



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 3J9G / pdb\_00003j9g  
EMDB ID : EMD-2699  
Title : Atomic model of the VipA/VipB, the type six secretion system contractile sheath of *Vibrio cholerae* from cryo-EM  
Authors : Kudryashev, M.; Wang, R.Y.-R.; Brackmann, M.; Scherer, S.; Maier, T.; Baker, D.; DiMaio, F.; Stahlberg, H.; Egelman, E.H.; Basler, M.  
Deposited on : 2015-01-16  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

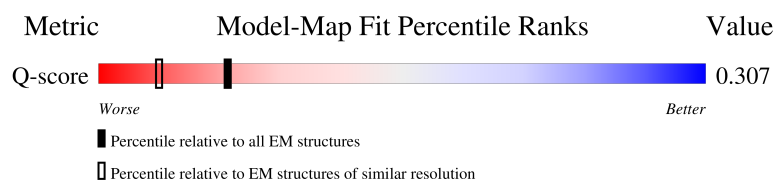
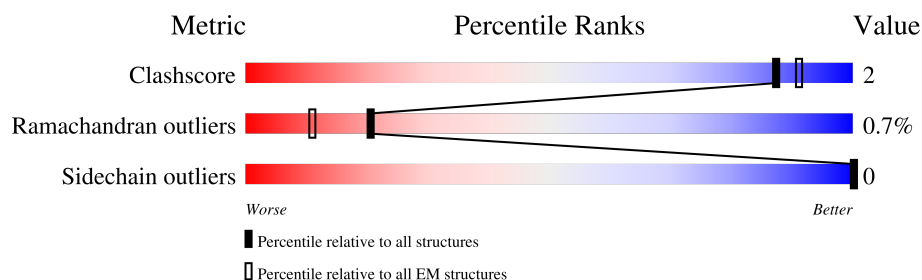
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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                       | 13950 ( 3.00 - 4.00 )                                    |

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   | 1     | 125    | <div> <div>64%</div> <div>95%</div> <div>5%</div> </div> |
| 1   | 3     | 125    | <div> <div>59%</div> <div>95%</div> <div>..</div> </div> |
| 1   | 5     | 125    | <div> <div>54%</div> <div>96%</div> <div>.</div> </div>  |
| 1   | 7     | 125    | <div> <div>53%</div> <div>96%</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--------------------|
| 1   | A     | 125    | 98%<br>94%<br>6%   |
| 1   | C     | 125    | 96%<br>96%<br>.    |
| 1   | E     | 125    | 97%<br>96%<br>.    |
| 1   | G     | 125    | 98%<br>96%<br>.    |
| 1   | I     | 125    | 98%<br>96%<br>.    |
| 1   | K     | 125    | 96%<br>96%<br>..   |
| 1   | M     | 125    | 59%<br>97%<br>.    |
| 1   | O     | 125    | 51%<br>95%<br>5%   |
| 1   | Q     | 125    | 50%<br>95%<br>5%   |
| 1   | S     | 125    | 60%<br>96%<br>..   |
| 1   | U     | 125    | 57%<br>96%<br>.    |
| 1   | W     | 125    | 49%<br>97%<br>.    |
| 1   | Y     | 125    | 54%<br>97%<br>.    |
| 1   | a     | 125    | 56%<br>94%<br>5% . |
| 1   | c     | 125    | 51%<br>96%<br>.    |
| 1   | e     | 125    | 56%<br>96%<br>.    |
| 1   | g     | 125    | 55%<br>97%<br>.    |
| 1   | i     | 125    | 49%<br>97%<br>.    |
| 1   | k     | 125    | 49%<br>97%<br>.    |
| 1   | m     | 125    | 59%<br>95%<br>5%   |
| 1   | o     | 125    | 59%<br>95%<br>5%   |
| 1   | q     | 125    | 58%<br>95%<br>5%   |
| 1   | s     | 125    | 54%<br>97%<br>.    |
| 1   | u     | 125    | 50%<br>95%<br>..   |
| 1   | w     | 125    | 47%<br>97%<br>.    |

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| Mol | Chain | Length | Quality of chain                            |
|-----|-------|--------|---------------------------------------------|
| 1   | y     | 125    | <div>59%</div> <div>96%</div> <div>.</div>  |
| 2   | 2     | 432    | <div>34%</div> <div>95%</div> <div>5%</div> |
| 2   | 4     | 432    | <div>35%</div> <div>95%</div> <div>.</div>  |
| 2   | 6     | 432    | <div>29%</div> <div>95%</div> <div>.</div>  |
| 2   | 8     | 432    | <div>25%</div> <div>95%</div> <div>.</div>  |
| 2   | B     | 432    | <div>69%</div> <div>95%</div> <div>.</div>  |
| 2   | D     | 432    | <div>70%</div> <div>95%</div> <div>.</div>  |
| 2   | F     | 432    | <div>74%</div> <div>95%</div> <div>.</div>  |
| 2   | H     | 432    | <div>76%</div> <div>95%</div> <div>5%</div> |
| 2   | J     | 432    | <div>76%</div> <div>95%</div> <div>5%</div> |
| 2   | L     | 432    | <div>71%</div> <div>95%</div> <div>.</div>  |
| 2   | N     | 432    | <div>25%</div> <div>95%</div> <div>.</div>  |
| 2   | P     | 432    | <div>24%</div> <div>95%</div> <div>.</div>  |
| 2   | R     | 432    | <div>27%</div> <div>95%</div> <div>.</div>  |
| 2   | T     | 432    | <div>34%</div> <div>95%</div> <div>5%</div> |
| 2   | V     | 432    | <div>33%</div> <div>95%</div> <div>5%</div> |
| 2   | X     | 432    | <div>29%</div> <div>95%</div> <div>.</div>  |
| 2   | Z     | 432    | <div>21%</div> <div>95%</div> <div>.</div>  |
| 2   | b     | 432    | <div>23%</div> <div>95%</div> <div>.</div>  |
| 2   | d     | 432    | <div>23%</div> <div>95%</div> <div>5%</div> |
| 2   | f     | 432    | <div>25%</div> <div>95%</div> <div>.</div>  |
| 2   | h     | 432    | <div>24%</div> <div>95%</div> <div>5%</div> |
| 2   | j     | 432    | <div>20%</div> <div>95%</div> <div>5%</div> |
| 2   | l     | 432    | <div>20%</div> <div>95%</div> <div>.</div>  |
| 2   | n     | 432    | <div>25%</div> <div>95%</div> <div>5%</div> |

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| Mol | Chain | Length | Quality of chain                             |    |
|-----|-------|--------|----------------------------------------------|----|
| 2   | p     | 432    | <div><div></div><div></div><div></div></div> | •  |
| 2   | r     | 432    | <div><div></div><div></div><div></div></div> | •  |
| 2   | t     | 432    | <div><div></div><div></div><div></div></div> | •  |
| 2   | v     | 432    | <div><div></div><div></div><div></div></div> | 5% |
| 2   | x     | 432    | <div><div></div><div></div><div></div></div> | 5% |
| 2   | z     | 432    | <div><div></div><div></div><div></div></div> | •  |



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 132930 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 VipA.

| Mol | Chain | Residues | Atoms        |          |          |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1   | A     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | C     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | E     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | G     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | I     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | K     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | M     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | O     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | Q     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | S     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | U     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | W     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | Y     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | a     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | c     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | e     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | g     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1   | i     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | k     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | m     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | o     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | q     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | s     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | u     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | w     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | y     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | 1     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | 3     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | 5     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |
| 1   | 7     | 125      | Total<br>963 | C<br>608 | N<br>160 | O<br>194 | S<br>1 | 0       | 0     |

- Molecule 2 is a protein called VipB.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2   | B     | 432      | Total<br>3468 | C<br>2215 | N<br>590 | O<br>650 | S<br>13 | 0       | 0     |
| 2   | D     | 432      | Total<br>3468 | C<br>2215 | N<br>590 | O<br>650 | S<br>13 | 0       | 0     |
| 2   | F     | 432      | Total<br>3468 | C<br>2215 | N<br>590 | O<br>650 | S<br>13 | 0       | 0     |
| 2   | H     | 432      | Total<br>3468 | C<br>2215 | N<br>590 | O<br>650 | S<br>13 | 0       | 0     |
| 2   | J     | 432      | Total<br>3468 | C<br>2215 | N<br>590 | O<br>650 | S<br>13 | 0       | 0     |
| 2   | L     | 432      | Total<br>3468 | C<br>2215 | N<br>590 | O<br>650 | S<br>13 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | N     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | P     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | R     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | T     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | V     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | X     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | Z     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | b     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | d     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | f     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | h     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | j     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | l     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | n     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | p     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | r     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | t     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | v     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | x     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | z     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | 2     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |

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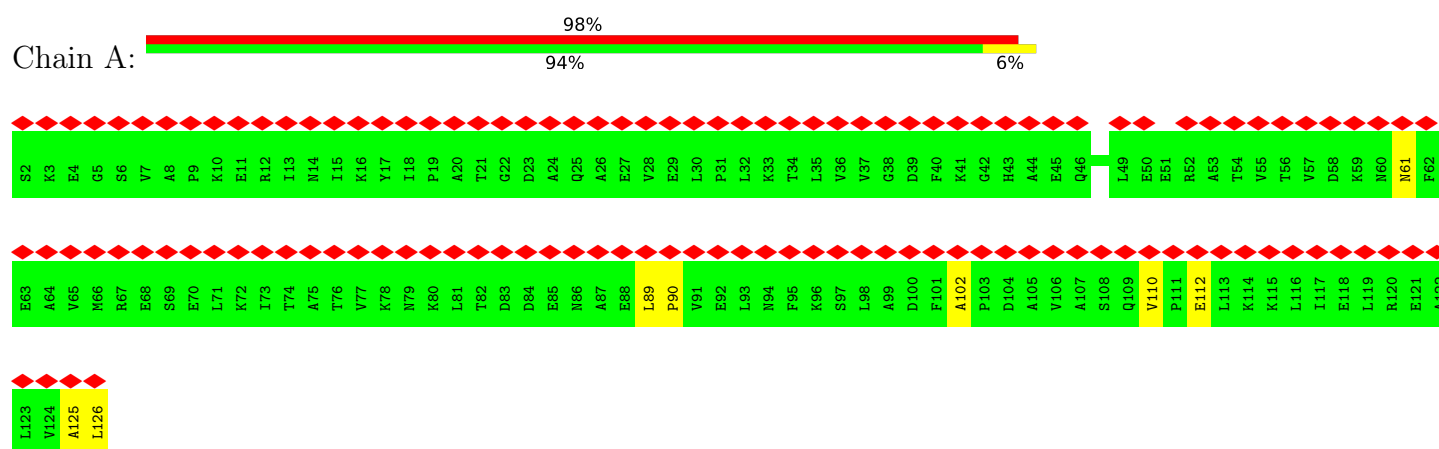
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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 4     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | 6     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |
| 2   | 8     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3468  | 2215 | 590 | 650 | 13 |         |       |

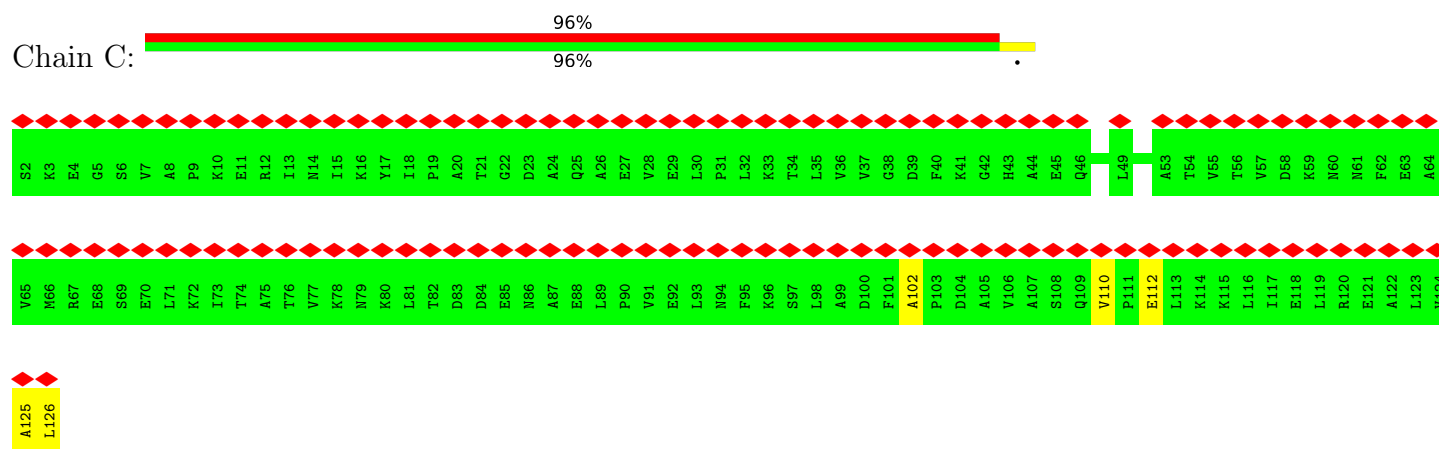
### 3 Residue-property plots

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.

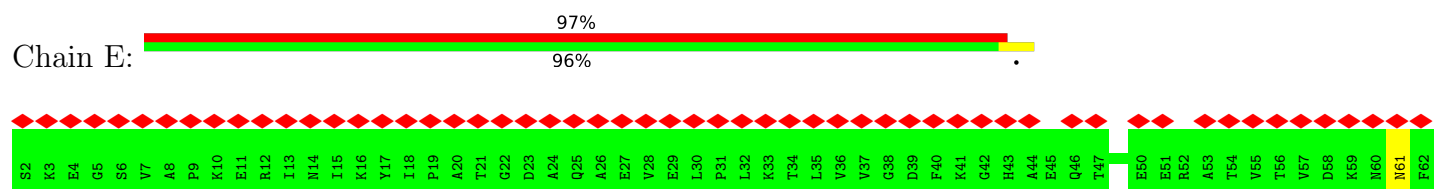
#### • Molecule 1: VipA

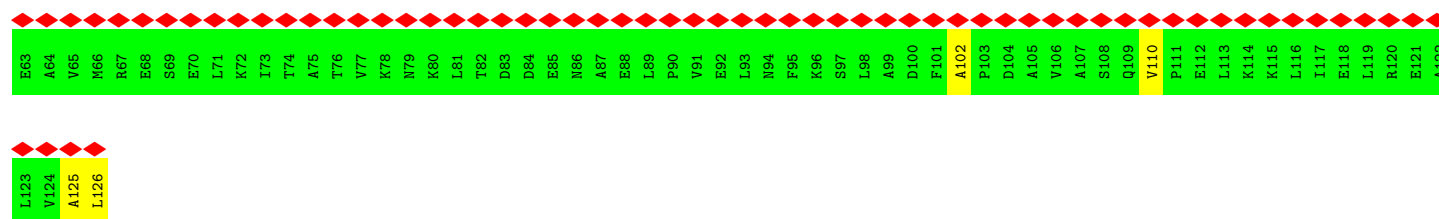


#### • Molecule 1: VipA

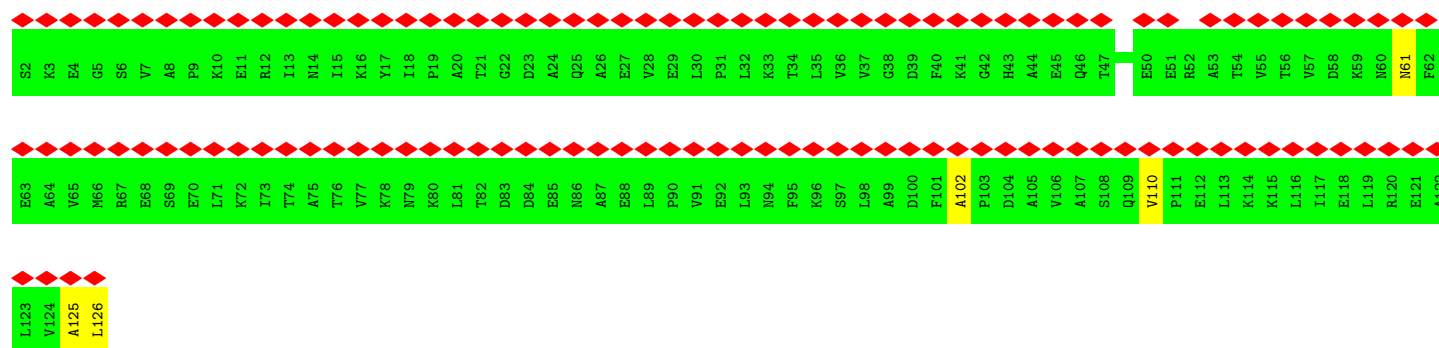


#### • Molecule 1: VipA

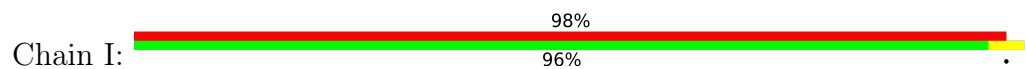




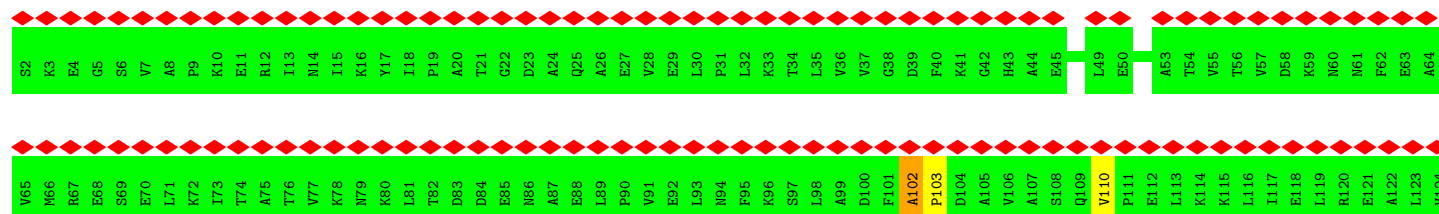
## • Molecule 1: VipA



## • Molecule 1: VipA

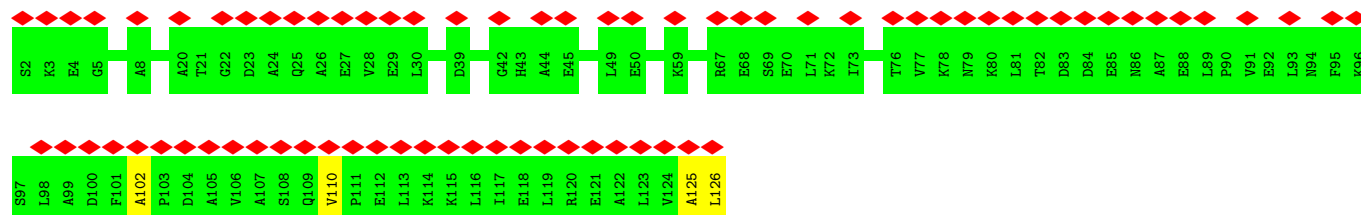


## • Molecule 1: VipA

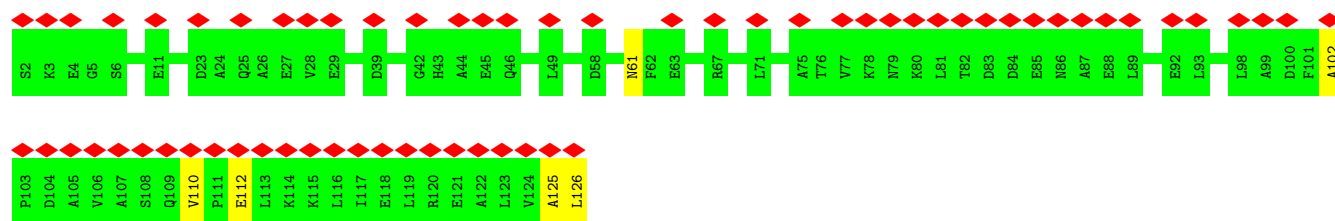




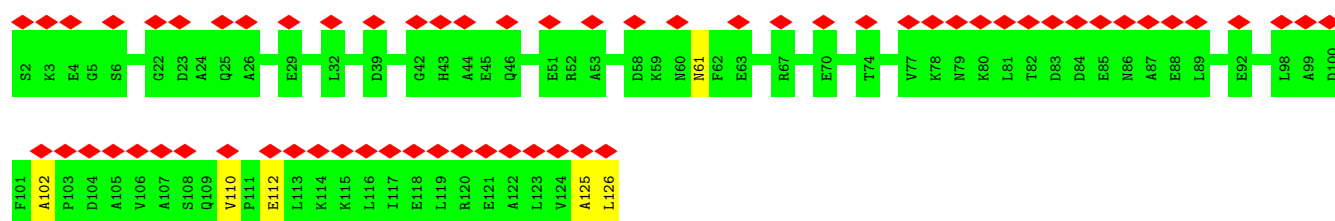
• Molecule 1: VipA



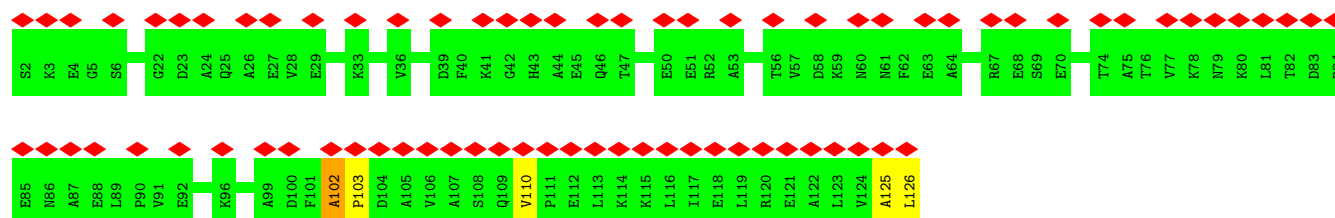
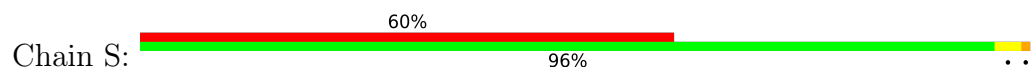
• Molecule 1: VipA



