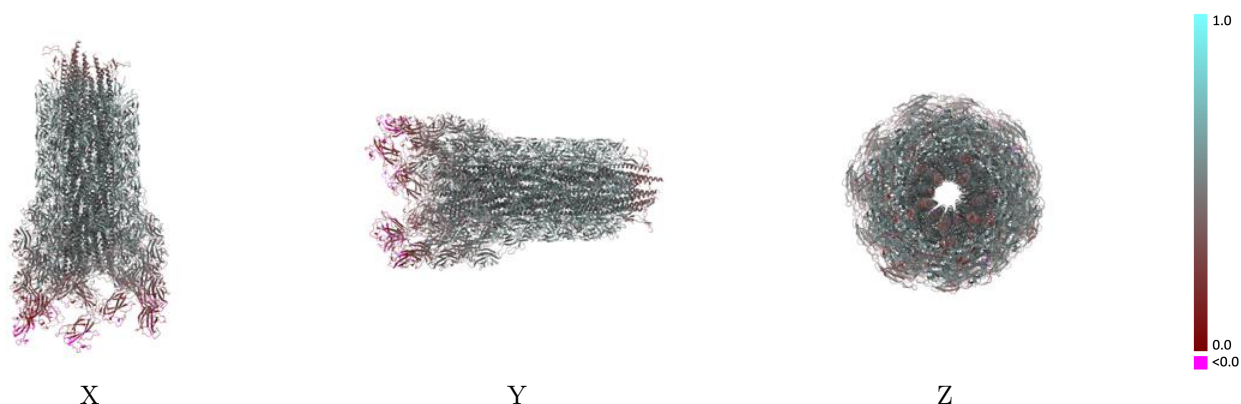
This section contains information regarding the fit between EMDB map EMD-37600 and PDB model 8WKI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



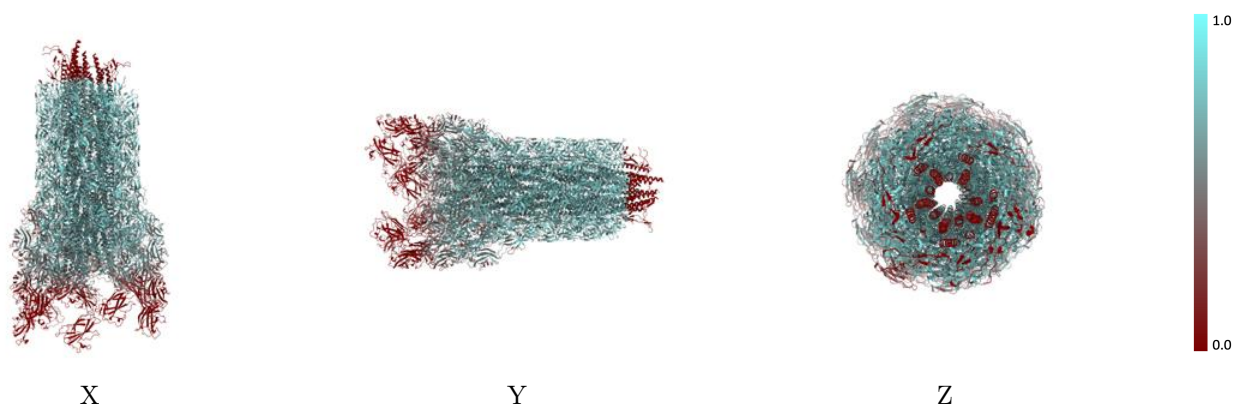
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



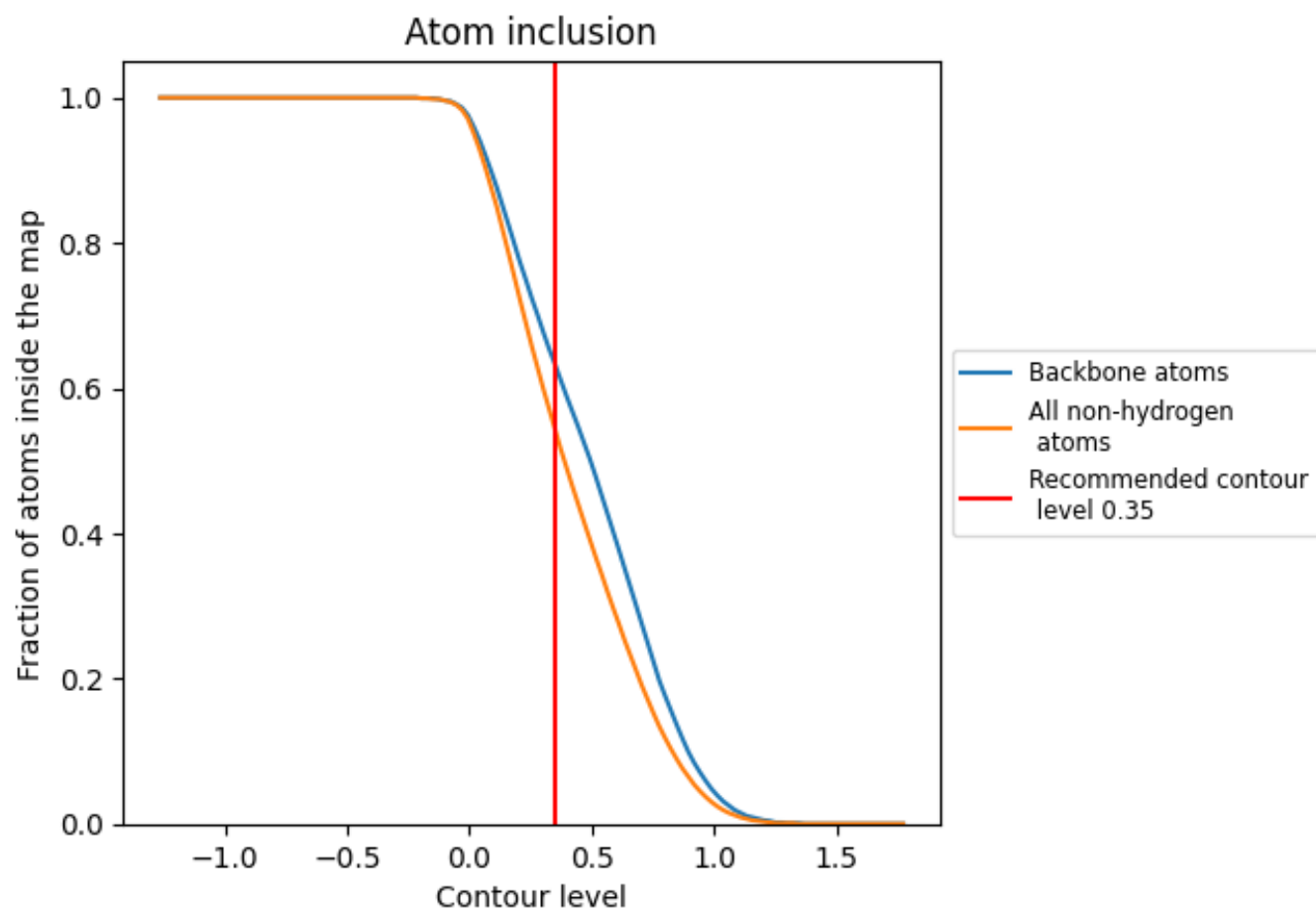
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5420   |  0.4590   |
| 0     |  0.6870   |  0.5200   |
| 1     |  0.6850   |  0.5230   |
| 2     |  0.7000   |  0.5280   |
| 3     |  0.7040   |  0.5250   |
| 4     |  0.6980   |  0.5180   |
| 5     |  0.6900   |  0.5190   |
| 6     |  0.6990   |  0.5230   |
| 7     |  0.7000   |  0.5200   |
| 8     |  0.7000   |  0.5210   |
| 9     |  0.6990   |  0.5260   |
| ZA    |  0.6910   |  0.5180   |
| ZB    |  0.7000   |  0.5220   |
| ZC    |  0.6940   |  0.5190   |
| ZD    |  0.6860  |  0.5150  |
| ZE    |  0.6730 |  0.5130 |
| ZF    |  0.4460 |  0.4510 |
| ZG    |  0.6020 |  0.4950 |
| ZH    |  0.6340 |  0.4920 |
| ZI    |  0.6440 |  0.4980 |
| ZJ    |  0.6340 |  0.4890 |
| ZK    |  0.6060 |  0.4800 |