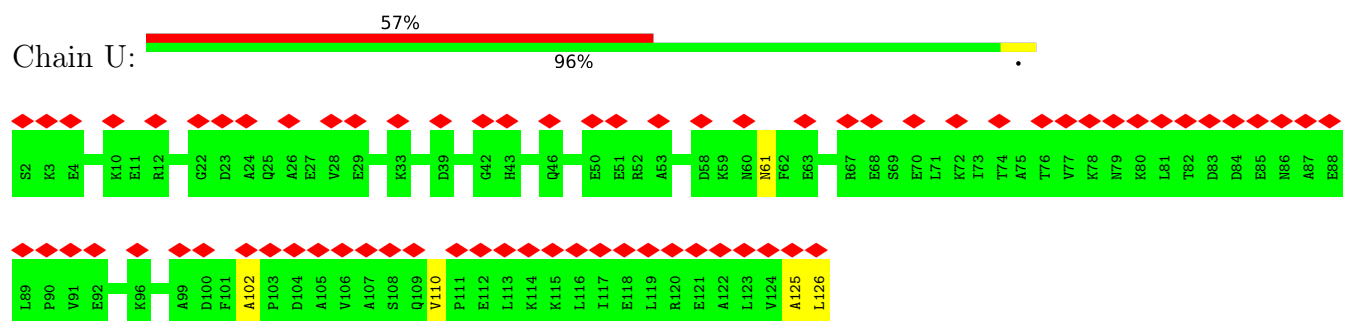
• Molecule 1: VipA



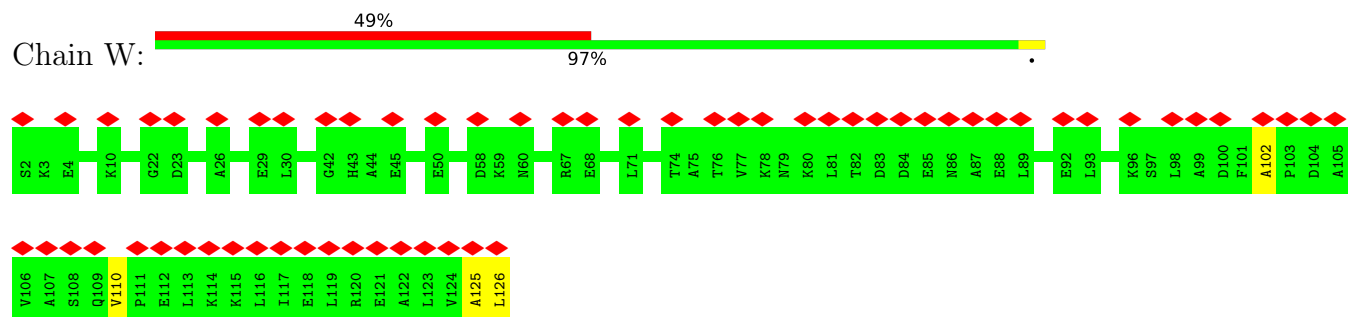
• Molecule 1: VipA



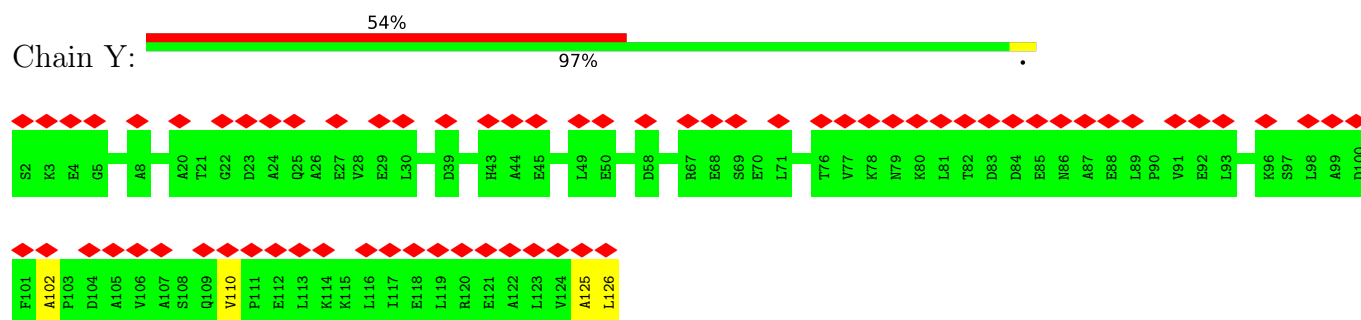
• Molecule 1: VipA



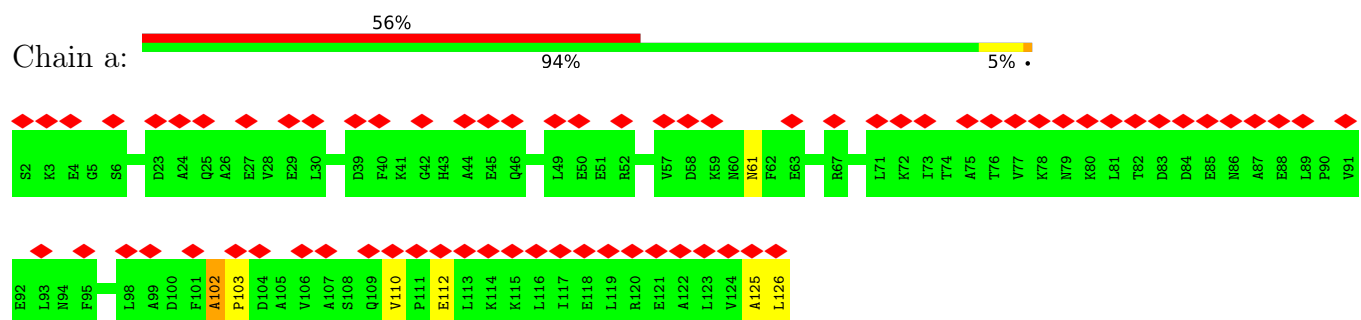
- Molecule 1: VipA



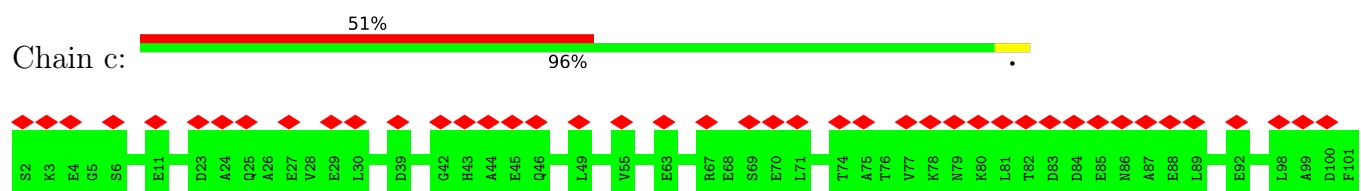
- Molecule 1: VipA

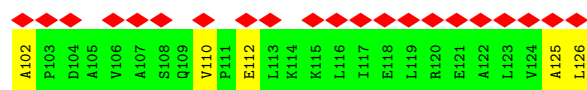


- Molecule 1: VipA

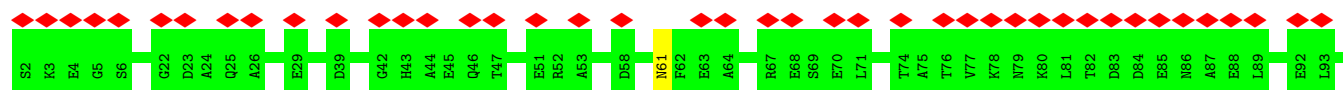


- Molecule 1: VipA

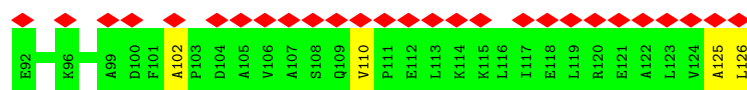
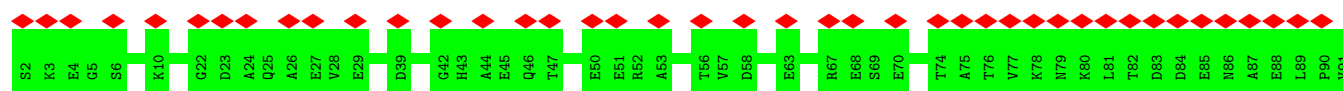




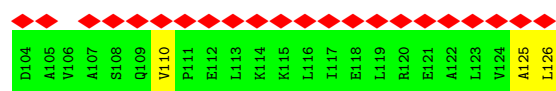
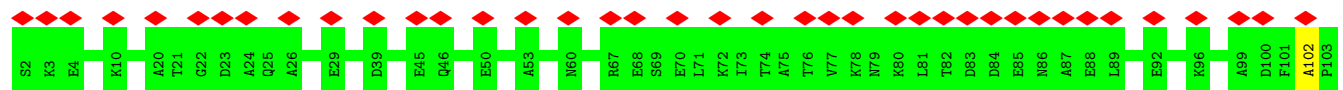
• Molecule 1: VipA



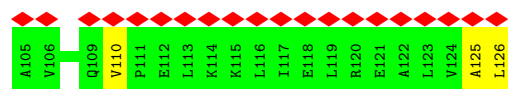
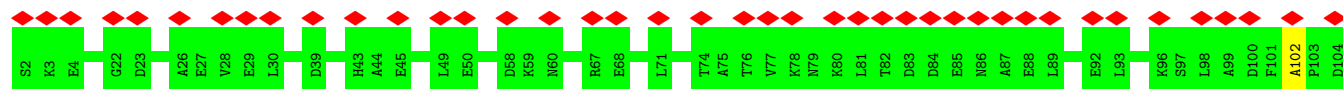
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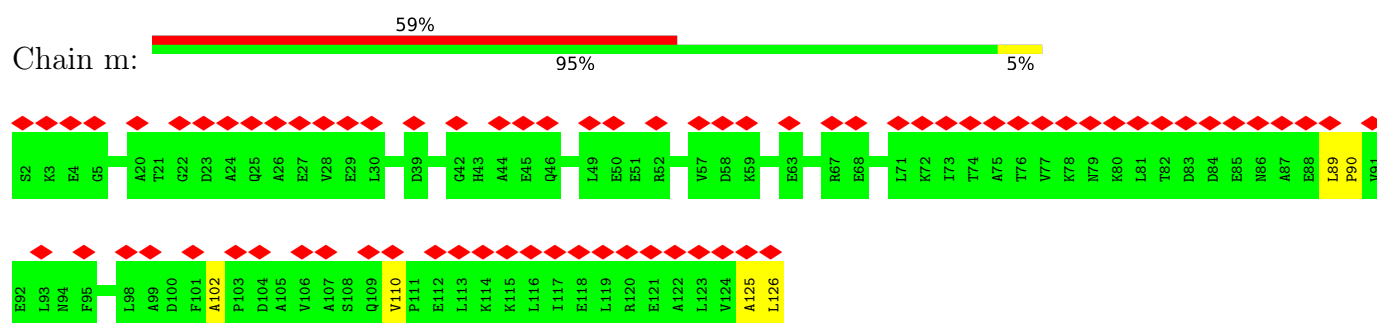
• Molecule 1: VipA



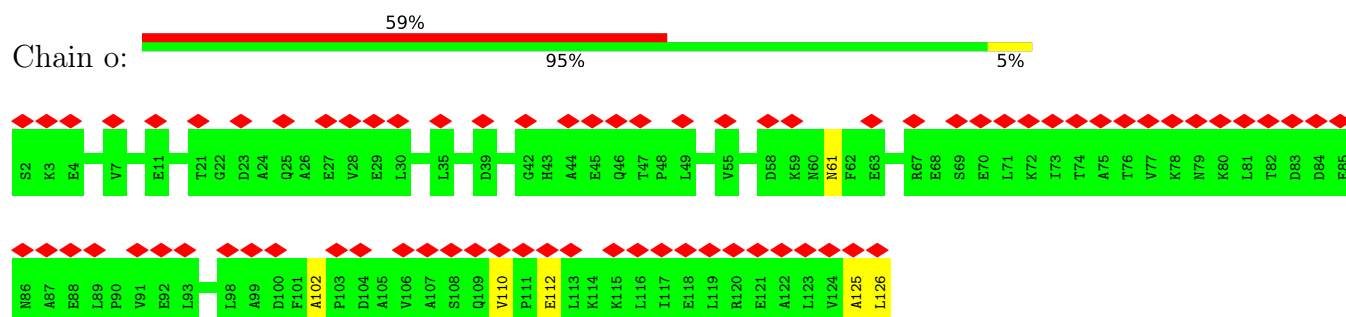
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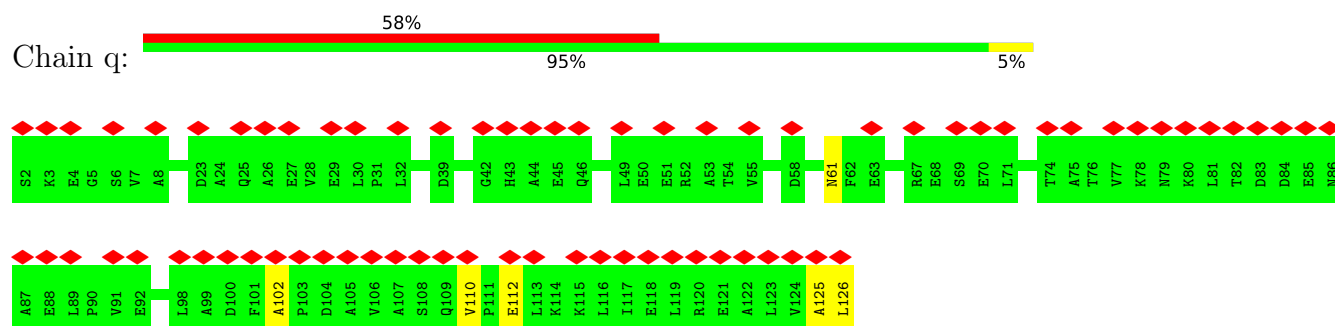
• Molecule 1: VipA



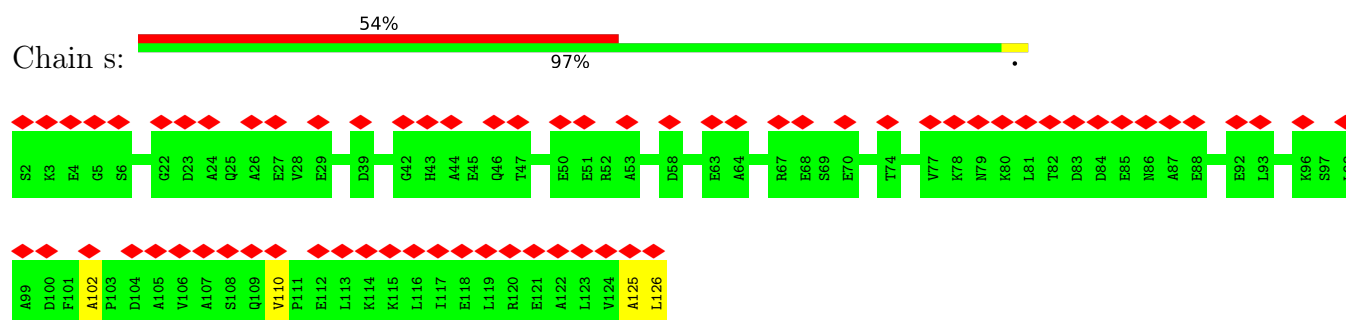
- Molecule 1: VipA



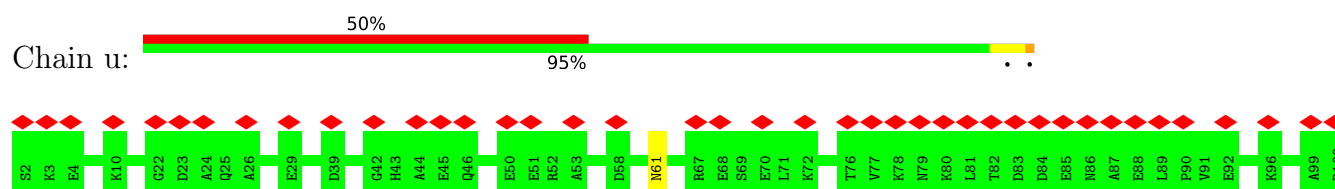
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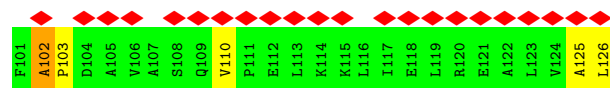


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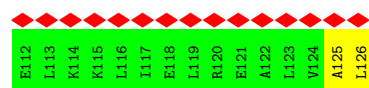
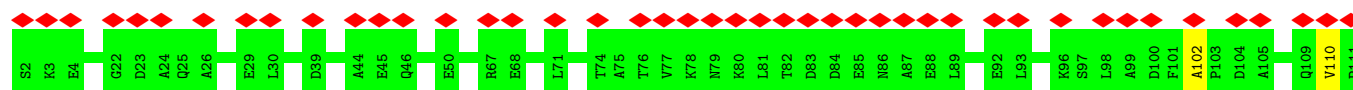


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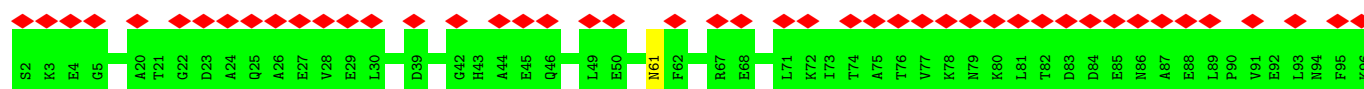




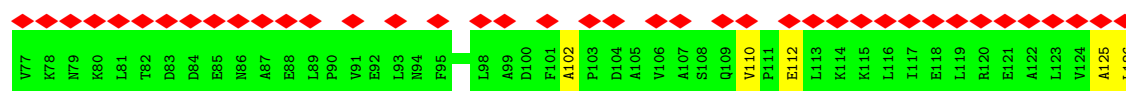
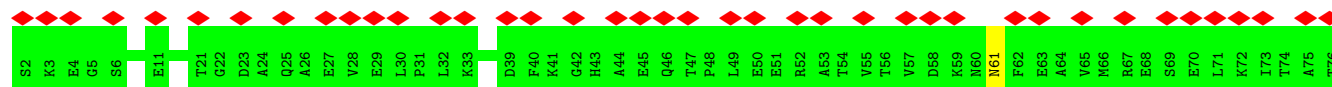
• Molecule 1: VipA



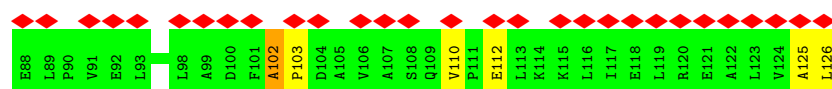
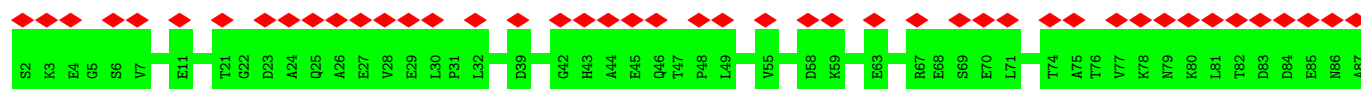
• Molecule 1: VipA



• Molecule 1: VipA

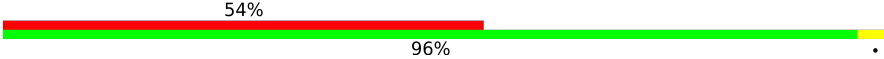


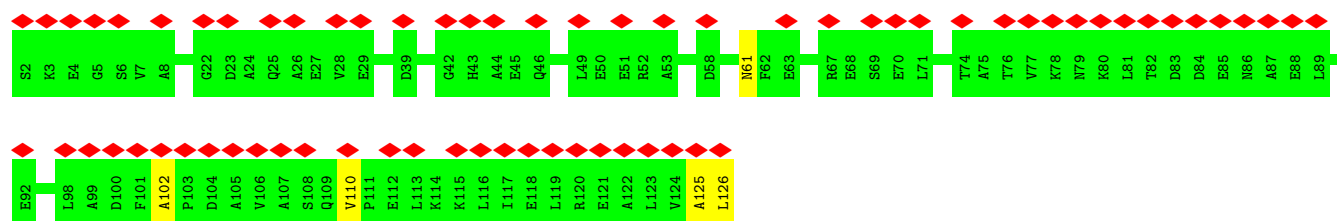
• Molecule 1: VipA



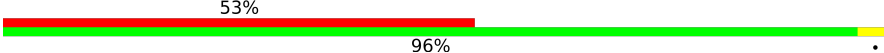
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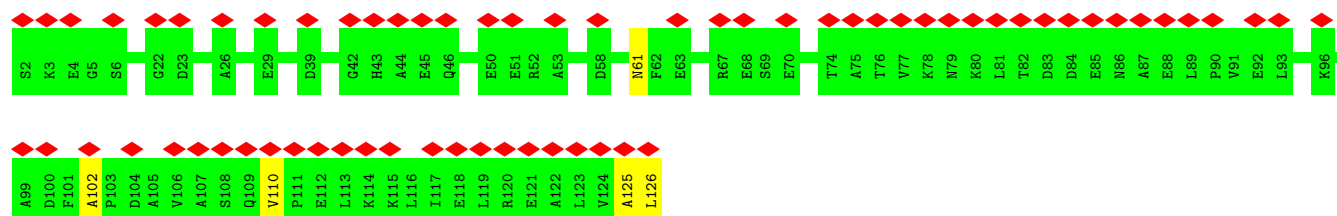


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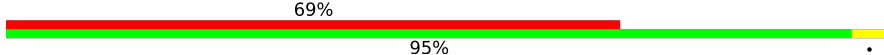


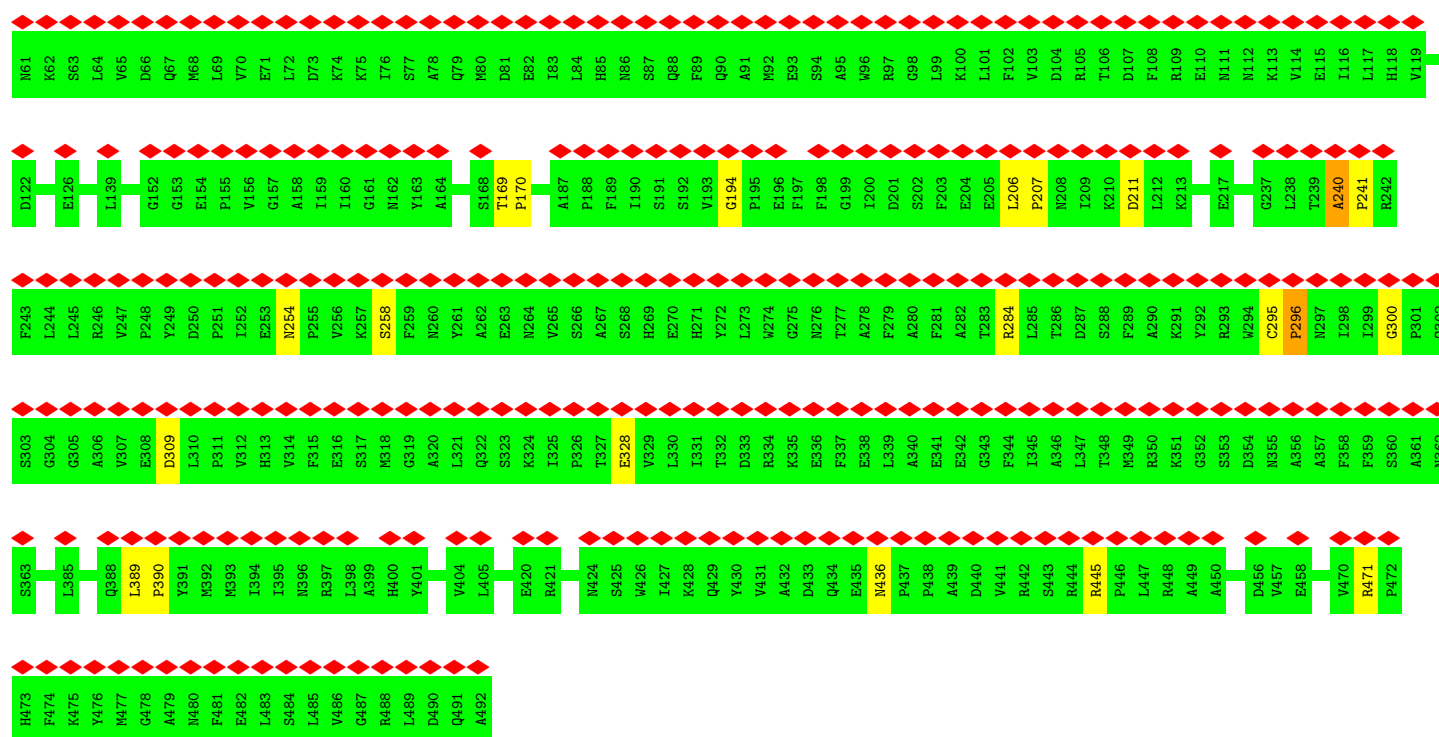
• Molecule 1: VipA

Chain 7: 

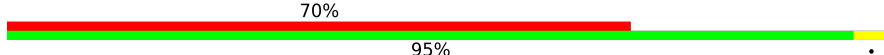


• Molecule 2: VipB

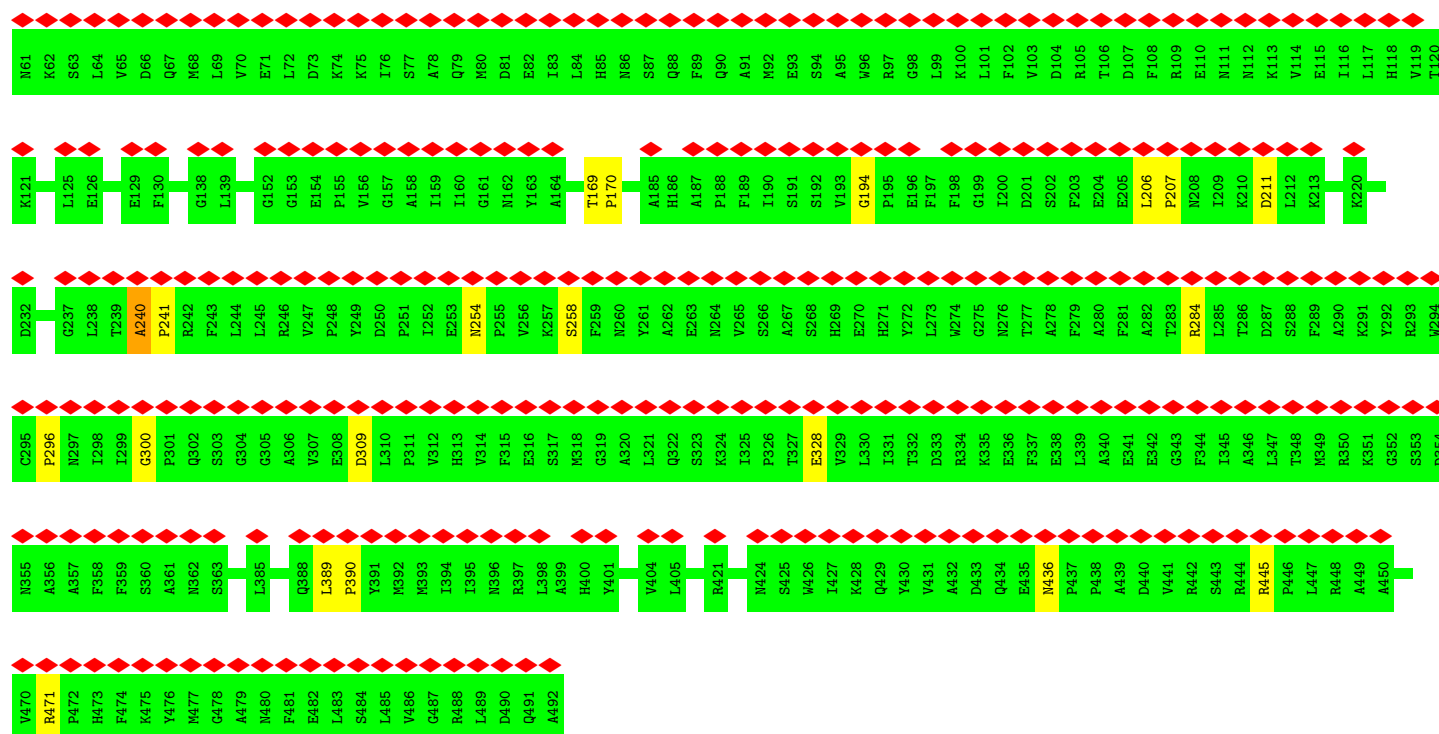
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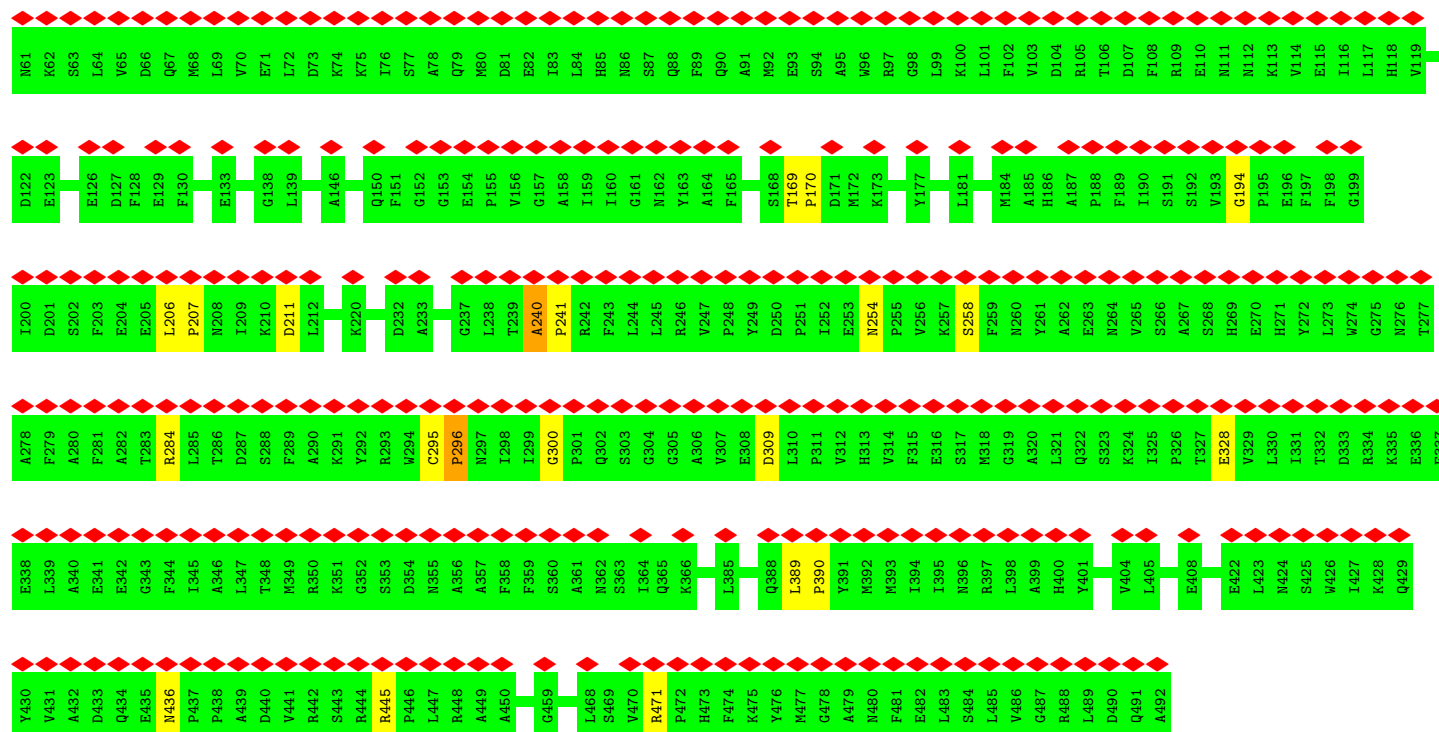
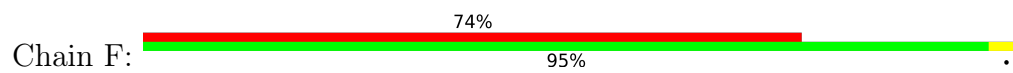
• Molecule 2: VipB

Chain D: 

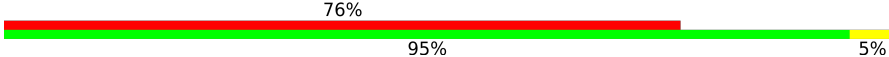


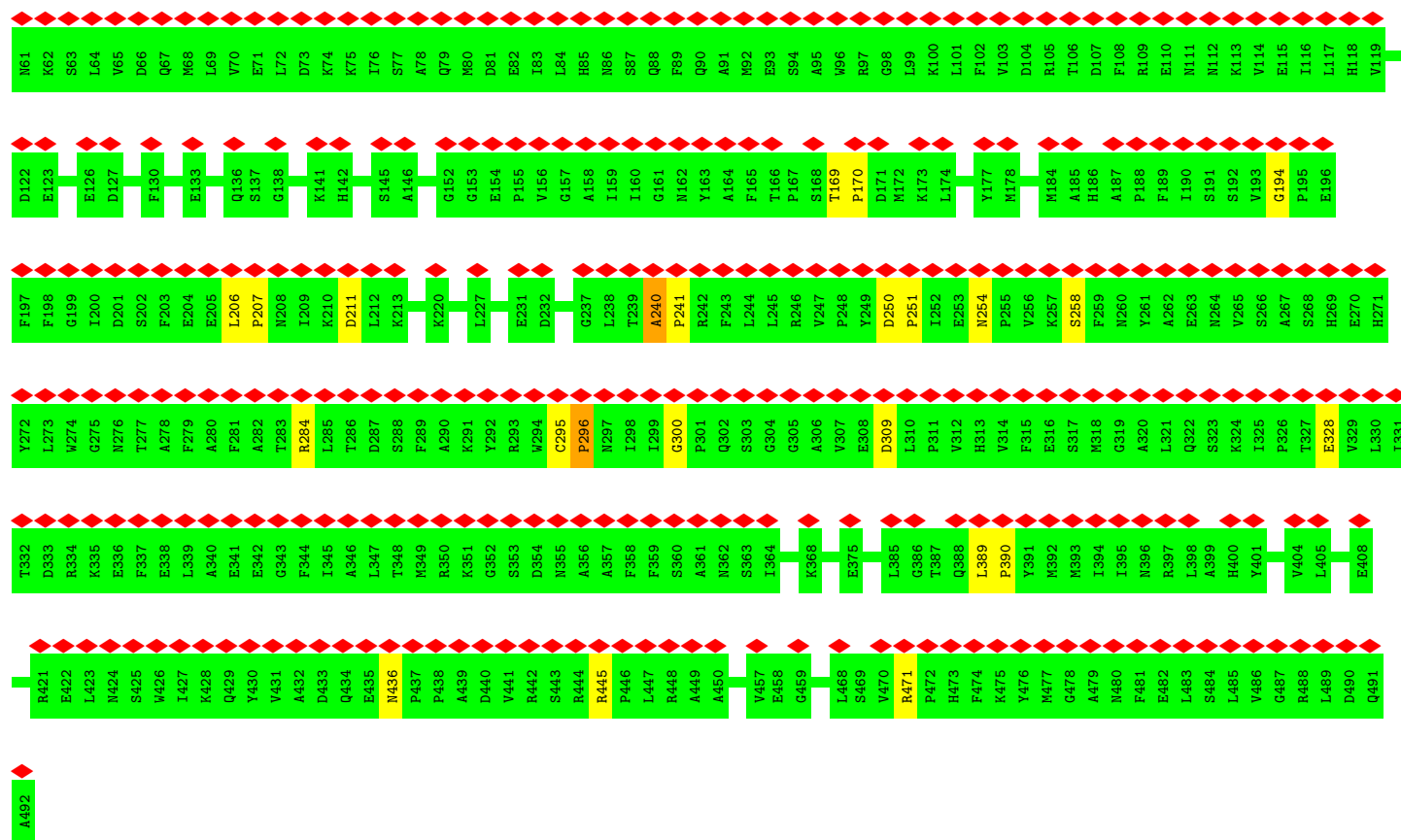


### • Molecule 2: VipB

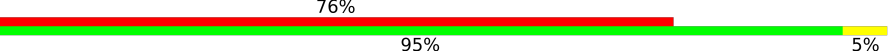


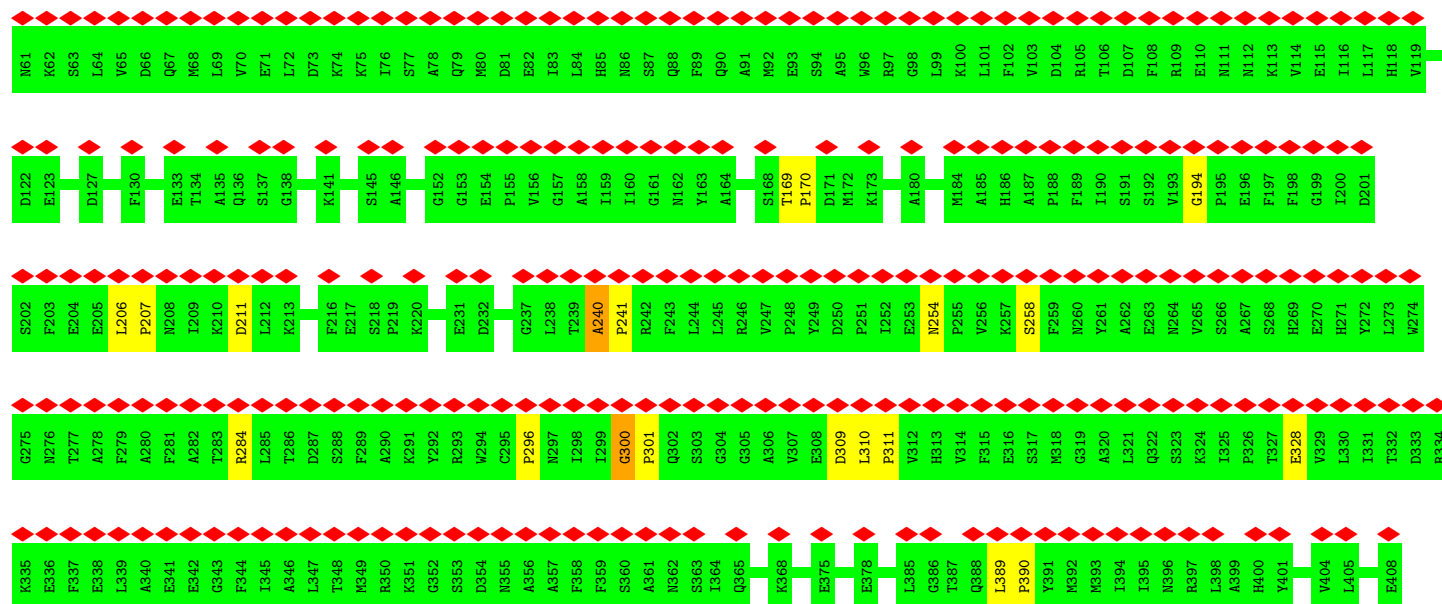
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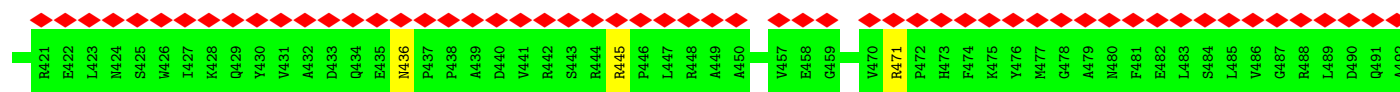
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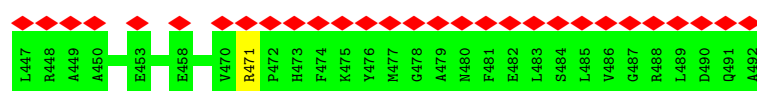
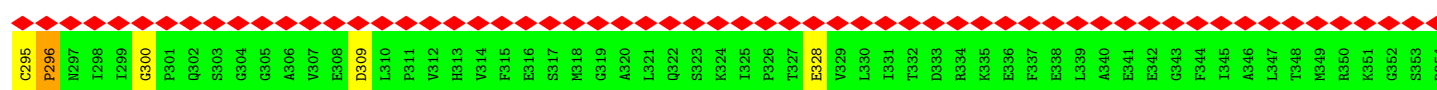
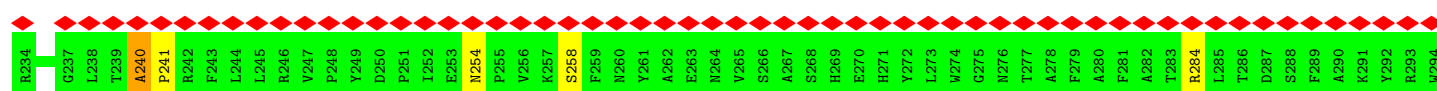
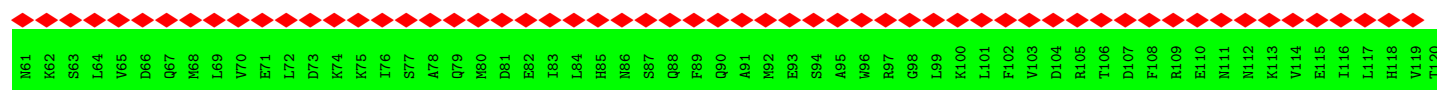
### • Molecule 2: VipB

Chain J: 

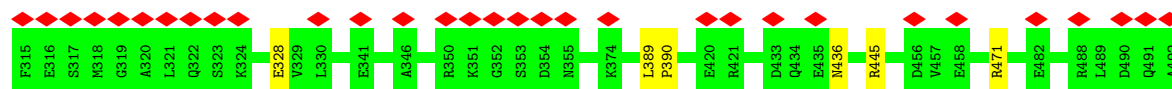
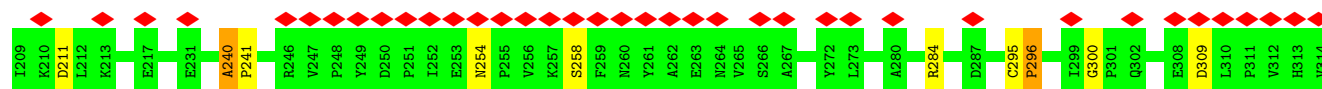
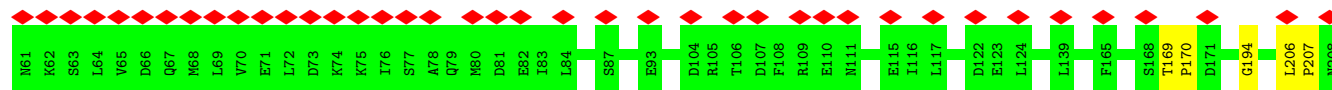




• Molecule 2: VipB

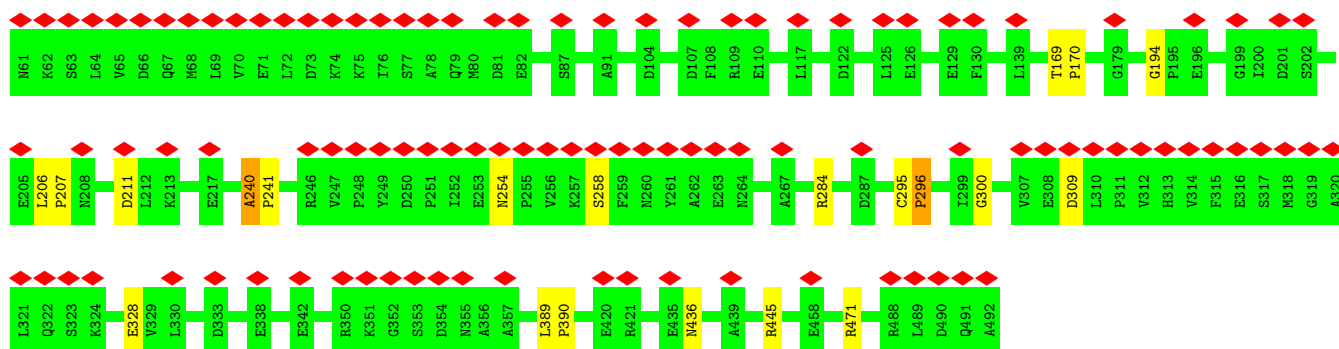


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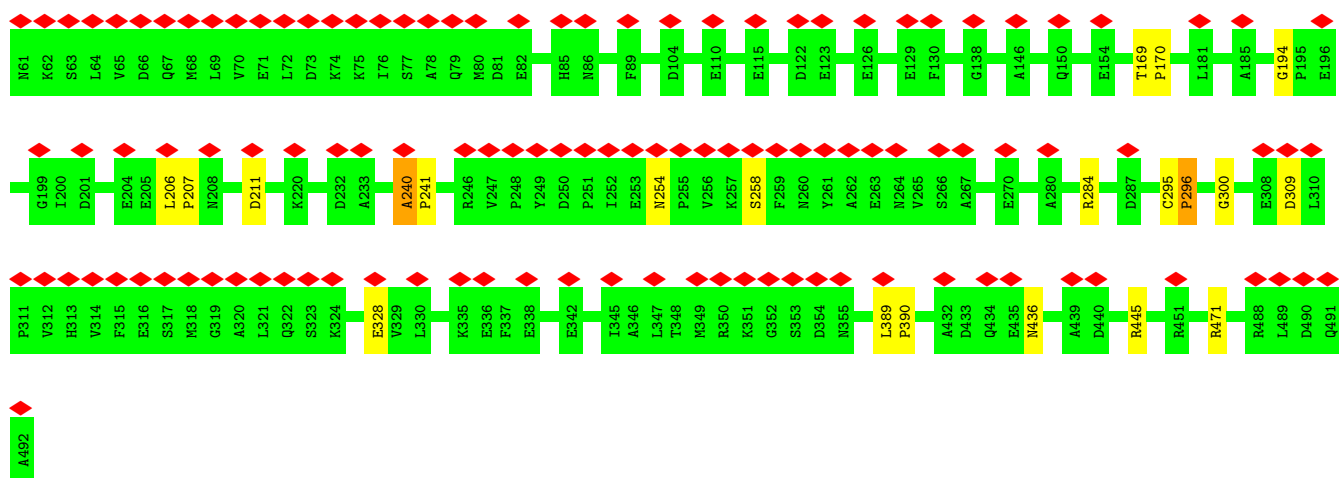


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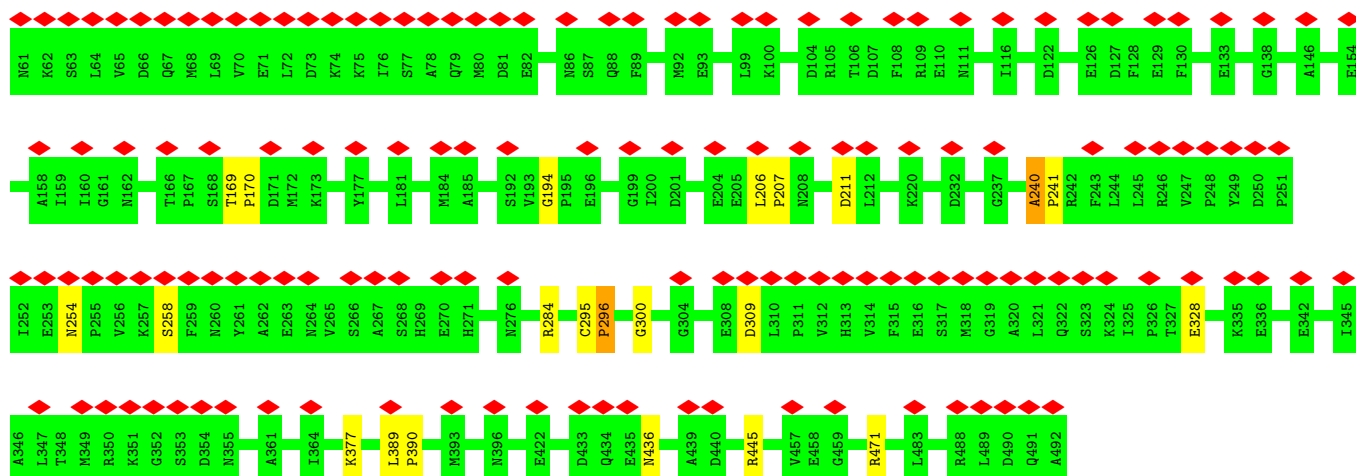




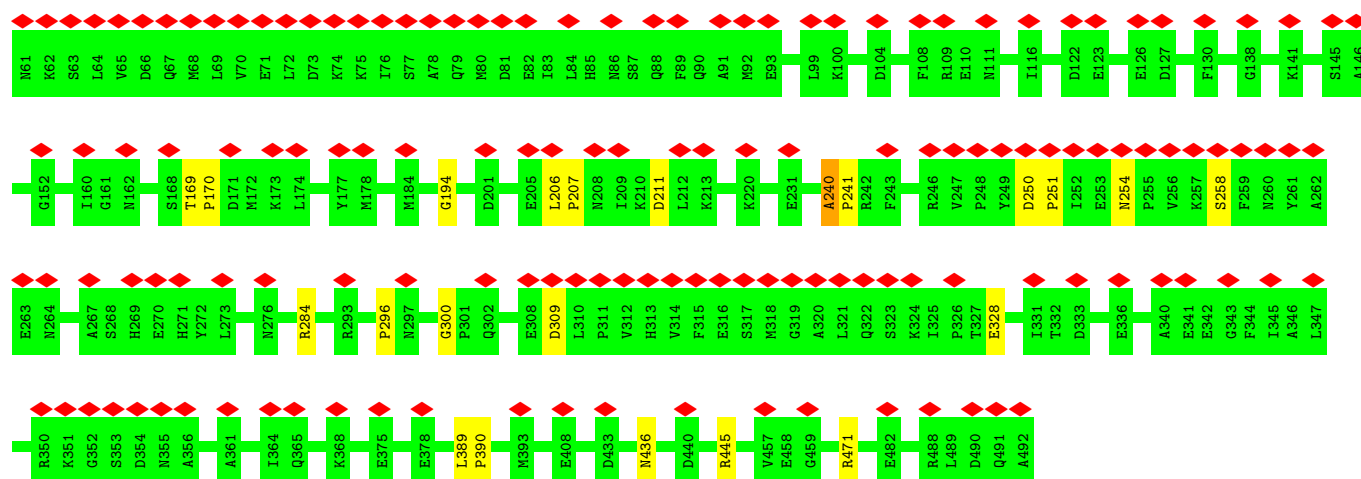
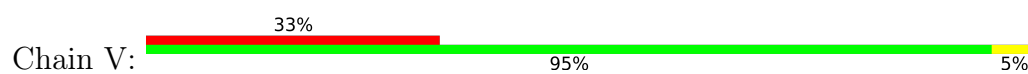
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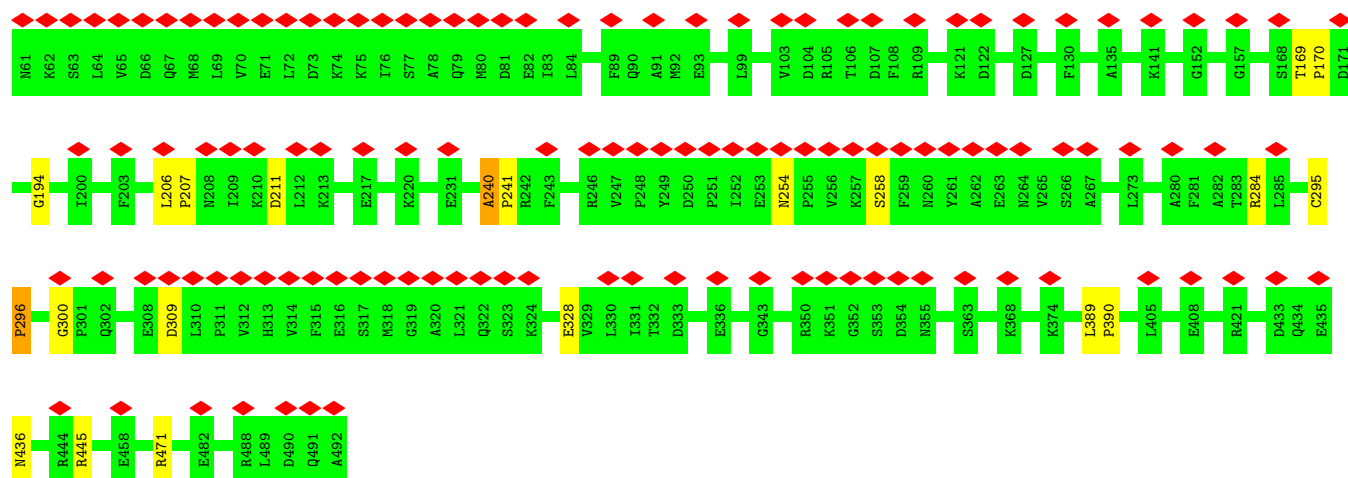
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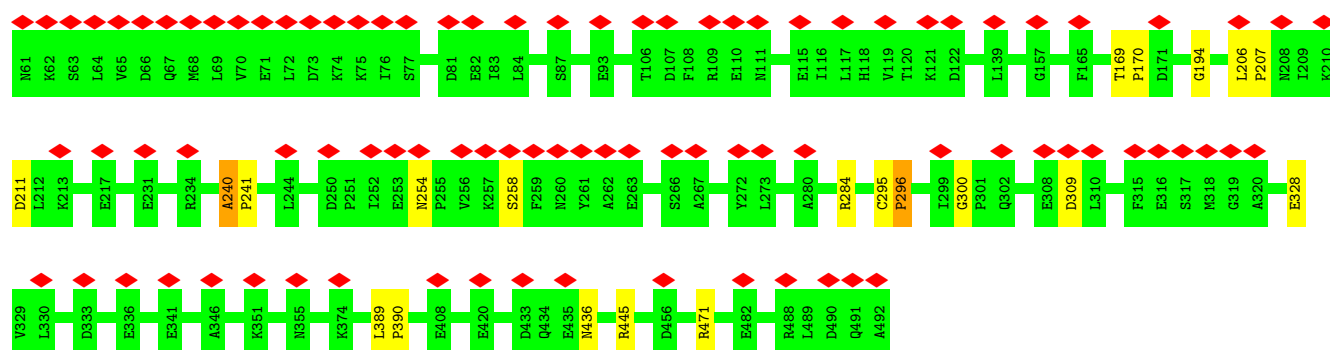
• Molecule 2: VipB