| ZL    |  0.6200 |  0.4840 |
| ZM    |  0.6340 |  0.4920 |
| ZN    |  0.6290 |  0.4840 |
| ZO    |  0.6130 |  0.4850 |
| 郑     |  0.6100 |  0.4790 |
| ZQ    |  0.5790 |  0.4750 |
| ZR    |  0.5760 |  0.4670 |
| ZS    |  0.5690 |  0.4650 |
| ZT    |  0.5340 |  0.4550 |
| ZU    |  0.5080 |  0.4460 |
| ZV    |  0.4910 |  0.4370 |
| ZW    |  0.4800 |  0.4340 |
| ZX    |  0.4570 |  0.4240 |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| ZY    |  0.4400   |  0.4130   |
| ZZ    |  0.4130   |  0.4010   |
| Za    |  0.3880   |  0.3920   |
| Zb    |  0.3760   |  0.3860   |
| Zc    |  0.3630   |  0.3800   |
| Zd    |  0.3300   |  0.3560   |
| Ze    |  0.2970   |  0.3500   |
| Zf    |  0.2660   |  0.3330   |
| Zg    |  0.2440   |  0.3040   |
| Zh    |  0.2240   |  0.3140   |
| r     |  0.3760   |  0.4510   |
| s     |  0.4570   |  0.4630   |
| t     |  0.4930   |  0.4710   |
| u     |  0.5110   |  0.4850   |
| v     |  0.5410   |  0.4830   |
| w     |  0.6050   |  0.5060   |
| x     |  0.6110   |  0.4960   |
| y     |  0.6250  |  0.5030  |
| z     |  0.6700 |  0.5150 |