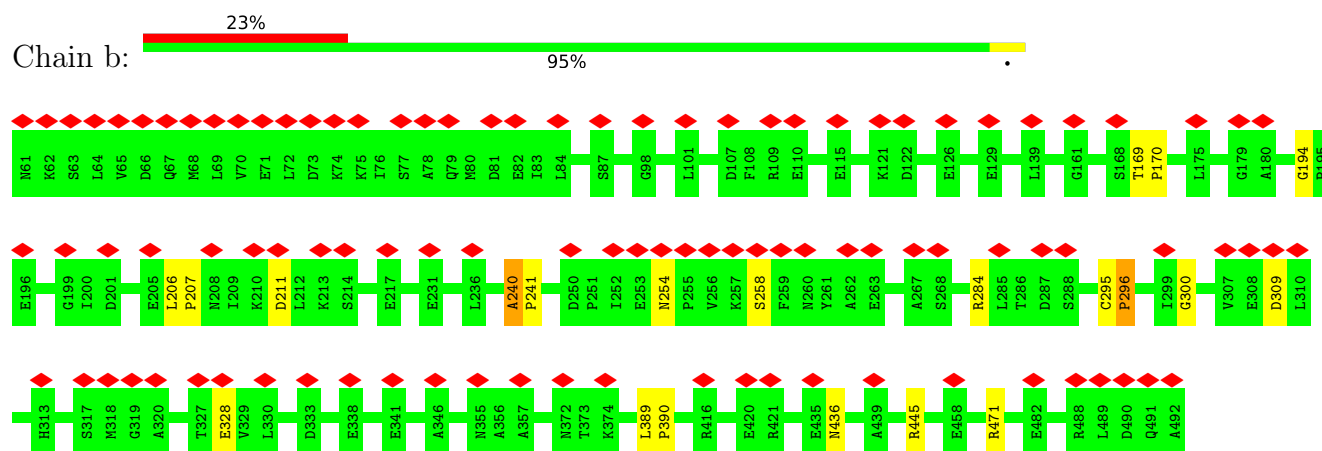
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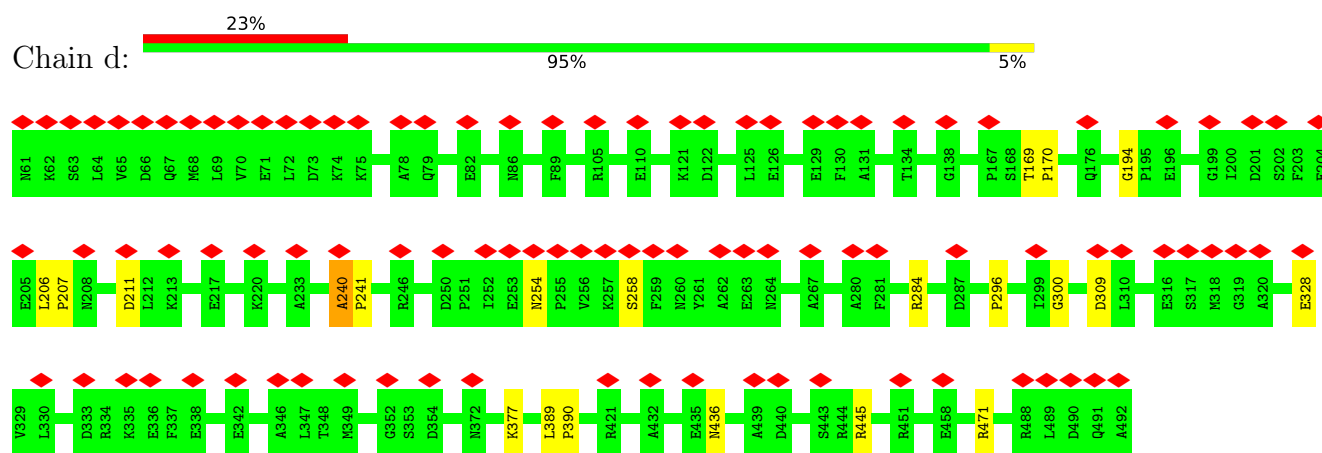
• Molecule 2: VipB



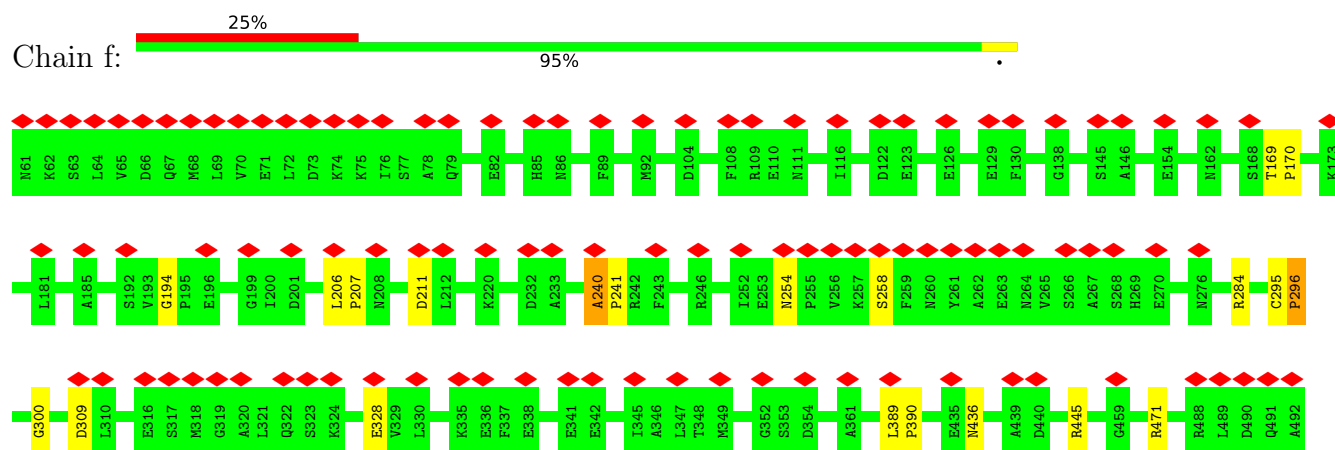
- Molecule 2: VipB



- Molecule 2: VipB

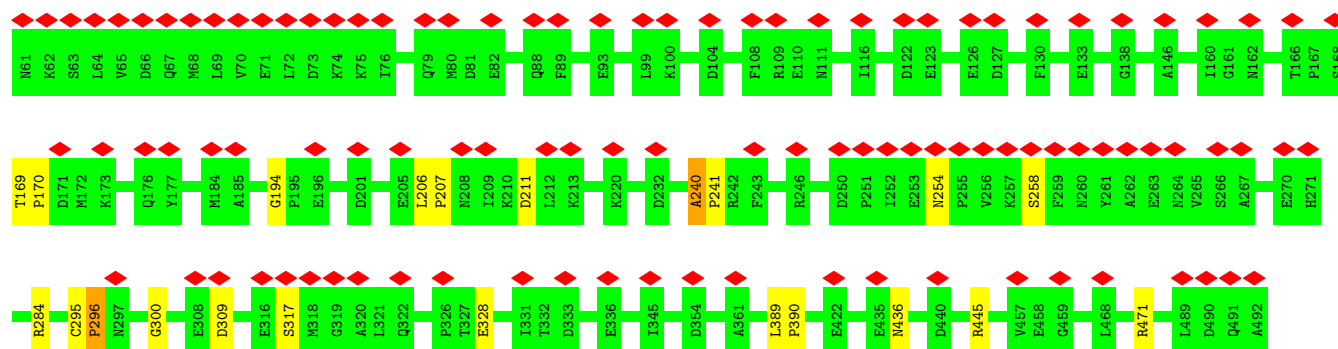


- Molecule 2: VipB

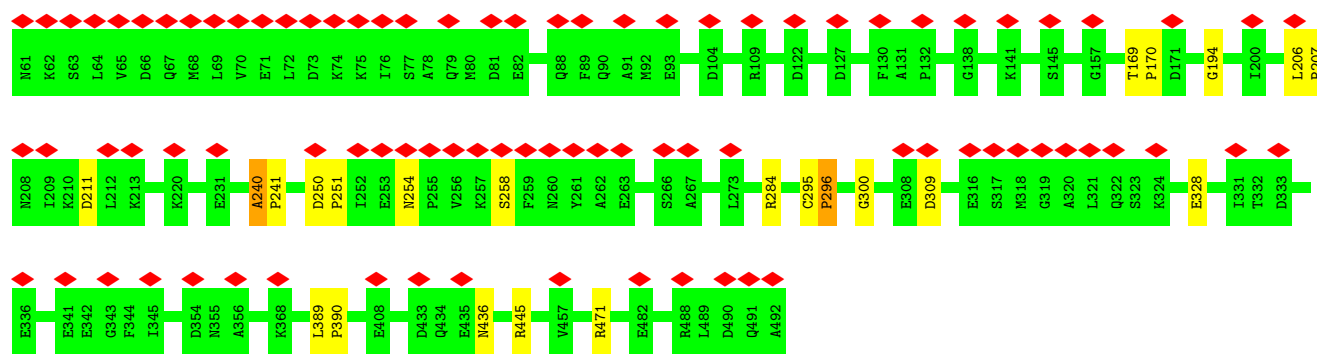


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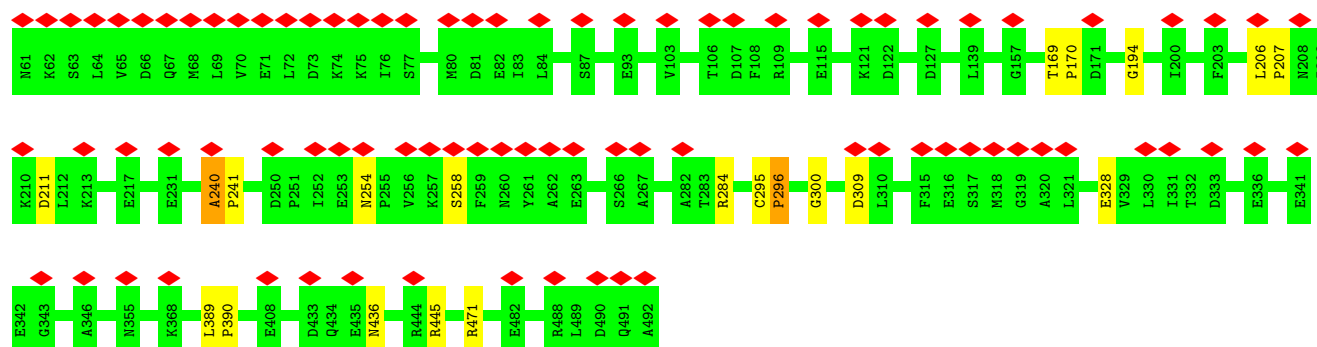




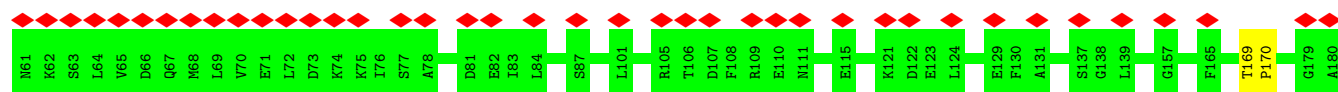
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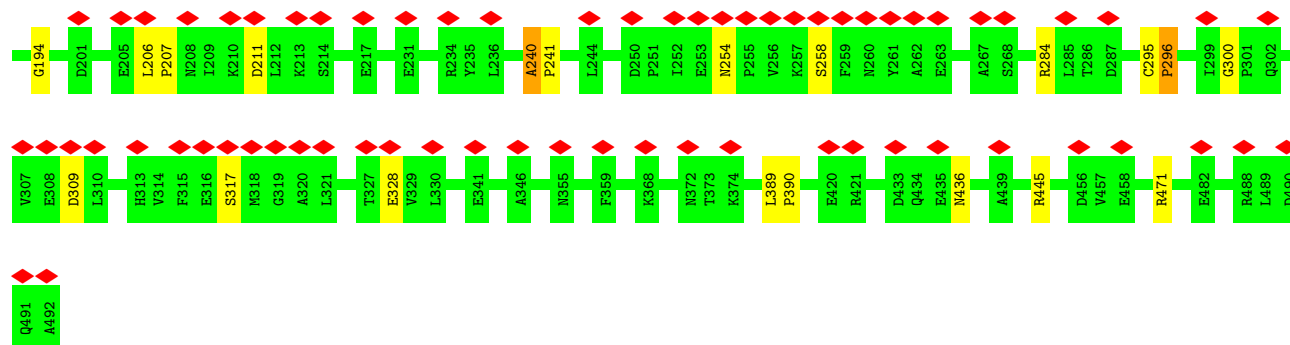
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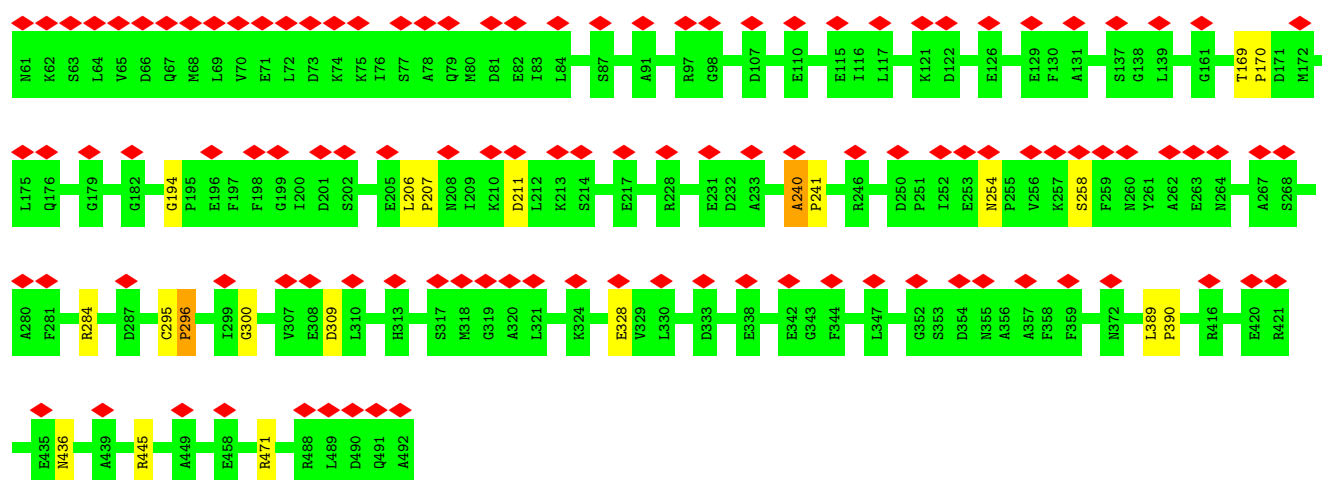
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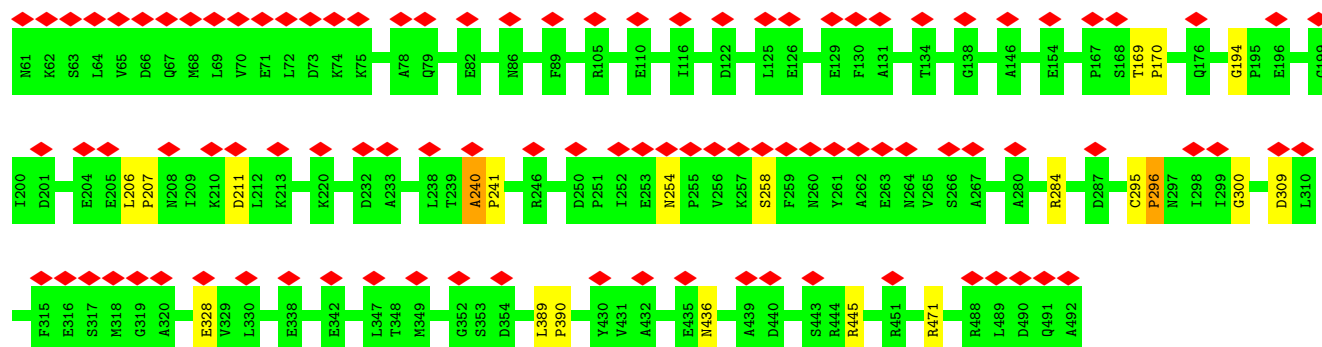




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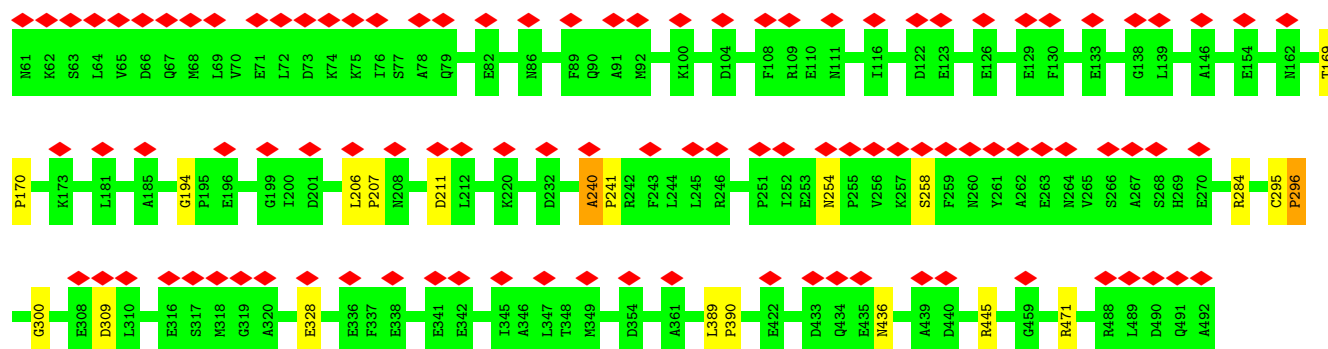


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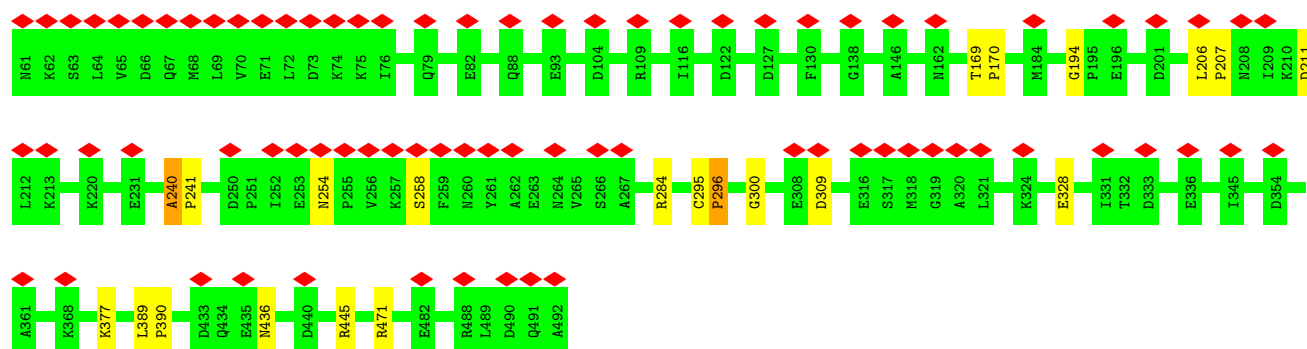


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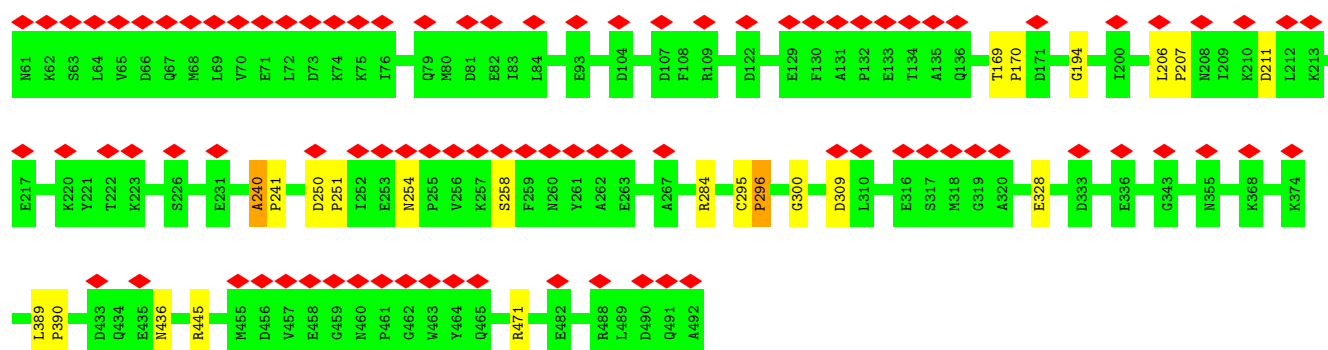




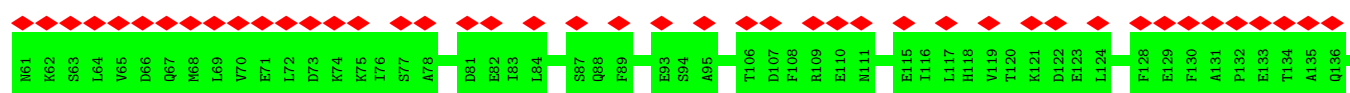
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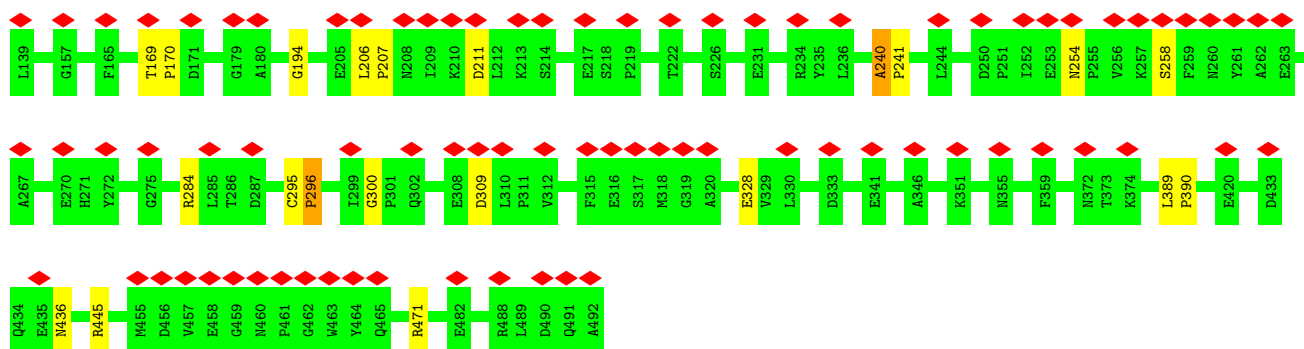


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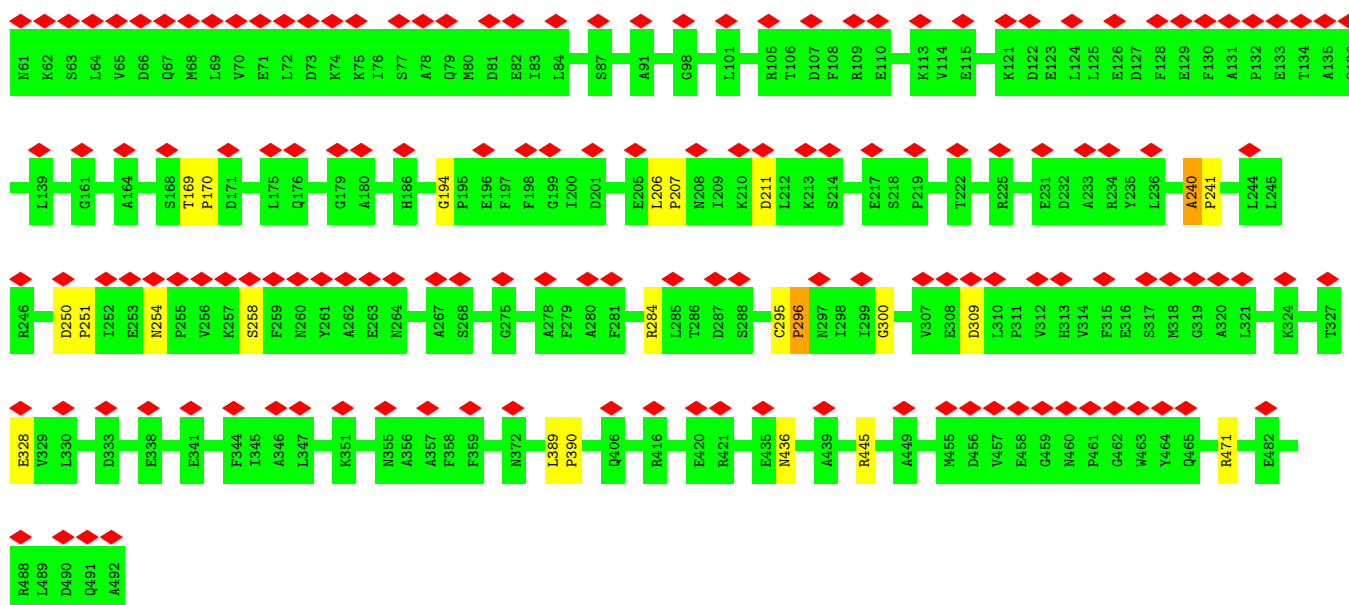


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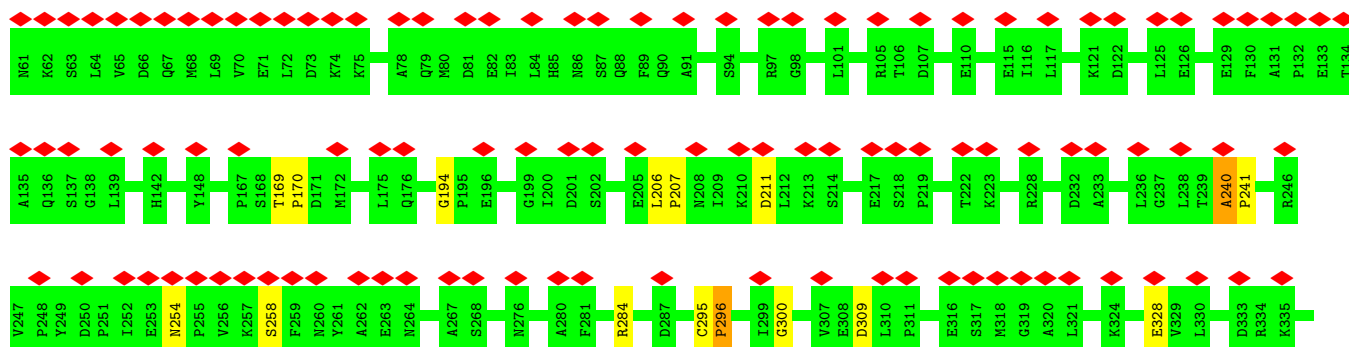


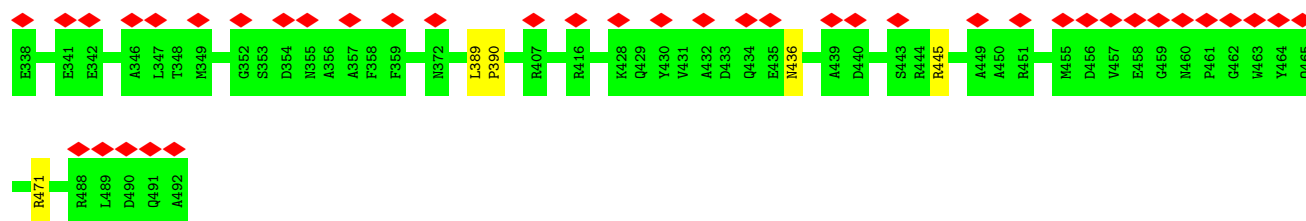


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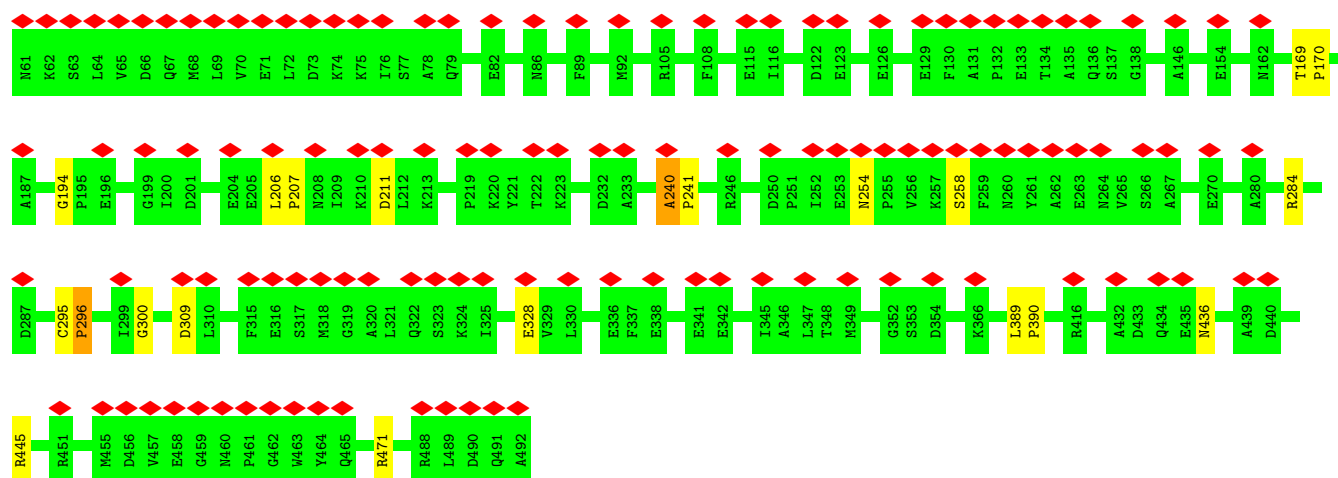


• Molecule 2: VipB

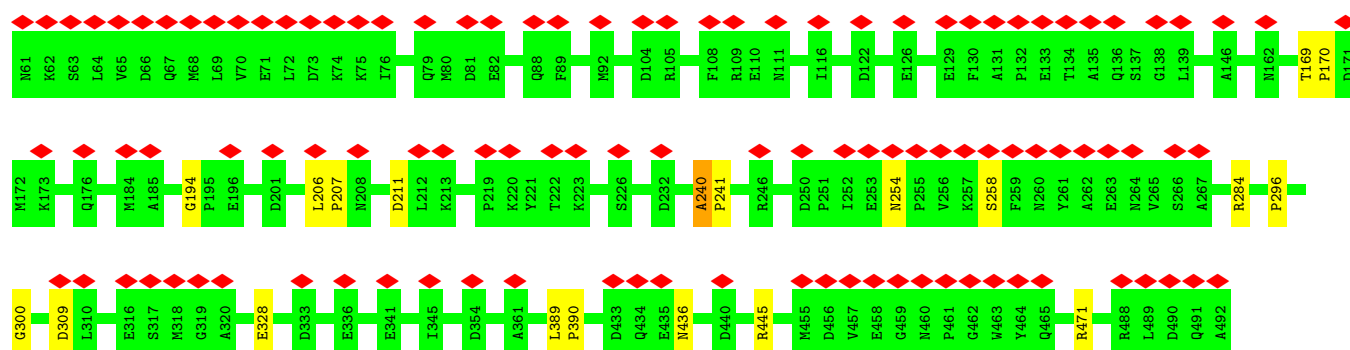




• Molecule 2: VipB



• Molecule 2: VipB



## 4 Experimental information

| Property                             | Value                                           | Source    |
|--------------------------------------|-------------------------------------------------|-----------|
| EM reconstruction method             | HELICAL                                         | Depositor |
| Imposed symmetry                     | HELICAL, twist=29.4°, rise=21.8 Å, axial sym=C6 | Depositor |
| Number of segments used              | 96000                                           | Depositor |
| Resolution determination method      | Not provided                                    |           |
| CTF correction method                | Phase Flip, CTF detection by CTFFIND            | Depositor |
| Microscope                           | FEI TITAN KRIOS                                 | Depositor |
| Voltage (kV)                         | 300                                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                              | Depositor |
| Minimum defocus (nm)                 | 400                                             | Depositor |
| Maximum defocus (nm)                 | 2000                                            | Depositor |
| Magnification                        | 29000                                           | Depositor |
| Image detector                       | GATAN K2 (4k x 4k)                              | Depositor |
| Maximum map value                    | 760.909                                         | Depositor |
| Minimum map value                    | -553.859                                        | Depositor |
| Average map value                    | -99.091                                         | Depositor |
| Map value standard deviation         | 111.770                                         | Depositor |
| Recommended contour level            | 120                                             | Depositor |
| Map size (Å)                         | 300.0, 300.0, 100.0                             | wwPDB     |
| Map dimensions                       | 600, 600, 200                                   | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                | wwPDB     |
| Pixel spacing (Å)                    | 0.5, 0.5, 0.5                                   | 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   | 1     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | 3     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | 5     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | 7     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | A     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | C     | 0.64         | 0/975       | 0.94        | 4/1321 (0.3%)  |
| 1   | E     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | G     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | I     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | K     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | M     | 0.64         | 0/975       | 0.94        | 4/1321 (0.3%)  |
| 1   | O     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | Q     | 0.64         | 0/975       | 0.94        | 4/1321 (0.3%)  |
| 1   | S     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | U     | 0.64         | 0/975       | 0.94        | 4/1321 (0.3%)  |
| 1   | W     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | Y     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | a     | 0.64         | 0/975       | 0.94        | 4/1321 (0.3%)  |
| 1   | c     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | e     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | g     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | i     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | k     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | m     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | o     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | q     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | s     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | u     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | w     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 1   | y     | 0.64         | 0/975       | 0.93        | 4/1321 (0.3%)  |
| 2   | 2     | 0.64         | 0/3556      | 0.95        | 12/4811 (0.2%) |
| 2   | 4     | 0.64         | 0/3556      | 0.95        | 12/4811 (0.2%) |
| 2   | 6     | 0.64         | 0/3556      | 0.95        | 12/4811 (0.2%) |
| 2   | 8     | 0.64         | 0/3556      | 0.95        | 12/4811 (0.2%) |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 2   | B     | 0.63         | 0/3556   | 0.94        | 12/4811 (0.2%)    |
| 2   | D     | 0.64         | 0/3556   | 0.94        | 12/4811 (0.2%)    |
| 2   | F     | 0.63         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | H     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | J     | 0.64         | 0/3556   | 0.94        | 12/4811 (0.2%)    |
| 2   | L     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | N     | 0.64         | 0/3556   | 0.94        | 12/4811 (0.2%)    |
| 2   | P     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | R     | 0.63         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | T     | 0.63         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | V     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | X     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | Z     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | b     | 0.64         | 0/3556   | 0.94        | 12/4811 (0.2%)    |
| 2   | d     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | f     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | h     | 0.64         | 0/3556   | 0.95        | 13/4811 (0.3%)    |
| 2   | j     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | l     | 0.63         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | n     | 0.64         | 0/3556   | 0.95        | 13/4811 (0.3%)    |
| 2   | p     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | r     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | t     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | v     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | x     | 0.63         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| 2   | z     | 0.64         | 0/3556   | 0.95        | 12/4811 (0.2%)    |
| All | All   | 0.64         | 0/135930 | 0.94        | 482/183960 (0.3%) |

There are no bond length outliers.

All (482) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | Q     | 110 | VAL  | CA-C-N | 6.10 | 126.28      | 119.32   |
| 1   | Q     | 110 | VAL  | C-N-CA | 6.10 | 126.28      | 119.32   |
| 1   | W     | 110 | VAL  | CA-C-N | 6.09 | 126.26      | 119.32   |
| 1   | W     | 110 | VAL  | C-N-CA | 6.09 | 126.26      | 119.32   |
| 1   | g     | 110 | VAL  | CA-C-N | 6.08 | 126.26      | 119.32   |
| 1   | g     | 110 | VAL  | C-N-CA | 6.08 | 126.26      | 119.32   |
| 1   | 3     | 110 | VAL  | CA-C-N | 6.08 | 126.25      | 119.32   |
| 1   | 3     | 110 | VAL  | C-N-CA | 6.08 | 126.25      | 119.32   |
| 1   | K     | 110 | VAL  | CA-C-N | 6.07 | 126.24      | 119.32   |
| 1   | K     | 110 | VAL  | C-N-CA | 6.07 | 126.24      | 119.32   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | i     | 110 | VAL  | CA-C-N | 6.07 | 126.24      | 119.32   |
| 1   | i     | 110 | VAL  | C-N-CA | 6.07 | 126.24      | 119.32   |
| 1   | O     | 110 | VAL  | CA-C-N | 6.07 | 126.24      | 119.32   |
| 1   | O     | 110 | VAL  | C-N-CA | 6.07 | 126.24      | 119.32   |
| 1   | 7     | 110 | VAL  | CA-C-N | 6.07 | 126.23      | 119.32   |
| 1   | 7     | 110 | VAL  | C-N-CA | 6.07 | 126.23      | 119.32   |
| 1   | C     | 110 | VAL  | CA-C-N | 6.05 | 126.22      | 119.32   |
| 1   | C     | 110 | VAL  | C-N-CA | 6.05 | 126.22      | 119.32   |
| 1   | y     | 110 | VAL  | CA-C-N | 6.05 | 126.22      | 119.32   |
| 1   | y     | 110 | VAL  | C-N-CA | 6.05 | 126.22      | 119.32   |
| 1   | G     | 110 | VAL  | CA-C-N | 6.05 | 126.22      | 119.32   |
| 1   | G     | 110 | VAL  | C-N-CA | 6.05 | 126.22      | 119.32   |
| 1   | M     | 110 | VAL  | CA-C-N | 6.05 | 126.22      | 119.32   |
| 1   | M     | 110 | VAL  | C-N-CA | 6.05 | 126.22      | 119.32   |
| 1   | q     | 110 | VAL  | CA-C-N | 6.04 | 126.21      | 119.32   |
| 1   | q     | 110 | VAL  | C-N-CA | 6.04 | 126.21      | 119.32   |
| 1   | w     | 110 | VAL  | CA-C-N | 6.04 | 126.21      | 119.32   |
| 1   | w     | 110 | VAL  | C-N-CA | 6.04 | 126.21      | 119.32   |
| 1   | Y     | 110 | VAL  | CA-C-N | 6.04 | 126.21      | 119.32   |
| 1   | Y     | 110 | VAL  | C-N-CA | 6.04 | 126.21      | 119.32   |
| 1   | e     | 110 | VAL  | CA-C-N | 6.04 | 126.21      | 119.32   |
| 1   | e     | 110 | VAL  | C-N-CA | 6.04 | 126.21      | 119.32   |
| 1   | E     | 110 | VAL  | CA-C-N | 6.03 | 126.20      | 119.32   |
| 1   | E     | 110 | VAL  | C-N-CA | 6.03 | 126.20      | 119.32   |
| 1   | a     | 110 | VAL  | CA-C-N | 6.03 | 126.20      | 119.32   |
| 1   | a     | 110 | VAL  | C-N-CA | 6.03 | 126.20      | 119.32   |
| 1   | o     | 110 | VAL  | CA-C-N | 6.03 | 126.19      | 119.32   |
| 1   | o     | 110 | VAL  | C-N-CA | 6.03 | 126.19      | 119.32   |
| 1   | 5     | 110 | VAL  | CA-C-N | 6.03 | 126.19      | 119.32   |
| 1   | 5     | 110 | VAL  | C-N-CA | 6.03 | 126.19      | 119.32   |
| 1   | I     | 110 | VAL  | CA-C-N | 6.03 | 126.19      | 119.32   |
| 1   | I     | 110 | VAL  | C-N-CA | 6.03 | 126.19      | 119.32   |
| 1   | k     | 110 | VAL  | CA-C-N | 6.02 | 126.18      | 119.32   |
| 1   | k     | 110 | VAL  | C-N-CA | 6.02 | 126.18      | 119.32   |
| 1   | u     | 110 | VAL  | CA-C-N | 6.02 | 126.18      | 119.32   |
| 1   | u     | 110 | VAL  | C-N-CA | 6.02 | 126.18      | 119.32   |
| 1   | l     | 110 | VAL  | CA-C-N | 6.02 | 126.18      | 119.32   |
| 1   | l     | 110 | VAL  | C-N-CA | 6.02 | 126.18      | 119.32   |
| 1   | m     | 110 | VAL  | CA-C-N | 6.02 | 126.18      | 119.32   |
| 1   | m     | 110 | VAL  | C-N-CA | 6.02 | 126.18      | 119.32   |
| 1   | A     | 110 | VAL  | CA-C-N | 6.01 | 126.18      | 119.32   |
| 1   | A     | 110 | VAL  | C-N-CA | 6.01 | 126.18      | 119.32   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | S     | 110 | VAL  | CA-C-N | 6.01 | 126.18      | 119.32   |
| 1   | S     | 110 | VAL  | C-N-CA | 6.01 | 126.18      | 119.32   |
| 1   | U     | 110 | VAL  | CA-C-N | 6.01 | 126.17      | 119.32   |
| 1   | U     | 110 | VAL  | C-N-CA | 6.01 | 126.17      | 119.32   |
| 1   | s     | 110 | VAL  | CA-C-N | 6.00 | 126.16      | 119.32   |
| 1   | s     | 110 | VAL  | C-N-CA | 6.00 | 126.16      | 119.32   |
| 1   | c     | 110 | VAL  | CA-C-N | 5.99 | 126.15      | 119.32   |
| 1   | c     | 110 | VAL  | C-N-CA | 5.99 | 126.15      | 119.32   |
| 2   | 4     | 436 | ASN  | CA-C-N | 5.85 | 123.87      | 119.66   |
| 2   | 4     | 436 | ASN  | C-N-CA | 5.85 | 123.87      | 119.66   |
| 2   | n     | 436 | ASN  | CA-C-N | 5.84 | 123.87      | 119.66   |
| 2   | n     | 436 | ASN  | C-N-CA | 5.84 | 123.87      | 119.66   |
| 2   | b     | 436 | ASN  | CA-C-N | 5.84 | 123.86      | 119.66   |
| 2   | b     | 436 | ASN  | C-N-CA | 5.84 | 123.86      | 119.66   |
| 2   | j     | 436 | ASN  | CA-C-N | 5.83 | 123.86      | 119.66   |
| 2   | j     | 436 | ASN  | C-N-CA | 5.83 | 123.86      | 119.66   |
| 2   | h     | 436 | ASN  | CA-C-N | 5.83 | 123.86      | 119.66   |
| 2   | h     | 436 | ASN  | C-N-CA | 5.83 | 123.86      | 119.66   |
| 2   | f     | 436 | ASN  | CA-C-N | 5.83 | 123.86      | 119.66   |
| 2   | f     | 436 | ASN  | C-N-CA | 5.83 | 123.86      | 119.66   |
| 2   | 8     | 436 | ASN  | CA-C-N | 5.83 | 123.86      | 119.66   |
| 2   | 8     | 436 | ASN  | C-N-CA | 5.83 | 123.86      | 119.66   |
| 2   | V     | 436 | ASN  | CA-C-N | 5.83 | 123.86      | 119.66   |
| 2   | V     | 436 | ASN  | C-N-CA | 5.83 | 123.86      | 119.66   |
| 2   | N     | 436 | ASN  | CA-C-N | 5.82 | 123.85      | 119.66   |
| 2   | N     | 436 | ASN  | C-N-CA | 5.82 | 123.85      | 119.66   |
| 2   | P     | 436 | ASN  | CA-C-N | 5.80 | 123.84      | 119.66   |
| 2   | P     | 436 | ASN  | C-N-CA | 5.80 | 123.84      | 119.66   |
| 2   | L     | 436 | ASN  | CA-C-N | 5.80 | 123.83      | 119.66   |
| 2   | L     | 436 | ASN  | C-N-CA | 5.80 | 123.83      | 119.66   |
| 2   | p     | 436 | ASN  | CA-C-N | 5.79 | 123.83      | 119.66   |
| 2   | p     | 436 | ASN  | C-N-CA | 5.79 | 123.83      | 119.66   |
| 2   | X     | 436 | ASN  | CA-C-N | 5.78 | 123.82      | 119.66   |
| 2   | X     | 436 | ASN  | C-N-CA | 5.78 | 123.82      | 119.66   |
| 2   | Z     | 436 | ASN  | CA-C-N | 5.78 | 123.82      | 119.66   |
| 2   | Z     | 436 | ASN  | C-N-CA | 5.78 | 123.82      | 119.66   |
| 2   | l     | 436 | ASN  | CA-C-N | 5.77 | 123.82      | 119.66   |
| 2   | l     | 436 | ASN  | C-N-CA | 5.77 | 123.82      | 119.66   |
| 2   | R     | 436 | ASN  | CA-C-N | 5.77 | 123.81      | 119.66   |
| 2   | R     | 436 | ASN  | C-N-CA | 5.77 | 123.81      | 119.66   |
| 2   | r     | 436 | ASN  | CA-C-N | 5.77 | 123.81      | 119.66   |
| 2   | r     | 436 | ASN  | C-N-CA | 5.77 | 123.81      | 119.66   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | d     | 436 | ASN  | CA-C-N | 5.77 | 123.81      | 119.66   |
| 2   | d     | 436 | ASN  | C-N-CA | 5.77 | 123.81      | 119.66   |
| 2   | F     | 436 | ASN  | CA-C-N | 5.76 | 123.81      | 119.66   |
| 2   | F     | 436 | ASN  | C-N-CA | 5.76 | 123.81      | 119.66   |
| 2   | v     | 436 | ASN  | CA-C-N | 5.76 | 123.81      | 119.66   |
| 2   | v     | 436 | ASN  | C-N-CA | 5.76 | 123.81      | 119.66   |
| 2   | x     | 436 | ASN  | CA-C-N | 5.76 | 123.81      | 119.66   |
| 2   | x     | 436 | ASN  | C-N-CA | 5.76 | 123.81      | 119.66   |
| 2   | B     | 436 | ASN  | CA-C-N | 5.73 | 123.78      | 119.66   |
| 2   | B     | 436 | ASN  | C-N-CA | 5.73 | 123.78      | 119.66   |
| 2   | 6     | 436 | ASN  | CA-C-N | 5.73 | 123.78      | 119.66   |
| 2   | 6     | 436 | ASN  | C-N-CA | 5.73 | 123.78      | 119.66   |
| 2   | z     | 436 | ASN  | CA-C-N | 5.72 | 123.78      | 119.66   |
| 2   | z     | 436 | ASN  | C-N-CA | 5.72 | 123.78      | 119.66   |
| 2   | 2     | 436 | ASN  | CA-C-N | 5.72 | 123.78      | 119.66   |
| 2   | 2     | 436 | ASN  | C-N-CA | 5.72 | 123.78      | 119.66   |
| 2   | T     | 436 | ASN  | CA-C-N | 5.72 | 123.78      | 119.66   |
| 2   | T     | 436 | ASN  | C-N-CA | 5.72 | 123.78      | 119.66   |
| 2   | H     | 436 | ASN  | CA-C-N | 5.71 | 123.77      | 119.66   |
| 2   | H     | 436 | ASN  | C-N-CA | 5.71 | 123.77      | 119.66   |
| 2   | D     | 436 | ASN  | CA-C-N | 5.71 | 123.77      | 119.66   |
| 2   | D     | 436 | ASN  | C-N-CA | 5.71 | 123.77      | 119.66   |
| 2   | J     | 436 | ASN  | CA-C-N | 5.71 | 123.77      | 119.66   |
| 2   | J     | 436 | ASN  | C-N-CA | 5.71 | 123.77      | 119.66   |
| 2   | t     | 436 | ASN  | CA-C-N | 5.71 | 123.77      | 119.66   |
| 2   | t     | 436 | ASN  | C-N-CA | 5.71 | 123.77      | 119.66   |
| 2   | R     | 254 | ASN  | CA-C-N | 5.59 | 125.56      | 120.03   |
| 2   | R     | 254 | ASN  | C-N-CA | 5.59 | 125.56      | 120.03   |
| 2   | D     | 254 | ASN  | CA-C-N | 5.57 | 125.55      | 120.03   |
| 2   | D     | 254 | ASN  | C-N-CA | 5.57 | 125.55      | 120.03   |
| 2   | H     | 254 | ASN  | CA-C-N | 5.57 | 125.54      | 120.03   |
| 2   | H     | 254 | ASN  | C-N-CA | 5.57 | 125.54      | 120.03   |
| 2   | d     | 254 | ASN  | CA-C-N | 5.57 | 125.54      | 120.03   |
| 2   | d     | 254 | ASN  | C-N-CA | 5.57 | 125.54      | 120.03   |
| 2   | L     | 254 | ASN  | CA-C-N | 5.56 | 125.53      | 120.03   |
| 2   | L     | 254 | ASN  | C-N-CA | 5.56 | 125.53      | 120.03   |
| 2   | Z     | 254 | ASN  | CA-C-N | 5.56 | 125.53      | 120.03   |
| 2   | Z     | 254 | ASN  | C-N-CA | 5.56 | 125.53      | 120.03   |
| 2   | z     | 254 | ASN  | CA-C-N | 5.55 | 125.53      | 120.03   |
| 2   | z     | 254 | ASN  | C-N-CA | 5.55 | 125.53      | 120.03   |
| 2   | 4     | 254 | ASN  | CA-C-N | 5.55 | 125.53      | 120.03   |
| 2   | 4     | 254 | ASN  | C-N-CA | 5.55 | 125.53      | 120.03   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | h     | 254 | ASN  | CA-C-N | 5.55 | 125.52      | 120.03   |
| 2   | h     | 254 | ASN  | C-N-CA | 5.55 | 125.52      | 120.03   |
| 2   | r     | 254 | ASN  | CA-C-N | 5.55 | 125.52      | 120.03   |
| 2   | r     | 254 | ASN  | C-N-CA | 5.55 | 125.52      | 120.03   |
| 2   | t     | 254 | ASN  | CA-C-N | 5.55 | 125.52      | 120.03   |
| 2   | t     | 254 | ASN  | C-N-CA | 5.55 | 125.52      | 120.03   |
| 2   | l     | 254 | ASN  | CA-C-N | 5.54 | 125.52      | 120.03   |
| 2   | l     | 254 | ASN  | C-N-CA | 5.54 | 125.52      | 120.03   |
| 2   | N     | 254 | ASN  | CA-C-N | 5.54 | 125.52      | 120.03   |
| 2   | N     | 254 | ASN  | C-N-CA | 5.54 | 125.52      | 120.03   |
| 2   | x     | 254 | ASN  | CA-C-N | 5.54 | 125.51      | 120.03   |
| 2   | x     | 254 | ASN  | C-N-CA | 5.54 | 125.51      | 120.03   |
| 2   | B     | 254 | ASN  | CA-C-N | 5.54 | 125.51      | 120.03   |
| 2   | B     | 254 | ASN  | C-N-CA | 5.54 | 125.51      | 120.03   |
| 2   | T     | 254 | ASN  | CA-C-N | 5.54 | 125.51      | 120.03   |
| 2   | T     | 254 | ASN  | C-N-CA | 5.54 | 125.51      | 120.03   |
| 2   | v     | 254 | ASN  | CA-C-N | 5.54 | 125.51      | 120.03   |
| 2   | v     | 254 | ASN  | C-N-CA | 5.54 | 125.51      | 120.03   |
| 2   | 2     | 254 | ASN  | CA-C-N | 5.54 | 125.51      | 120.03   |
| 2   | 2     | 254 | ASN  | C-N-CA | 5.54 | 125.51      | 120.03   |
| 2   | R     | 445 | ARG  | CA-C-N | 5.53 | 125.20      | 119.56   |
| 2   | R     | 445 | ARG  | C-N-CA | 5.53 | 125.20      | 119.56   |
| 2   | j     | 254 | ASN  | CA-C-N | 5.53 | 125.51      | 120.03   |
| 2   | j     | 254 | ASN  | C-N-CA | 5.53 | 125.51      | 120.03   |
| 2   | V     | 445 | ARG  | CA-C-N | 5.53 | 125.20      | 119.56   |
| 2   | V     | 445 | ARG  | C-N-CA | 5.53 | 125.20      | 119.56   |
| 2   | F     | 254 | ASN  | CA-C-N | 5.53 | 125.50      | 120.03   |
| 2   | F     | 254 | ASN  | C-N-CA | 5.53 | 125.50      | 120.03   |
| 2   | b     | 254 | ASN  | CA-C-N | 5.52 | 125.49      | 120.03   |
| 2   | b     | 254 | ASN  | C-N-CA | 5.52 | 125.49      | 120.03   |
| 2   | V     | 254 | ASN  | CA-C-N | 5.52 | 125.49      | 120.03   |
| 2   | V     | 254 | ASN  | C-N-CA | 5.52 | 125.49      | 120.03   |
| 2   | 8     | 254 | ASN  | CA-C-N | 5.52 | 125.49      | 120.03   |
| 2   | 8     | 254 | ASN  | C-N-CA | 5.52 | 125.49      | 120.03   |
| 2   | 8     | 445 | ARG  | CA-C-N | 5.52 | 125.19      | 119.56   |
| 2   | 8     | 445 | ARG  | C-N-CA | 5.52 | 125.19      | 119.56   |
| 2   | J     | 254 | ASN  | CA-C-N | 5.51 | 125.49      | 120.03   |
| 2   | J     | 254 | ASN  | C-N-CA | 5.51 | 125.49      | 120.03   |
| 2   | P     | 254 | ASN  | CA-C-N | 5.51 | 125.49      | 120.03   |
| 2   | P     | 254 | ASN  | C-N-CA | 5.51 | 125.49      | 120.03   |
| 2   | p     | 254 | ASN  | CA-C-N | 5.51 | 125.49      | 120.03   |
| 2   | p     | 254 | ASN  | C-N-CA | 5.51 | 125.49      | 120.03   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | L     | 445 | ARG  | CA-C-N | 5.51 | 125.18      | 119.56   |
| 2   | L     | 445 | ARG  | C-N-CA | 5.51 | 125.18      | 119.56   |
| 2   | p     | 445 | ARG  | CA-C-N | 5.50 | 125.17      | 119.56   |
| 2   | p     | 445 | ARG  | C-N-CA | 5.50 | 125.17      | 119.56   |
| 2   | X     | 254 | ASN  | CA-C-N | 5.50 | 125.47      | 120.03   |
| 2   | X     | 254 | ASN  | C-N-CA | 5.50 | 125.47      | 120.03   |
| 2   | d     | 445 | ARG  | CA-C-N | 5.50 | 125.17      | 119.56   |
| 2   | d     | 445 | ARG  | C-N-CA | 5.50 | 125.17      | 119.56   |
| 2   | n     | 445 | ARG  | CA-C-N | 5.50 | 125.17      | 119.56   |
| 2   | n     | 445 | ARG  | C-N-CA | 5.50 | 125.17      | 119.56   |
| 2   | f     | 254 | ASN  | CA-C-N | 5.49 | 125.47      | 120.03   |
| 2   | f     | 254 | ASN  | C-N-CA | 5.49 | 125.47      | 120.03   |
| 2   | Z     | 445 | ARG  | CA-C-N | 5.49 | 125.16      | 119.56   |
| 2   | Z     | 445 | ARG  | C-N-CA | 5.49 | 125.16      | 119.56   |
| 2   | n     | 254 | ASN  | CA-C-N | 5.49 | 125.46      | 120.03   |
| 2   | n     | 254 | ASN  | C-N-CA | 5.49 | 125.46      | 120.03   |
| 2   | t     | 445 | ARG  | CA-C-N | 5.49 | 125.16      | 119.56   |
| 2   | t     | 445 | ARG  | C-N-CA | 5.49 | 125.16      | 119.56   |
| 2   | 6     | 254 | ASN  | CA-C-N | 5.49 | 125.46      | 120.03   |
| 2   | 6     | 254 | ASN  | C-N-CA | 5.49 | 125.46      | 120.03   |
| 2   | H     | 445 | ARG  | CA-C-N | 5.48 | 125.15      | 119.56   |
| 2   | H     | 445 | ARG  | C-N-CA | 5.48 | 125.15      | 119.56   |
| 2   | h     | 445 | ARG  | CA-C-N | 5.48 | 125.15      | 119.56   |
| 2   | h     | 445 | ARG  | C-N-CA | 5.48 | 125.15      | 119.56   |
| 2   | J     | 445 | ARG  | CA-C-N | 5.48 | 125.15      | 119.56   |
| 2   | J     | 445 | ARG  | C-N-CA | 5.48 | 125.15      | 119.56   |
| 2   | j     | 445 | ARG  | CA-C-N | 5.47 | 125.14      | 119.56   |
| 2   | j     | 445 | ARG  | C-N-CA | 5.47 | 125.14      | 119.56   |
| 2   | z     | 445 | ARG  | CA-C-N | 5.47 | 125.14      | 119.56   |
| 2   | z     | 445 | ARG  | C-N-CA | 5.47 | 125.14      | 119.56   |
| 2   | l     | 445 | ARG  | CA-C-N | 5.47 | 125.14      | 119.56   |
| 2   | l     | 445 | ARG  | C-N-CA | 5.47 | 125.14      | 119.56   |
| 2   | X     | 445 | ARG  | CA-C-N | 5.47 | 125.14      | 119.56   |
| 2   | X     | 445 | ARG  | C-N-CA | 5.47 | 125.14      | 119.56   |
| 2   | 4     | 445 | ARG  | CA-C-N | 5.47 | 125.14      | 119.56   |
| 2   | 4     | 445 | ARG  | C-N-CA | 5.47 | 125.14      | 119.56   |
| 2   | 6     | 445 | ARG  | CA-C-N | 5.47 | 125.14      | 119.56   |
| 2   | 6     | 445 | ARG  | C-N-CA | 5.47 | 125.14      | 119.56   |
| 2   | f     | 445 | ARG  | CA-C-N | 5.46 | 125.13      | 119.56   |
| 2   | f     | 445 | ARG  | C-N-CA | 5.46 | 125.13      | 119.56   |
| 2   | v     | 445 | ARG  | CA-C-N | 5.46 | 125.13      | 119.56   |
| 2   | v     | 445 | ARG  | C-N-CA | 5.46 | 125.13      | 119.56   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | B     | 445 | ARG  | CA-C-N | 5.46 | 125.13      | 119.56   |
| 2   | B     | 445 | ARG  | C-N-CA | 5.46 | 125.13      | 119.56   |
| 2   | D     | 445 | ARG  | CA-C-N | 5.46 | 125.12      | 119.56   |
| 2   | D     | 445 | ARG  | C-N-CA | 5.46 | 125.12      | 119.56   |
| 2   | b     | 445 | ARG  | CA-C-N | 5.46 | 125.13      | 119.56   |
| 2   | b     | 445 | ARG  | C-N-CA | 5.46 | 125.13      | 119.56   |
| 2   | r     | 445 | ARG  | CA-C-N | 5.46 | 125.13      | 119.56   |
| 2   | r     | 445 | ARG  | C-N-CA | 5.46 | 125.13      | 119.56   |
| 2   | N     | 445 | ARG  | CA-C-N | 5.45 | 125.12      | 119.56   |
| 2   | N     | 445 | ARG  | C-N-CA | 5.45 | 125.12      | 119.56   |
| 2   | T     | 445 | ARG  | CA-C-N | 5.44 | 125.11      | 119.56   |
| 2   | T     | 445 | ARG  | C-N-CA | 5.44 | 125.11      | 119.56   |
| 2   | F     | 445 | ARG  | CA-C-N | 5.44 | 125.11      | 119.56   |
| 2   | F     | 445 | ARG  | C-N-CA | 5.44 | 125.11      | 119.56   |
| 2   | P     | 445 | ARG  | CA-C-N | 5.44 | 125.11      | 119.56   |
| 2   | P     | 445 | ARG  | C-N-CA | 5.44 | 125.11      | 119.56   |
| 2   | 2     | 445 | ARG  | CA-C-N | 5.44 | 125.11      | 119.56   |
| 2   | 2     | 445 | ARG  | C-N-CA | 5.44 | 125.11      | 119.56   |
| 2   | x     | 445 | ARG  | CA-C-N | 5.43 | 125.10      | 119.56   |
| 2   | x     | 445 | ARG  | C-N-CA | 5.43 | 125.10      | 119.56   |
| 2   | 4     | 471 | ARG  | CA-C-N | 5.29 | 125.50      | 120.31   |
| 2   | 4     | 471 | ARG  | C-N-CA | 5.29 | 125.50      | 120.31   |
| 2   | V     | 194 | GLY  | CA-C-N | 5.28 | 124.91      | 119.05   |
| 2   | V     | 194 | GLY  | C-N-CA | 5.28 | 124.91      | 119.05   |
| 2   | 4     | 194 | GLY  | CA-C-N | 5.28 | 124.91      | 119.05   |
| 2   | 4     | 194 | GLY  | C-N-CA | 5.28 | 124.91      | 119.05   |
| 2   | t     | 471 | ARG  | CA-C-N | 5.28 | 125.48      | 120.31   |
| 2   | t     | 471 | ARG  | C-N-CA | 5.28 | 125.48      | 120.31   |
| 2   | b     | 194 | GLY  | CA-C-N | 5.27 | 124.90      | 119.05   |
| 2   | b     | 194 | GLY  | C-N-CA | 5.27 | 124.90      | 119.05   |
| 2   | x     | 194 | GLY  | CA-C-N | 5.27 | 124.90      | 119.05   |
| 2   | x     | 194 | GLY  | C-N-CA | 5.27 | 124.90      | 119.05   |
| 2   | R     | 471 | ARG  | CA-C-N | 5.27 | 125.47      | 120.31   |
| 2   | R     | 471 | ARG  | C-N-CA | 5.27 | 125.47      | 120.31   |
| 2   | 6     | 471 | ARG  | CA-C-N | 5.27 | 125.47      | 120.31   |
| 2   | 6     | 471 | ARG  | C-N-CA | 5.27 | 125.47      | 120.31   |
| 2   | X     | 471 | ARG  | CA-C-N | 5.26 | 125.47      | 120.31   |
| 2   | X     | 471 | ARG  | C-N-CA | 5.26 | 125.47      | 120.31   |
| 2   | l     | 471 | ARG  | CA-C-N | 5.26 | 125.47      | 120.31   |
| 2   | l     | 471 | ARG  | C-N-CA | 5.26 | 125.47      | 120.31   |
| 2   | X     | 194 | GLY  | CA-C-N | 5.26 | 124.89      | 119.05   |
| 2   | X     | 194 | GLY  | C-N-CA | 5.26 | 124.89      | 119.05   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | n     | 471 | ARG  | CA-C-N | 5.26 | 125.47      | 120.31   |
| 2   | n     | 471 | ARG  | C-N-CA | 5.26 | 125.47      | 120.31   |
| 2   | v     | 471 | ARG  | CA-C-N | 5.26 | 125.47      | 120.31   |
| 2   | v     | 471 | ARG  | C-N-CA | 5.26 | 125.47      | 120.31   |
| 2   | B     | 471 | ARG  | CA-C-N | 5.26 | 125.46      | 120.31   |
| 2   | B     | 471 | ARG  | C-N-CA | 5.26 | 125.46      | 120.31   |
| 2   | z     | 194 | GLY  | CA-C-N | 5.26 | 124.89      | 119.05   |
| 2   | z     | 194 | GLY  | C-N-CA | 5.26 | 124.89      | 119.05   |
| 2   | t     | 194 | GLY  | CA-C-N | 5.25 | 124.88      | 119.05   |
| 2   | t     | 194 | GLY  | C-N-CA | 5.25 | 124.88      | 119.05   |
| 2   | n     | 194 | GLY  | CA-C-N | 5.25 | 124.88      | 119.05   |
| 2   | n     | 194 | GLY  | C-N-CA | 5.25 | 124.88      | 119.05   |
| 2   | d     | 194 | GLY  | CA-C-N | 5.25 | 124.88      | 119.05   |
| 2   | d     | 194 | GLY  | C-N-CA | 5.25 | 124.88      | 119.05   |
| 2   | J     | 471 | ARG  | CA-C-N | 5.25 | 125.45      | 120.31   |
| 2   | J     | 471 | ARG  | C-N-CA | 5.25 | 125.45      | 120.31   |
| 2   | v     | 194 | GLY  | CA-C-N | 5.25 | 124.87      | 119.05   |
| 2   | v     | 194 | GLY  | C-N-CA | 5.25 | 124.87      | 119.05   |
| 2   | J     | 194 | GLY  | CA-C-N | 5.24 | 124.87      | 119.05   |
| 2   | J     | 194 | GLY  | C-N-CA | 5.24 | 124.87      | 119.05   |
| 2   | L     | 471 | ARG  | CA-C-N | 5.24 | 125.45      | 120.31   |
| 2   | L     | 471 | ARG  | C-N-CA | 5.24 | 125.45      | 120.31   |
| 2   | h     | 194 | GLY  | CA-C-N | 5.24 | 124.87      | 119.05   |
| 2   | h     | 194 | GLY  | C-N-CA | 5.24 | 124.87      | 119.05   |
| 2   | H     | 471 | ARG  | CA-C-N | 5.24 | 125.44      | 120.31   |
| 2   | H     | 471 | ARG  | C-N-CA | 5.24 | 125.44      | 120.31   |
| 2   | L     | 194 | GLY  | CA-C-N | 5.24 | 124.87      | 119.05   |
| 2   | L     | 194 | GLY  | C-N-CA | 5.24 | 124.87      | 119.05   |
| 2   | f     | 471 | ARG  | CA-C-N | 5.24 | 125.45      | 120.31   |
| 2   | f     | 471 | ARG  | C-N-CA | 5.24 | 125.45      | 120.31   |
| 2   | H     | 194 | GLY  | CA-C-N | 5.24 | 124.86      | 119.05   |
| 2   | H     | 194 | GLY  | C-N-CA | 5.24 | 124.86      | 119.05   |
| 2   | R     | 194 | GLY  | CA-C-N | 5.24 | 124.86      | 119.05   |
| 2   | R     | 194 | GLY  | C-N-CA | 5.24 | 124.86      | 119.05   |
| 2   | j     | 471 | ARG  | CA-C-N | 5.24 | 125.44      | 120.31   |
| 2   | j     | 471 | ARG  | C-N-CA | 5.24 | 125.44      | 120.31   |
| 2   | z     | 471 | ARG  | CA-C-N | 5.24 | 125.44      | 120.31   |
| 2   | z     | 471 | ARG  | C-N-CA | 5.24 | 125.44      | 120.31   |
| 2   | P     | 471 | ARG  | CA-C-N | 5.24 | 125.44      | 120.31   |
| 2   | P     | 471 | ARG  | C-N-CA | 5.24 | 125.44      | 120.31   |
| 2   | T     | 194 | GLY  | CA-C-N | 5.24 | 124.86      | 119.05   |
| 2   | T     | 194 | GLY  | C-N-CA | 5.24 | 124.86      | 119.05   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | Z     | 194 | GLY  | CA-C-N | 5.24 | 124.86      | 119.05   |
| 2   | Z     | 194 | GLY  | C-N-CA | 5.24 | 124.86      | 119.05   |
| 2   | j     | 194 | GLY  | CA-C-N | 5.23 | 124.86      | 119.05   |
| 2   | j     | 194 | GLY  | C-N-CA | 5.23 | 124.86      | 119.05   |
| 2   | p     | 194 | GLY  | CA-C-N | 5.23 | 124.86      | 119.05   |
| 2   | p     | 194 | GLY  | C-N-CA | 5.23 | 124.86      | 119.05   |
| 2   | P     | 194 | GLY  | CA-C-N | 5.23 | 124.86      | 119.05   |
| 2   | P     | 194 | GLY  | C-N-CA | 5.23 | 124.86      | 119.05   |
| 2   | f     | 194 | GLY  | CA-C-N | 5.23 | 124.86      | 119.05   |
| 2   | f     | 194 | GLY  | C-N-CA | 5.23 | 124.86      | 119.05   |
| 2   | r     | 471 | ARG  | CA-C-N | 5.23 | 125.44      | 120.31   |
| 2   | r     | 471 | ARG  | C-N-CA | 5.23 | 125.44      | 120.31   |
| 2   | 2     | 471 | ARG  | CA-C-N | 5.23 | 125.44      | 120.31   |
| 2   | 2     | 471 | ARG  | C-N-CA | 5.23 | 125.44      | 120.31   |
| 2   | h     | 471 | ARG  | CA-C-N | 5.23 | 125.44      | 120.31   |
| 2   | h     | 471 | ARG  | C-N-CA | 5.23 | 125.44      | 120.31   |
| 2   | F     | 471 | ARG  | CA-C-N | 5.23 | 125.43      | 120.31   |
| 2   | F     | 471 | ARG  | C-N-CA | 5.23 | 125.43      | 120.31   |
| 2   | r     | 194 | GLY  | CA-C-N | 5.23 | 124.85      | 119.05   |
| 2   | r     | 194 | GLY  | C-N-CA | 5.23 | 124.85      | 119.05   |
| 2   | l     | 194 | GLY  | CA-C-N | 5.23 | 124.85      | 119.05   |
| 2   | l     | 194 | GLY  | C-N-CA | 5.23 | 124.85      | 119.05   |
| 2   | 8     | 471 | ARG  | CA-C-N | 5.23 | 125.43      | 120.31   |
| 2   | 8     | 471 | ARG  | C-N-CA | 5.23 | 125.43      | 120.31   |
| 2   | N     | 194 | GLY  | CA-C-N | 5.22 | 124.85      | 119.05   |
| 2   | N     | 194 | GLY  | C-N-CA | 5.22 | 124.85      | 119.05   |
| 2   | Z     | 471 | ARG  | CA-C-N | 5.22 | 125.43      | 120.31   |
| 2   | Z     | 471 | ARG  | C-N-CA | 5.22 | 125.43      | 120.31   |
| 2   | d     | 471 | ARG  | CA-C-N | 5.22 | 125.43      | 120.31   |
| 2   | d     | 471 | ARG  | C-N-CA | 5.22 | 125.43      | 120.31   |
| 2   | x     | 471 | ARG  | CA-C-N | 5.22 | 125.43      | 120.31   |
| 2   | x     | 471 | ARG  | C-N-CA | 5.22 | 125.43      | 120.31   |
| 2   | T     | 471 | ARG  | CA-C-N | 5.22 | 125.43      | 120.31   |
| 2   | T     | 471 | ARG  | C-N-CA | 5.22 | 125.43      | 120.31   |
| 2   | V     | 471 | ARG  | CA-C-N | 5.22 | 125.43      | 120.31   |
| 2   | V     | 471 | ARG  | C-N-CA | 5.22 | 125.43      | 120.31   |
| 2   | 6     | 194 | GLY  | CA-C-N | 5.22 | 124.85      | 119.05   |
| 2   | 6     | 194 | GLY  | C-N-CA | 5.22 | 124.85      | 119.05   |
| 2   | B     | 194 | GLY  | CA-C-N | 5.22 | 124.84      | 119.05   |
| 2   | B     | 194 | GLY  | C-N-CA | 5.22 | 124.84      | 119.05   |
| 2   | D     | 194 | GLY  | CA-C-N | 5.22 | 124.84      | 119.05   |
| 2   | D     | 194 | GLY  | C-N-CA | 5.22 | 124.84      | 119.05   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | F     | 194 | GLY  | CA-C-N | 5.22 | 124.84      | 119.05   |
| 2   | F     | 194 | GLY  | C-N-CA | 5.22 | 124.84      | 119.05   |
| 2   | p     | 471 | ARG  | CA-C-N | 5.22 | 125.42      | 120.31   |
| 2   | p     | 471 | ARG  | C-N-CA | 5.22 | 125.42      | 120.31   |
| 2   | b     | 471 | ARG  | CA-C-N | 5.21 | 125.42      | 120.31   |
| 2   | b     | 471 | ARG  | C-N-CA | 5.21 | 125.42      | 120.31   |
| 2   | D     | 471 | ARG  | CA-C-N | 5.21 | 125.42      | 120.31   |
| 2   | D     | 471 | ARG  | C-N-CA | 5.21 | 125.42      | 120.31   |
| 2   | 2     | 194 | GLY  | CA-C-N | 5.20 | 124.82      | 119.05   |
| 2   | 2     | 194 | GLY  | C-N-CA | 5.20 | 124.82      | 119.05   |
| 2   | 8     | 194 | GLY  | CA-C-N | 5.19 | 124.81      | 119.05   |
| 2   | 8     | 194 | GLY  | C-N-CA | 5.19 | 124.81      | 119.05   |
| 2   | N     | 471 | ARG  | CA-C-N | 5.18 | 125.39      | 120.31   |
| 2   | N     | 471 | ARG  | C-N-CA | 5.18 | 125.39      | 120.31   |
| 2   | z     | 300 | GLY  | CA-C-N | 5.12 | 124.74      | 119.05   |
| 2   | z     | 300 | GLY  | C-N-CA | 5.12 | 124.74      | 119.05   |
| 2   | 8     | 300 | GLY  | CA-C-N | 5.11 | 124.72      | 119.05   |
| 2   | 8     | 300 | GLY  | C-N-CA | 5.11 | 124.72      | 119.05   |
| 1   | Q     | 102 | ALA  | CA-C-N | 5.10 | 125.39      | 119.47   |
| 1   | Q     | 102 | ALA  | C-N-CA | 5.10 | 125.39      | 119.47   |
| 1   | Y     | 102 | ALA  | CA-C-N | 5.10 | 125.39      | 119.47   |
| 1   | Y     | 102 | ALA  | C-N-CA | 5.10 | 125.39      | 119.47   |
| 1   | e     | 102 | ALA  | CA-C-N | 5.10 | 125.39      | 119.47   |
| 1   | e     | 102 | ALA  | C-N-CA | 5.10 | 125.39      | 119.47   |
| 1   | o     | 102 | ALA  | CA-C-N | 5.10 | 125.39      | 119.47   |
| 1   | o     | 102 | ALA  | C-N-CA | 5.10 | 125.39      | 119.47   |
| 2   | H     | 300 | GLY  | CA-C-N | 5.10 | 124.71      | 119.05   |
| 2   | H     | 300 | GLY  | C-N-CA | 5.10 | 124.71      | 119.05   |
| 2   | N     | 300 | GLY  | CA-C-N | 5.10 | 124.71      | 119.05   |
| 2   | N     | 300 | GLY  | C-N-CA | 5.10 | 124.71      | 119.05   |
| 2   | p     | 300 | GLY  | CA-C-N | 5.10 | 124.71      | 119.05   |
| 2   | p     | 300 | GLY  | C-N-CA | 5.10 | 124.71      | 119.05   |
| 2   | T     | 300 | GLY  | CA-C-N | 5.10 | 124.71      | 119.05   |
| 2   | T     | 300 | GLY  | C-N-CA | 5.10 | 124.71      | 119.05   |
| 2   | 4     | 300 | GLY  | CA-C-N | 5.10 | 124.71      | 119.05   |
| 2   | 4     | 300 | GLY  | C-N-CA | 5.10 | 124.71      | 119.05   |
| 2   | h     | 300 | GLY  | CA-C-N | 5.10 | 124.71      | 119.05   |
| 2   | h     | 300 | GLY  | C-N-CA | 5.10 | 124.71      | 119.05   |
| 2   | J     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | J     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |
| 2   | R     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | R     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | i     | 102 | ALA  | CA-C-N | 5.09 | 125.38      | 119.47   |
| 1   | i     | 102 | ALA  | C-N-CA | 5.09 | 125.38      | 119.47   |
| 2   | D     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | D     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |
| 1   | U     | 102 | ALA  | CA-C-N | 5.09 | 125.38      | 119.47   |
| 1   | U     | 102 | ALA  | C-N-CA | 5.09 | 125.38      | 119.47   |
| 2   | j     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | j     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |
| 2   | X     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | X     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |
| 1   | M     | 102 | ALA  | CA-C-N | 5.09 | 125.37      | 119.47   |
| 1   | M     | 102 | ALA  | C-N-CA | 5.09 | 125.37      | 119.47   |
| 2   | v     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | v     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |
| 2   | B     | 300 | GLY  | CA-C-N | 5.09 | 124.69      | 119.05   |
| 2   | B     | 300 | GLY  | C-N-CA | 5.09 | 124.69      | 119.05   |
| 2   | F     | 300 | GLY  | CA-C-N | 5.09 | 124.70      | 119.05   |
| 2   | F     | 300 | GLY  | C-N-CA | 5.09 | 124.70      | 119.05   |
| 1   | g     | 102 | ALA  | CA-C-N | 5.08 | 125.37      | 119.47   |
| 1   | g     | 102 | ALA  | C-N-CA | 5.08 | 125.37      | 119.47   |
| 2   | P     | 300 | GLY  | CA-C-N | 5.08 | 124.69      | 119.05   |
| 2   | P     | 300 | GLY  | C-N-CA | 5.08 | 124.69      | 119.05   |
| 1   | a     | 102 | ALA  | CA-C-N | 5.08 | 125.37      | 119.47   |
| 1   | a     | 102 | ALA  | C-N-CA | 5.08 | 125.37      | 119.47   |
| 2   | t     | 300 | GLY  | CA-C-N | 5.08 | 124.69      | 119.05   |
| 2   | t     | 300 | GLY  | C-N-CA | 5.08 | 124.69      | 119.05   |
| 1   | s     | 102 | ALA  | CA-C-N | 5.08 | 125.36      | 119.47   |
| 1   | s     | 102 | ALA  | C-N-CA | 5.08 | 125.36      | 119.47   |
| 2   | f     | 300 | GLY  | CA-C-N | 5.08 | 124.69      | 119.05   |
| 2   | f     | 300 | GLY  | C-N-CA | 5.08 | 124.69      | 119.05   |
| 1   | l     | 102 | ALA  | CA-C-N | 5.08 | 125.36      | 119.47   |
| 1   | l     | 102 | ALA  | C-N-CA | 5.08 | 125.36      | 119.47   |
| 1   | S     | 102 | ALA  | CA-C-N | 5.08 | 125.36      | 119.47   |
| 1   | S     | 102 | ALA  | C-N-CA | 5.08 | 125.36      | 119.47   |
| 2   | V     | 300 | GLY  | CA-C-N | 5.08 | 124.68      | 119.05   |
| 2   | V     | 300 | GLY  | C-N-CA | 5.08 | 124.68      | 119.05   |
| 1   | m     | 102 | ALA  | CA-C-N | 5.07 | 125.36      | 119.47   |
| 1   | m     | 102 | ALA  | C-N-CA | 5.07 | 125.36      | 119.47   |
| 1   | y     | 102 | ALA  | CA-C-N | 5.07 | 125.35      | 119.47   |
| 1   | y     | 102 | ALA  | C-N-CA | 5.07 | 125.35      | 119.47   |
| 1   | C     | 102 | ALA  | CA-C-N | 5.07 | 125.35      | 119.47   |
| 1   | C     | 102 | ALA  | C-N-CA | 5.07 | 125.35      | 119.47   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | Z     | 300 | GLY  | CA-C-N | 5.07 | 124.68      | 119.05   |
| 2   | Z     | 300 | GLY  | C-N-CA | 5.07 | 124.68      | 119.05   |
| 2   | d     | 300 | GLY  | CA-C-N | 5.07 | 124.67      | 119.05   |
| 2   | d     | 300 | GLY  | C-N-CA | 5.07 | 124.67      | 119.05   |
| 2   | r     | 300 | GLY  | CA-C-N | 5.07 | 124.67      | 119.05   |
| 2   | r     | 300 | GLY  | C-N-CA | 5.07 | 124.67      | 119.05   |
| 2   | x     | 300 | GLY  | CA-C-N | 5.07 | 124.67      | 119.05   |
| 2   | x     | 300 | GLY  | C-N-CA | 5.07 | 124.67      | 119.05   |
| 2   | b     | 300 | GLY  | CA-C-N | 5.06 | 124.67      | 119.05   |
| 2   | b     | 300 | GLY  | C-N-CA | 5.06 | 124.67      | 119.05   |
| 1   | 3     | 102 | ALA  | CA-C-N | 5.06 | 125.34      | 119.47   |
| 1   | 3     | 102 | ALA  | C-N-CA | 5.06 | 125.34      | 119.47   |
| 1   | c     | 102 | ALA  | CA-C-N | 5.06 | 125.34      | 119.47   |
| 1   | c     | 102 | ALA  | C-N-CA | 5.06 | 125.34      | 119.47   |
| 1   | k     | 102 | ALA  | CA-C-N | 5.06 | 125.34      | 119.47   |
| 1   | k     | 102 | ALA  | C-N-CA | 5.06 | 125.34      | 119.47   |
| 1   | A     | 102 | ALA  | CA-C-N | 5.06 | 125.34      | 119.47   |
| 1   | A     | 102 | ALA  | C-N-CA | 5.06 | 125.34      | 119.47   |
| 2   | n     | 300 | GLY  | CA-C-N | 5.06 | 124.66      | 119.05   |
| 2   | n     | 300 | GLY  | C-N-CA | 5.06 | 124.66      | 119.05   |
| 1   | 5     | 102 | ALA  | CA-C-N | 5.06 | 125.34      | 119.47   |
| 1   | 5     | 102 | ALA  | C-N-CA | 5.06 | 125.34      | 119.47   |
| 1   | I     | 102 | ALA  | CA-C-N | 5.05 | 125.33      | 119.47   |
| 1   | I     | 102 | ALA  | C-N-CA | 5.05 | 125.33      | 119.47   |
| 1   | w     | 102 | ALA  | CA-C-N | 5.05 | 125.33      | 119.47   |
| 1   | w     | 102 | ALA  | C-N-CA | 5.05 | 125.33      | 119.47   |
| 1   | 7     | 102 | ALA  | CA-C-N | 5.05 | 125.33      | 119.47   |
| 1   | 7     | 102 | ALA  | C-N-CA | 5.05 | 125.33      | 119.47   |
| 1   | G     | 102 | ALA  | CA-C-N | 5.05 | 125.33      | 119.47   |
| 1   | G     | 102 | ALA  | C-N-CA | 5.05 | 125.33      | 119.47   |
| 2   | L     | 300 | GLY  | CA-C-N | 5.05 | 124.66      | 119.05   |
| 2   | L     | 300 | GLY  | C-N-CA | 5.05 | 124.66      | 119.05   |
| 1   | K     | 102 | ALA  | CA-C-N | 5.05 | 125.32      | 119.47   |
| 1   | K     | 102 | ALA  | C-N-CA | 5.05 | 125.32      | 119.47   |
| 1   | E     | 102 | ALA  | CA-C-N | 5.04 | 125.32      | 119.47   |
| 1   | E     | 102 | ALA  | C-N-CA | 5.04 | 125.32      | 119.47   |
| 2   | 2     | 300 | GLY  | CA-C-N | 5.04 | 124.64      | 119.05   |
| 2   | 2     | 300 | GLY  | C-N-CA | 5.04 | 124.64      | 119.05   |
| 1   | W     | 102 | ALA  | CA-C-N | 5.04 | 125.31      | 119.47   |
| 1   | W     | 102 | ALA  | C-N-CA | 5.04 | 125.31      | 119.47   |
| 1   | O     | 102 | ALA  | CA-C-N | 5.03 | 125.31      | 119.47   |
| 1   | O     | 102 | ALA  | C-N-CA | 5.03 | 125.31      | 119.47   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | q     | 102 | ALA  | CA-C-N | 5.03 | 125.30      | 119.47   |
| 1   | q     | 102 | ALA  | C-N-CA | 5.03 | 125.30      | 119.47   |
| 2   | 6     | 300 | GLY  | CA-C-N | 5.03 | 124.64      | 119.05   |
| 2   | 6     | 300 | GLY  | C-N-CA | 5.03 | 124.64      | 119.05   |
| 2   | l     | 300 | GLY  | CA-C-N | 5.02 | 124.63      | 119.05   |
| 2   | l     | 300 | GLY  | C-N-CA | 5.02 | 124.63      | 119.05   |
| 1   | u     | 102 | ALA  | CA-C-N | 5.02 | 125.29      | 119.47   |
| 1   | u     | 102 | ALA  | C-N-CA | 5.02 | 125.29      | 119.47   |
| 2   | n     | 317 | SER  | CA-C-O | 5.01 | 120.85      | 117.94   |
| 2   | h     | 317 | SER  | CA-C-O | 5.00 | 120.84      | 117.94   |

There are no chirality outliers.

There are no planarity outliers.

## 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   | 1     | 963   | 0        | 986      | 4       | 0            |
| 1   | 3     | 963   | 0        | 986      | 4       | 0            |
| 1   | 5     | 963   | 0        | 986      | 3       | 0            |
| 1   | 7     | 963   | 0        | 986      | 4       | 0            |
| 1   | A     | 963   | 0        | 986      | 6       | 0            |
| 1   | C     | 963   | 0        | 986      | 3       | 0            |
| 1   | E     | 963   | 0        | 986      | 3       | 0            |
| 1   | G     | 963   | 0        | 986      | 4       | 0            |
| 1   | I     | 963   | 0        | 986      | 3       | 0            |
| 1   | K     | 963   | 0        | 986      | 3       | 0            |
| 1   | M     | 963   | 0        | 986      | 2       | 0            |
| 1   | O     | 963   | 0        | 986      | 5       | 0            |
| 1   | Q     | 963   | 0        | 986      | 5       | 0            |
| 1   | S     | 963   | 0        | 986      | 4       | 0            |
| 1   | U     | 963   | 0        | 986      | 3       | 0            |
| 1   | W     | 963   | 0        | 986      | 3       | 0            |
| 1   | Y     | 963   | 0        | 986      | 2       | 0            |
| 1   | a     | 963   | 0        | 986      | 5       | 0            |
| 1   | c     | 963   | 0        | 986      | 4       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | e     | 963    | 0        | 986      | 3       | 0            |
| 1   | g     | 963    | 0        | 986      | 3       | 0            |
| 1   | i     | 963    | 0        | 986      | 2       | 0            |
| 1   | k     | 963    | 0        | 986      | 3       | 0            |
| 1   | m     | 963    | 0        | 986      | 4       | 0            |
| 1   | o     | 963    | 0        | 986      | 5       | 0            |
| 1   | q     | 963    | 0        | 986      | 4       | 0            |
| 1   | s     | 963    | 0        | 986      | 3       | 0            |
| 1   | u     | 963    | 0        | 986      | 4       | 0            |
| 1   | w     | 963    | 0        | 986      | 3       | 0            |
| 1   | y     | 963    | 0        | 986      | 3       | 0            |
| 2   | 2     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | 4     | 3468   | 0        | 3386     | 13      | 0            |
| 2   | 6     | 3468   | 0        | 3386     | 13      | 0            |
| 2   | 8     | 3468   | 0        | 3386     | 12      | 0            |
| 2   | B     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | D     | 3468   | 0        | 3386     | 13      | 0            |
| 2   | F     | 3468   | 0        | 3386     | 13      | 0            |
| 2   | H     | 3468   | 0        | 3386     | 16      | 0            |
| 2   | J     | 3468   | 0        | 3386     | 15      | 0            |
| 2   | L     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | N     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | P     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | R     | 3468   | 0        | 3386     | 15      | 0            |
| 2   | T     | 3468   | 0        | 3386     | 15      | 0            |
| 2   | V     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | X     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | Z     | 3468   | 0        | 3386     | 15      | 0            |
| 2   | b     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | d     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | f     | 3468   | 0        | 3386     | 13      | 0            |
| 2   | h     | 3468   | 0        | 3386     | 15      | 0            |
| 2   | j     | 3468   | 0        | 3386     | 16      | 0            |
| 2   | l     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | n     | 3468   | 0        | 3386     | 13      | 0            |
| 2   | p     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | r     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | t     | 3468   | 0        | 3386     | 14      | 0            |
| 2   | v     | 3468   | 0        | 3386     | 15      | 0            |
| 2   | x     | 3468   | 0        | 3386     | 16      | 0            |
| 2   | z     | 3468   | 0        | 3386     | 13      | 0            |
| All | All   | 132930 | 0        | 131160   | 530     | 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 2.

All (530) 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:G:126:LEU:HG | 1:G:126:LEU:O  | 1.92                     | 0.69              |
| 1:g:126:LEU:HG | 1:g:126:LEU:O  | 1.92                     | 0.69              |
| 1:A:126:LEU:O  | 1:A:126:LEU:HG | 1.92                     | 0.69              |
| 1:O:126:LEU:O  | 1:O:126:LEU:HG | 1.92                     | 0.69              |
| 1:y:126:LEU:O  | 1:y:126:LEU:HG | 1.92                     | 0.69              |
| 1:S:126:LEU:HG | 1:S:126:LEU:O  | 1.92                     | 0.69              |
| 1:u:126:LEU:HG | 1:u:126:LEU:O  | 1.92                     | 0.69              |
| 1:7:126:LEU:O  | 1:7:126:LEU:HG | 1.92                     | 0.69              |
| 1:Y:126:LEU:O  | 1:Y:126:LEU:HG | 1.92                     | 0.69              |
| 1:c:126:LEU:O  | 1:c:126:LEU:HG | 1.92                     | 0.69              |
| 1:o:126:LEU:O  | 1:o:126:LEU:HG | 1.92                     | 0.69              |
| 1:U:126:LEU:O  | 1:U:126:LEU:HG | 1.92                     | 0.69              |
| 1:k:126:LEU:O  | 1:k:126:LEU:HG | 1.92                     | 0.69              |
| 1:C:126:LEU:O  | 1:C:126:LEU:HG | 1.92                     | 0.68              |
| 1:3:126:LEU:HG | 1:3:126:LEU:O  | 1.92                     | 0.68              |
| 1:W:126:LEU:O  | 1:W:126:LEU:HG | 1.92                     | 0.68              |
| 1:m:126:LEU:O  | 1:m:126:LEU:HG | 1.92                     | 0.68              |
| 1:a:126:LEU:O  | 1:a:126:LEU:HG | 1.92                     | 0.68              |
| 1:E:126:LEU:HG | 1:E:126:LEU:O  | 1.92                     | 0.68              |
| 1:e:126:LEU:O  | 1:e:126:LEU:HG | 1.92                     | 0.68              |
| 1:5:126:LEU:O  | 1:5:126:LEU:HG | 1.92                     | 0.68              |
| 1:K:126:LEU:O  | 1:K:126:LEU:HG | 1.92                     | 0.68              |
| 1:s:126:LEU:HG | 1:s:126:LEU:O  | 1.92                     | 0.68              |
| 1:q:126:LEU:O  | 1:q:126:LEU:HG | 1.92                     | 0.68              |
| 1:w:126:LEU:O  | 1:w:126:LEU:HG | 1.92                     | 0.68              |
| 1:1:126:LEU:HG | 1:1:126:LEU:O  | 1.92                     | 0.68              |
| 1:Q:126:LEU:HG | 1:Q:126:LEU:O  | 1.92                     | 0.68              |
| 1:i:126:LEU:HG | 1:i:126:LEU:O  | 1.92                     | 0.68              |
| 1:I:126:LEU:HG | 1:I:126:LEU:O  | 1.92                     | 0.67              |
| 1:M:126:LEU:O  | 1:M:126:LEU:HG | 1.92                     | 0.67              |
| 1:e:125:ALA:O  | 1:e:126:LEU:C  | 2.51                     | 0.54              |
| 1:w:125:ALA:O  | 1:w:126:LEU:C  | 2.51                     | 0.54              |
| 1:U:125:ALA:O  | 1:U:126:LEU:C  | 2.51                     | 0.54              |
| 1:i:125:ALA:O  | 1:i:126:LEU:C  | 2.51                     | 0.54              |
| 1:5:125:ALA:O  | 1:5:126:LEU:C  | 2.51                     | 0.54              |
| 1:K:125:ALA:O  | 1:K:126:LEU:C  | 2.51                     | 0.53              |
| 1:M:125:ALA:O  | 1:M:126:LEU:C  | 2.51                     | 0.53              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:125:ALA:O   | 1:E:126:LEU:C   | 2.51                     | 0.53              |
| 1:m:125:ALA:O   | 1:m:126:LEU:C   | 2.51                     | 0.53              |
| 1:s:125:ALA:O   | 1:s:126:LEU:C   | 2.51                     | 0.53              |
| 1:u:125:ALA:O   | 1:u:126:LEU:C   | 2.51                     | 0.53              |
| 1:I:125:ALA:O   | 1:I:126:LEU:C   | 2.51                     | 0.53              |
| 1:Q:125:ALA:O   | 1:Q:126:LEU:C   | 2.51                     | 0.53              |
| 1:l:125:ALA:O   | 1:l:126:LEU:C   | 2.51                     | 0.53              |
| 1:G:125:ALA:O   | 1:G:126:LEU:C   | 2.51                     | 0.53              |
| 1:Y:125:ALA:O   | 1:Y:126:LEU:C   | 2.51                     | 0.53              |
| 1:a:125:ALA:O   | 1:a:126:LEU:C   | 2.51                     | 0.53              |
| 1:S:125:ALA:O   | 1:S:126:LEU:C   | 2.51                     | 0.53              |
| 1:k:125:ALA:O   | 1:k:126:LEU:C   | 2.51                     | 0.53              |
| 1:q:125:ALA:O   | 1:q:126:LEU:C   | 2.51                     | 0.53              |
| 1:A:125:ALA:O   | 1:A:126:LEU:C   | 2.51                     | 0.53              |
| 1:C:125:ALA:O   | 1:C:126:LEU:C   | 2.51                     | 0.53              |
| 2:D:240:ALA:HB3 | 2:D:241:PRO:HD3 | 1.91                     | 0.53              |
| 2:b:240:ALA:HB3 | 2:b:241:PRO:HD3 | 1.91                     | 0.53              |
| 1:g:125:ALA:O   | 1:g:126:LEU:C   | 2.51                     | 0.53              |
| 1:o:125:ALA:O   | 1:o:126:LEU:C   | 2.51                     | 0.53              |
| 1:y:125:ALA:O   | 1:y:126:LEU:C   | 2.51                     | 0.53              |
| 1:7:125:ALA:O   | 1:7:126:LEU:C   | 2.51                     | 0.53              |
| 2:B:240:ALA:HB3 | 2:B:241:PRO:HD3 | 1.92                     | 0.52              |
| 1:W:125:ALA:O   | 1:W:126:LEU:C   | 2.51                     | 0.52              |
| 2:d:240:ALA:HB3 | 2:d:241:PRO:HD3 | 1.91                     | 0.52              |
| 2:P:240:ALA:HB3 | 2:P:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:R:240:ALA:HB3 | 2:R:241:PRO:HD3 | 1.92                     | 0.52              |
| 1:c:125:ALA:O   | 1:c:126:LEU:C   | 2.51                     | 0.52              |
| 2:p:240:ALA:HB3 | 2:p:241:PRO:HD3 | 1.91                     | 0.52              |
| 2:4:240:ALA:HB3 | 2:4:241:PRO:HD3 | 1.91                     | 0.52              |
| 2:2:240:ALA:HB3 | 2:2:241:PRO:HD3 | 1.91                     | 0.52              |
| 1:3:125:ALA:O   | 1:3:126:LEU:C   | 2.51                     | 0.52              |
| 2:F:240:ALA:HB3 | 2:F:241:PRO:HD3 | 1.92                     | 0.52              |
| 1:O:125:ALA:O   | 1:O:126:LEU:C   | 2.51                     | 0.52              |
| 2:f:240:ALA:HB3 | 2:f:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:r:240:ALA:HB3 | 2:r:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:N:240:ALA:HB3 | 2:N:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:6:240:ALA:HB3 | 2:6:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:t:240:ALA:HB3 | 2:t:241:PRO:HD3 | 1.91                     | 0.52              |
| 2:T:240:ALA:HB3 | 2:T:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:z:240:ALA:HB3 | 2:z:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:Z:240:ALA:HB3 | 2:Z:241:PRO:HD3 | 1.91                     | 0.52              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:n:240:ALA:HB3 | 2:n:241:PRO:HD3 | 1.92                     | 0.52              |
| 2:L:240:ALA:HB3 | 2:L:241:PRO:HD3 | 1.91                     | 0.52              |
| 2:f:169:THR:HB  | 2:f:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:l:240:ALA:HB3 | 2:l:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:F:169:THR:HB  | 2:F:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:R:169:THR:HB  | 2:R:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:X:240:ALA:HB3 | 2:X:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:6:169:THR:HB  | 2:6:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:h:240:ALA:HB3 | 2:h:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:r:169:THR:HB  | 2:r:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:t:169:THR:HB  | 2:t:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:8:240:ALA:HB3 | 2:8:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:J:240:ALA:HB3 | 2:J:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:T:169:THR:HB  | 2:T:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:V:240:ALA:HB3 | 2:V:241:PRO:CD  | 2.41                     | 0.51              |
| 2:2:240:ALA:HB3 | 2:2:241:PRO:CD  | 2.41                     | 0.51              |
| 2:D:169:THR:HB  | 2:D:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:L:240:ALA:HB3 | 2:L:241:PRO:CD  | 2.41                     | 0.51              |
| 2:Z:240:ALA:HB3 | 2:Z:241:PRO:CD  | 2.41                     | 0.51              |
| 2:b:240:ALA:HB3 | 2:b:241:PRO:CD  | 2.41                     | 0.51              |
| 2:j:240:ALA:HB3 | 2:j:241:PRO:HD3 | 1.92                     | 0.51              |
| 2:v:240:ALA:HB3 | 2:v:241:PRO:CD  | 2.41                     | 0.51              |
| 2:x:240:ALA:HB3 | 2:x:241:PRO:HD3 | 1.92                     | 0.51              |
| 2:8:169:THR:HB  | 2:8:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:H:240:ALA:HB3 | 2:H:241:PRO:HD3 | 1.92                     | 0.51              |
| 2:L:169:THR:HB  | 2:L:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:V:240:ALA:HB3 | 2:V:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:d:169:THR:HB  | 2:d:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:z:240:ALA:HB3 | 2:z:241:PRO:CD  | 2.41                     | 0.51              |
| 2:B:240:ALA:HB3 | 2:B:241:PRO:CD  | 2.41                     | 0.51              |
| 2:N:169:THR:HB  | 2:N:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:T:240:ALA:HB3 | 2:T:241:PRO:CD  | 2.41                     | 0.51              |
| 2:Z:169:THR:HB  | 2:Z:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:b:240:ALA:CB  | 2:b:241:PRO:CD  | 2.89                     | 0.51              |
| 2:l:240:ALA:HB3 | 2:l:241:PRO:CD  | 2.41                     | 0.51              |
| 2:v:240:ALA:HB3 | 2:v:241:PRO:HD3 | 1.91                     | 0.51              |
| 2:2:240:ALA:CB  | 2:2:241:PRO:CD  | 2.89                     | 0.51              |
| 2:4:240:ALA:HB3 | 2:4:241:PRO:CD  | 2.41                     | 0.51              |
| 2:6:240:ALA:HB3 | 2:6:241:PRO:CD  | 2.41                     | 0.51              |
| 2:8:240:ALA:HB3 | 2:8:241:PRO:CD  | 2.41                     | 0.51              |
| 2:B:240:ALA:CB  | 2:B:241:PRO:CD  | 2.89                     | 0.51              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:N:240:ALA:CB  | 2:N:241:PRO:CD  | 2.89                     | 0.51              |
| 2:P:240:ALA:CB  | 2:P:241:PRO:CD  | 2.89                     | 0.51              |
| 2:X:169:THR:HB  | 2:X:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:d:240:ALA:HB3 | 2:d:241:PRO:CD  | 2.41                     | 0.51              |
| 2:f:240:ALA:HB3 | 2:f:241:PRO:CD  | 2.41                     | 0.51              |
| 2:j:328:GLU:OE1 | 2:j:328:GLU:N   | 2.38                     | 0.51              |
| 2:t:240:ALA:HB3 | 2:t:241:PRO:CD  | 2.41                     | 0.51              |
| 2:4:169:THR:HB  | 2:4:170:PRO:HD3 | 1.92                     | 0.51              |
| 2:4:328:GLU:OE1 | 2:4:328:GLU:N   | 2.38                     | 0.51              |
| 2:P:240:ALA:HB3 | 2:P:241:PRO:CD  | 2.41                     | 0.50              |
| 2:X:240:ALA:HB3 | 2:X:241:PRO:CD  | 2.41                     | 0.50              |
| 2:h:169:THR:HB  | 2:h:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:h:240:ALA:HB3 | 2:h:241:PRO:CD  | 2.41                     | 0.50              |
| 2:n:240:ALA:CB  | 2:n:241:PRO:CD  | 2.89                     | 0.50              |
| 2:p:240:ALA:CB  | 2:p:241:PRO:CD  | 2.89                     | 0.50              |
| 2:z:169:THR:HB  | 2:z:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:B:169:THR:HB  | 2:B:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:D:240:ALA:HB3 | 2:D:241:PRO:CD  | 2.41                     | 0.50              |
| 2:F:240:ALA:HB3 | 2:F:241:PRO:CD  | 2.41                     | 0.50              |
| 2:L:240:ALA:CB  | 2:L:241:PRO:CD  | 2.89                     | 0.50              |
| 2:Z:328:GLU:OE1 | 2:Z:328:GLU:N   | 2.38                     | 0.50              |
| 2:l:169:THR:HB  | 2:l:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:n:169:THR:HB  | 2:n:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:D:240:ALA:CB  | 2:D:241:PRO:CD  | 2.89                     | 0.50              |
| 2:H:169:THR:HB  | 2:H:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:R:240:ALA:HB3 | 2:R:241:PRO:CD  | 2.41                     | 0.50              |
| 2:Z:240:ALA:CB  | 2:Z:241:PRO:CD  | 2.89                     | 0.50              |
| 2:d:240:ALA:CB  | 2:d:241:PRO:CD  | 2.89                     | 0.50              |
| 2:l:328:GLU:OE1 | 2:l:328:GLU:N   | 2.38                     | 0.50              |
| 2:p:240:ALA:HB3 | 2:p:241:PRO:CD  | 2.41                     | 0.50              |
| 2:H:240:ALA:HB3 | 2:H:241:PRO:CD  | 2.41                     | 0.50              |
| 2:J:240:ALA:HB3 | 2:J:241:PRO:CD  | 2.41                     | 0.50              |
| 2:b:169:THR:HB  | 2:b:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:z:240:ALA:CB  | 2:z:241:PRO:CD  | 2.89                     | 0.50              |
| 2:2:169:THR:HB  | 2:2:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:4:240:ALA:CB  | 2:4:241:PRO:CD  | 2.89                     | 0.50              |
| 2:V:328:GLU:OE1 | 2:V:328:GLU:N   | 2.38                     | 0.50              |
| 2:r:240:ALA:HB3 | 2:r:241:PRO:CD  | 2.41                     | 0.50              |
| 2:J:169:THR:HB  | 2:J:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:N:240:ALA:HB3 | 2:N:241:PRO:CD  | 2.41                     | 0.50              |
| 2:X:240:ALA:CB  | 2:X:241:PRO:CD  | 2.89                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:j:169:THR:HB  | 2:j:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:p:328:GLU:OE1 | 2:p:328:GLU:N   | 2.38                     | 0.50              |
| 2:t:240:ALA:CB  | 2:t:241:PRO:CD  | 2.89                     | 0.50              |
| 2:R:240:ALA:CB  | 2:R:241:PRO:CD  | 2.89                     | 0.50              |
| 2:b:328:GLU:OE1 | 2:b:328:GLU:N   | 2.38                     | 0.50              |
| 2:x:169:THR:HB  | 2:x:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:8:240:ALA:CB  | 2:8:241:PRO:CD  | 2.89                     | 0.50              |
| 2:h:240:ALA:CB  | 2:h:241:PRO:CD  | 2.89                     | 0.50              |
| 2:j:240:ALA:HB3 | 2:j:241:PRO:CD  | 2.41                     | 0.50              |
| 2:l:240:ALA:CB  | 2:l:241:PRO:CD  | 2.89                     | 0.50              |
| 2:P:169:THR:HB  | 2:P:170:PRO:HD3 | 1.92                     | 0.50              |
| 2:T:240:ALA:CB  | 2:T:241:PRO:CD  | 2.89                     | 0.50              |
| 2:n:240:ALA:HB3 | 2:n:241:PRO:CD  | 2.41                     | 0.50              |
| 2:r:240:ALA:CB  | 2:r:241:PRO:CD  | 2.89                     | 0.50              |
| 2:x:240:ALA:HB3 | 2:x:241:PRO:CD  | 2.41                     | 0.50              |
| 2:F:240:ALA:CB  | 2:F:241:PRO:CD  | 2.89                     | 0.49              |
| 2:H:240:ALA:CB  | 2:H:241:PRO:CD  | 2.89                     | 0.49              |
| 2:J:240:ALA:CB  | 2:J:241:PRO:CD  | 2.89                     | 0.49              |
| 2:n:328:GLU:OE1 | 2:n:328:GLU:N   | 2.38                     | 0.49              |
| 2:x:328:GLU:OE1 | 2:x:328:GLU:N   | 2.38                     | 0.49              |
| 2:6:240:ALA:CB  | 2:6:241:PRO:CD  | 2.89                     | 0.49              |
| 2:f:240:ALA:CB  | 2:f:241:PRO:CD  | 2.89                     | 0.49              |
| 2:j:240:ALA:CB  | 2:j:241:PRO:CD  | 2.89                     | 0.49              |
| 2:p:169:THR:HB  | 2:p:170:PRO:HD3 | 1.92                     | 0.49              |
| 2:v:169:THR:HB  | 2:v:170:PRO:HD3 | 1.92                     | 0.49              |
| 2:z:328:GLU:OE1 | 2:z:328:GLU:N   | 2.38                     | 0.49              |
| 2:V:240:ALA:CB  | 2:V:241:PRO:CD  | 2.89                     | 0.49              |
| 2:x:240:ALA:CB  | 2:x:241:PRO:CD  | 2.89                     | 0.49              |
| 2:d:328:GLU:OE1 | 2:d:328:GLU:N   | 2.38                     | 0.49              |
| 2:v:240:ALA:CB  | 2:v:241:PRO:CD  | 2.89                     | 0.49              |
| 2:V:169:THR:HB  | 2:V:170:PRO:HD3 | 1.92                     | 0.49              |
| 1:O:126:LEU:O   | 1:O:126:LEU:CG  | 2.61                     | 0.49              |
| 2:v:328:GLU:OE1 | 2:v:328:GLU:N   | 2.38                     | 0.49              |
| 2:2:328:GLU:OE1 | 2:2:328:GLU:N   | 2.38                     | 0.49              |
| 2:H:328:GLU:OE1 | 2:H:328:GLU:N   | 2.38                     | 0.49              |
| 1:W:126:LEU:O   | 1:W:126:LEU:CG  | 2.61                     | 0.49              |
| 1:m:126:LEU:O   | 1:m:126:LEU:CG  | 2.61                     | 0.49              |
| 1:o:126:LEU:O   | 1:o:126:LEU:CG  | 2.61                     | 0.49              |
| 2:B:240:ALA:CB  | 2:B:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:N:240:ALA:CB  | 2:N:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:b:240:ALA:CB  | 2:b:241:PRO:HD3 | 2.43                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:n:240:ALA:CB  | 2:n:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:J:240:ALA:CB  | 2:J:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:L:240:ALA:CB  | 2:L:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:Z:240:ALA:CB  | 2:Z:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:j:240:ALA:CB  | 2:j:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:2:240:ALA:CB  | 2:2:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:V:240:ALA:CB  | 2:V:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:X:240:ALA:CB  | 2:X:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:x:240:ALA:CB  | 2:x:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:z:240:ALA:CB  | 2:z:241:PRO:HD3 | 2.43                     | 0.48              |
| 1:A:126:LEU:O   | 1:A:126:LEU:CG  | 2.61                     | 0.48              |
| 2:l:240:ALA:CB  | 2:l:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:v:240:ALA:CB  | 2:v:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:H:240:ALA:CB  | 2:H:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:P:240:ALA:CB  | 2:P:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:X:328:GLU:OE1 | 2:X:328:GLU:N   | 2.38                     | 0.48              |
| 2:Z:206:LEU:HB2 | 2:Z:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:L:206:LEU:HB2 | 2:L:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:n:206:LEU:HB2 | 2:n:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:z:206:LEU:HB2 | 2:z:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:X:206:LEU:HB2 | 2:X:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:h:240:ALA:CB  | 2:h:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:p:240:ALA:CB  | 2:p:241:PRO:HD3 | 2.43                     | 0.48              |
| 2:2:206:LEU:HB2 | 2:2:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:6:328:GLU:OE1 | 2:6:328:GLU:N   | 2.38                     | 0.48              |
| 2:N:206:LEU:HB2 | 2:N:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:l:206:LEU:HB2 | 2:l:207:PRO:HD3 | 1.96                     | 0.48              |
| 2:h:328:GLU:OE1 | 2:h:328:GLU:N   | 2.38                     | 0.47              |
| 2:t:240:ALA:CB  | 2:t:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:6:240:ALA:CB  | 2:6:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:8:240:ALA:CB  | 2:8:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:D:211:ASP:OD1 | 2:D:211:ASP:C   | 2.58                     | 0.47              |
| 2:D:240:ALA:CB  | 2:D:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:R:389:LEU:N   | 2:R:390:PRO:CD  | 2.77                     | 0.47              |
| 2:T:211:ASP:OD1 | 2:T:211:ASP:C   | 2.58                     | 0.47              |
| 2:b:206:LEU:HB2 | 2:b:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:r:389:LEU:N   | 2:r:390:PRO:CD  | 2.77                     | 0.47              |
| 2:D:389:LEU:N   | 2:D:390:PRO:CD  | 2.78                     | 0.47              |
| 2:T:240:ALA:CB  | 2:T:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:b:211:ASP:OD1 | 2:b:211:ASP:C   | 2.58                     | 0.47              |
| 2:d:389:LEU:N   | 2:d:390:PRO:CD  | 2.77                     | 0.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:f:240:ALA:CB  | 2:f:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:p:206:LEU:HB2 | 2:p:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:t:211:ASP:C   | 2:t:211:ASP:OD1 | 2.58                     | 0.47              |
| 2:6:389:LEU:N   | 2:6:390:PRO:CD  | 2.77                     | 0.47              |
| 2:B:206:LEU:HB2 | 2:B:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:B:211:ASP:OD1 | 2:B:211:ASP:C   | 2.58                     | 0.47              |
| 2:F:206:LEU:HB2 | 2:F:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:d:211:ASP:OD1 | 2:d:211:ASP:C   | 2.58                     | 0.47              |
| 2:d:240:ALA:CB  | 2:d:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:f:206:LEU:HB2 | 2:f:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:f:389:LEU:N   | 2:f:390:PRO:CD  | 2.78                     | 0.47              |
| 2:r:211:ASP:C   | 2:r:211:ASP:OD1 | 2.58                     | 0.47              |
| 2:2:211:ASP:C   | 2:2:211:ASP:OD1 | 2.58                     | 0.47              |
| 2:4:389:LEU:N   | 2:4:390:PRO:CD  | 2.77                     | 0.47              |
| 2:F:240:ALA:CB  | 2:F:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:F:389:LEU:N   | 2:F:390:PRO:CD  | 2.78                     | 0.47              |
| 2:J:206:LEU:HB2 | 2:J:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:R:211:ASP:C   | 2:R:211:ASP:OD1 | 2.58                     | 0.47              |
| 2:t:206:LEU:HB2 | 2:t:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:P:206:LEU:HB2 | 2:P:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:T:206:LEU:HB2 | 2:T:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:r:240:ALA:CB  | 2:r:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:4:240:ALA:CB  | 2:4:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:8:206:LEU:HB2 | 2:8:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:F:211:ASP:C   | 2:F:211:ASP:OD1 | 2.58                     | 0.47              |
| 2:J:389:LEU:N   | 2:J:390:PRO:CD  | 2.78                     | 0.47              |
| 2:L:389:LEU:N   | 2:L:390:PRO:CD  | 2.77                     | 0.47              |
| 2:N:328:GLU:OE1 | 2:N:328:GLU:N   | 2.38                     | 0.47              |
| 2:P:389:LEU:N   | 2:P:390:PRO:CD  | 2.78                     | 0.47              |
| 2:R:206:LEU:HB2 | 2:R:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:R:240:ALA:CB  | 2:R:241:PRO:HD3 | 2.43                     | 0.47              |
| 2:T:389:LEU:N   | 2:T:390:PRO:CD  | 2.77                     | 0.47              |
| 2:V:211:ASP:OD1 | 2:V:211:ASP:C   | 2.58                     | 0.47              |
| 2:Z:389:LEU:N   | 2:Z:390:PRO:CD  | 2.77                     | 0.47              |
| 2:j:206:LEU:HB2 | 2:j:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:j:389:LEU:N   | 2:j:390:PRO:CD  | 2.77                     | 0.47              |
| 2:p:389:LEU:N   | 2:p:390:PRO:CD  | 2.78                     | 0.47              |
| 2:t:389:LEU:N   | 2:t:390:PRO:CD  | 2.78                     | 0.47              |
| 2:x:389:LEU:N   | 2:x:390:PRO:CD  | 2.78                     | 0.47              |
| 2:4:206:LEU:HB2 | 2:4:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:4:211:ASP:OD1 | 2:4:211:ASP:C   | 2.58                     | 0.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:6:206:LEU:HB2 | 2:6:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:6:211:ASP:OD1 | 2:6:211:ASP:C   | 2.58                     | 0.47              |
| 2:z:389:LEU:N   | 2:z:390:PRO:CD  | 2.77                     | 0.47              |
| 2:h:206:LEU:HB2 | 2:h:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:v:211:ASP:OD1 | 2:v:211:ASP:C   | 2.58                     | 0.47              |
| 2:d:206:LEU:HB2 | 2:d:207:PRO:HD3 | 1.96                     | 0.47              |
| 2:B:389:LEU:N   | 2:B:390:PRO:CD  | 2.78                     | 0.46              |
| 2:H:206:LEU:HB2 | 2:H:207:PRO:HD3 | 1.96                     | 0.46              |
| 2:N:211:ASP:OD1 | 2:N:211:ASP:C   | 2.58                     | 0.46              |
| 2:b:389:LEU:N   | 2:b:390:PRO:CD  | 2.78                     | 0.46              |
| 2:f:211:ASP:C   | 2:f:211:ASP:OD1 | 2.58                     | 0.46              |
| 2:h:211:ASP:C   | 2:h:211:ASP:OD1 | 2.58                     | 0.46              |
| 2:8:328:GLU:OE1 | 2:8:328:GLU:N   | 2.38                     | 0.46              |
| 2:8:389:LEU:N   | 2:8:390:PRO:CD  | 2.77                     | 0.46              |
| 2:D:206:LEU:HB2 | 2:D:207:PRO:HD3 | 1.96                     | 0.46              |
| 2:X:211:ASP:OD1 | 2:X:211:ASP:C   | 2.58                     | 0.46              |
| 2:h:389:LEU:N   | 2:h:390:PRO:CD  | 2.77                     | 0.46              |
| 2:r:206:LEU:HB2 | 2:r:207:PRO:HD3 | 1.96                     | 0.46              |
| 2:x:206:LEU:HB2 | 2:x:207:PRO:HD3 | 1.96                     | 0.46              |
| 2:2:389:LEU:N   | 2:2:390:PRO:CD  | 2.78                     | 0.46              |
| 2:H:389:LEU:N   | 2:H:390:PRO:CD  | 2.77                     | 0.46              |
| 1:1:112:GLU:OE1 | 1:1:112:GLU:N   | 2.39                     | 0.46              |
| 1:a:112:GLU:OE1 | 1:a:112:GLU:N   | 2.39                     | 0.46              |
| 2:P:211:ASP:C   | 2:P:211:ASP:OD1 | 2.58                     | 0.46              |
| 2:T:284:ARG:HA  | 2:T:284:ARG:NE  | 2.31                     | 0.46              |
| 1:A:112:GLU:OE1 | 1:A:112:GLU:N   | 2.39                     | 0.46              |
| 2:N:389:LEU:N   | 2:N:390:PRO:CD  | 2.77                     | 0.46              |
| 2:b:284:ARG:HA  | 2:b:284:ARG:NE  | 2.31                     | 0.46              |
| 2:l:211:ASP:OD1 | 2:l:211:ASP:C   | 2.58                     | 0.46              |
| 2:n:211:ASP:OD1 | 2:n:211:ASP:C   | 2.58                     | 0.46              |
| 2:n:389:LEU:N   | 2:n:390:PRO:CD  | 2.77                     | 0.46              |
| 2:t:284:ARG:HA  | 2:t:284:ARG:NE  | 2.31                     | 0.46              |
| 2:v:389:LEU:N   | 2:v:390:PRO:CD  | 2.77                     | 0.46              |
| 2:x:211:ASP:OD1 | 2:x:211:ASP:C   | 2.58                     | 0.46              |
| 2:D:284:ARG:NE  | 2:D:284:ARG:HA  | 2.31                     | 0.46              |
| 2:H:211:ASP:C   | 2:H:211:ASP:OD1 | 2.58                     | 0.46              |
| 2:H:284:ARG:HA  | 2:H:284:ARG:NE  | 2.31                     | 0.46              |
| 2:L:284:ARG:HA  | 2:L:284:ARG:NE  | 2.31                     | 0.46              |
| 1:Q:112:GLU:OE1 | 1:Q:112:GLU:N   | 2.39                     | 0.46              |
| 2:V:389:LEU:N   | 2:V:390:PRO:CD  | 2.77                     | 0.46              |
| 2:X:284:ARG:NE  | 2:X:284:ARG:HA  | 2.31                     | 0.46              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:h:284:ARG:HA  | 2:h:284:ARG:NE  | 2.31                     | 0.46              |
| 2:p:211:ASP:OD1 | 2:p:211:ASP:C   | 2.58                     | 0.46              |
| 1:q:112:GLU:OE1 | 1:q:112:GLU:N   | 2.39                     | 0.46              |
| 2:v:206:LEU:HB2 | 2:v:207:PRO:HD3 | 1.96                     | 0.46              |
| 2:2:284:ARG:HA  | 2:2:284:ARG:NE  | 2.31                     | 0.46              |
| 2:6:284:ARG:HA  | 2:6:284:ARG:NE  | 2.31                     | 0.46              |
| 2:J:284:ARG:HA  | 2:J:284:ARG:NE  | 2.31                     | 0.46              |
| 2:T:328:GLU:OE1 | 2:T:328:GLU:N   | 2.38                     | 0.46              |
| 2:V:284:ARG:HA  | 2:V:284:ARG:NE  | 2.31                     | 0.46              |
| 2:j:284:ARG:HA  | 2:j:284:ARG:NE  | 2.31                     | 0.46              |
| 2:v:284:ARG:HA  | 2:v:284:ARG:NE  | 2.31                     | 0.46              |
| 2:B:284:ARG:NE  | 2:B:284:ARG:HA  | 2.31                     | 0.46              |
| 2:Z:284:ARG:NE  | 2:Z:284:ARG:HA  | 2.31                     | 0.46              |
| 2:l:389:LEU:N   | 2:l:390:PRO:CD  | 2.77                     | 0.46              |
| 2:r:284:ARG:HA  | 2:r:284:ARG:NE  | 2.31                     | 0.46              |
| 2:8:284:ARG:NE  | 2:8:284:ARG:HA  | 2.31                     | 0.46              |
| 2:N:284:ARG:NE  | 2:N:284:ARG:HA  | 2.31                     | 0.46              |
| 2:V:206:LEU:HB2 | 2:V:207:PRO:HD3 | 1.96                     | 0.46              |
| 2:d:284:ARG:NE  | 2:d:284:ARG:HA  | 2.31                     | 0.46              |
| 2:l:284:ARG:HA  | 2:l:284:ARG:NE  | 2.31                     | 0.46              |
| 2:R:284:ARG:HA  | 2:R:284:ARG:NE  | 2.31                     | 0.45              |
| 2:X:389:LEU:N   | 2:X:390:PRO:CD  | 2.77                     | 0.45              |
| 2:j:211:ASP:OD1 | 2:j:211:ASP:C   | 2.58                     | 0.45              |
| 2:x:284:ARG:HA  | 2:x:284:ARG:NE  | 2.31                     | 0.45              |
| 2:z:211:ASP:OD1 | 2:z:211:ASP:C   | 2.58                     | 0.45              |
| 1:o:112:GLU:OE1 | 1:o:112:GLU:N   | 2.39                     | 0.45              |
| 1:3:112:GLU:OE1 | 1:3:112:GLU:N   | 2.39                     | 0.45              |
| 1:C:112:GLU:OE1 | 1:C:112:GLU:N   | 2.39                     | 0.45              |
| 1:O:112:GLU:OE1 | 1:O:112:GLU:N   | 2.39                     | 0.45              |
| 1:c:112:GLU:OE1 | 1:c:112:GLU:N   | 2.39                     | 0.45              |
| 2:4:284:ARG:HA  | 2:4:284:ARG:NE  | 2.31                     | 0.45              |
| 2:n:284:ARG:NE  | 2:n:284:ARG:HA  | 2.31                     | 0.45              |
| 2:p:284:ARG:NE  | 2:p:284:ARG:HA  | 2.31                     | 0.45              |
| 2:z:284:ARG:NE  | 2:z:284:ARG:HA  | 2.31                     | 0.45              |
| 2:J:211:ASP:OD1 | 2:J:211:ASP:C   | 2.58                     | 0.45              |
| 1:S:126:LEU:O   | 1:S:126:LEU:CG  | 2.61                     | 0.45              |
| 2:F:284:ARG:HA  | 2:F:284:ARG:NE  | 2.31                     | 0.45              |
| 2:Z:211:ASP:C   | 2:Z:211:ASP:OD1 | 2.58                     | 0.45              |
| 2:t:328:GLU:OE1 | 2:t:328:GLU:N   | 2.38                     | 0.44              |
| 2:L:211:ASP:OD1 | 2:L:211:ASP:C   | 2.58                     | 0.44              |
| 2:P:284:ARG:HA  | 2:P:284:ARG:NE  | 2.31                     | 0.44              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:s:126:LEU:O   | 1:s:126:LEU:CG | 2.61                     | 0.44              |
| 2:f:284:ARG:NE  | 2:f:284:ARG:HA | 2.31                     | 0.44              |
| 2:8:211:ASP:OD1 | 2:8:211:ASP:C  | 2.58                     | 0.44              |
| 2:P:328:GLU:OE1 | 2:P:328:GLU:N  | 2.38                     | 0.44              |
| 2:F:328:GLU:OE1 | 2:F:328:GLU:N  | 2.38                     | 0.44              |
| 2:P:284:ARG:HA  | 2:P:284:ARG:CZ | 2.48                     | 0.44              |
| 2:p:284:ARG:HA  | 2:p:284:ARG:CZ | 2.48                     | 0.43              |
| 2:n:284:ARG:HA  | 2:n:284:ARG:CZ | 2.48                     | 0.43              |
| 2:N:284:ARG:HA  | 2:N:284:ARG:CZ | 2.48                     | 0.43              |
| 2:R:284:ARG:HA  | 2:R:284:ARG:CZ | 2.48                     | 0.43              |
| 2:r:284:ARG:HA  | 2:r:284:ARG:CZ | 2.49                     | 0.43              |
| 1:w:126:LEU:O   | 1:w:126:LEU:CG | 2.61                     | 0.43              |
| 2:4:284:ARG:HA  | 2:4:284:ARG:CZ | 2.49                     | 0.43              |
| 1:G:126:LEU:O   | 1:G:126:LEU:CG | 2.61                     | 0.43              |
| 2:d:284:ARG:HA  | 2:d:284:ARG:CZ | 2.49                     | 0.43              |
| 2:6:284:ARG:HA  | 2:6:284:ARG:CZ | 2.49                     | 0.43              |
| 2:D:284:ARG:HA  | 2:D:284:ARG:CZ | 2.48                     | 0.43              |
| 2:F:284:ARG:HA  | 2:F:284:ARG:CZ | 2.48                     | 0.43              |
| 2:f:284:ARG:HA  | 2:f:284:ARG:CZ | 2.49                     | 0.43              |
| 2:B:284:ARG:HA  | 2:B:284:ARG:CZ | 2.48                     | 0.43              |
| 2:J:328:GLU:OE1 | 2:J:328:GLU:N  | 2.38                     | 0.43              |
| 2:T:284:ARG:HA  | 2:T:284:ARG:CZ | 2.48                     | 0.43              |
| 2:2:284:ARG:HA  | 2:2:284:ARG:CZ | 2.49                     | 0.43              |
| 2:L:284:ARG:HA  | 2:L:284:ARG:CZ | 2.48                     | 0.43              |
| 2:b:284:ARG:HA  | 2:b:284:ARG:CZ | 2.48                     | 0.43              |
| 2:t:284:ARG:HA  | 2:t:284:ARG:CZ | 2.48                     | 0.43              |
| 2:X:284:ARG:HA  | 2:X:284:ARG:CZ | 2.48                     | 0.42              |
| 2:f:328:GLU:OE1 | 2:f:328:GLU:N  | 2.38                     | 0.42              |
| 2:l:284:ARG:HA  | 2:l:284:ARG:CZ | 2.48                     | 0.42              |
| 2:D:328:GLU:OE1 | 2:D:328:GLU:N  | 2.38                     | 0.42              |
| 2:Z:284:ARG:HA  | 2:Z:284:ARG:CZ | 2.48                     | 0.42              |
| 1:g:126:LEU:O   | 1:g:126:LEU:CG | 2.61                     | 0.42              |
| 2:v:284:ARG:HA  | 2:v:284:ARG:CZ | 2.48                     | 0.42              |
| 2:V:284:ARG:HA  | 2:V:284:ARG:CZ | 2.48                     | 0.42              |
| 2:8:284:ARG:HA  | 2:8:284:ARG:CZ | 2.49                     | 0.42              |
| 2:H:284:ARG:HA  | 2:H:284:ARG:CZ | 2.48                     | 0.42              |
| 2:h:284:ARG:HA  | 2:h:284:ARG:CZ | 2.49                     | 0.42              |
| 2:J:284:ARG:HA  | 2:J:284:ARG:CZ | 2.49                     | 0.42              |
| 2:R:328:GLU:OE1 | 2:R:328:GLU:N  | 2.38                     | 0.42              |
| 2:j:284:ARG:HA  | 2:j:284:ARG:CZ | 2.48                     | 0.42              |
| 2:z:284:ARG:HA  | 2:z:284:ARG:CZ | 2.49                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:x:284:ARG:HA  | 2:x:284:ARG:CZ  | 2.48                     | 0.42              |
| 2:D:206:LEU:N   | 2:D:207:PRO:CD  | 2.83                     | 0.41              |
| 2:2:250:ASP:HA  | 2:2:251:PRO:HD3 | 1.95                     | 0.41              |
| 2:4:206:LEU:N   | 2:4:207:PRO:CD  | 2.83                     | 0.41              |
| 2:J:206:LEU:N   | 2:J:207:PRO:CD  | 2.83                     | 0.41              |
| 2:R:206:LEU:N   | 2:R:207:PRO:CD  | 2.83                     | 0.41              |
| 2:6:206:LEU:N   | 2:6:207:PRO:CD  | 2.83                     | 0.41              |
| 2:B:206:LEU:N   | 2:B:207:PRO:CD  | 2.83                     | 0.41              |
| 2:F:206:LEU:N   | 2:F:207:PRO:CD  | 2.83                     | 0.41              |
| 2:P:206:LEU:N   | 2:P:207:PRO:CD  | 2.83                     | 0.41              |
| 2:d:206:LEU:N   | 2:d:207:PRO:CD  | 2.83                     | 0.41              |
| 2:f:206:LEU:N   | 2:f:207:PRO:CD  | 2.83                     | 0.41              |
| 2:r:206:LEU:N   | 2:r:207:PRO:CD  | 2.83                     | 0.41              |
| 2:t:206:LEU:N   | 2:t:207:PRO:CD  | 2.83                     | 0.41              |
| 1:3:102:ALA:HA  | 1:3:103:PRO:HD3 | 1.92                     | 0.41              |
| 2:8:206:LEU:N   | 2:8:207:PRO:CD  | 2.83                     | 0.41              |
| 2:L:206:LEU:N   | 2:L:207:PRO:CD  | 2.83                     | 0.41              |
| 1:7:126:LEU:O   | 1:7:126:LEU:CG  | 2.61                     | 0.41              |
| 2:T:206:LEU:N   | 2:T:207:PRO:CD  | 2.83                     | 0.41              |
| 2:X:206:LEU:N   | 2:X:207:PRO:CD  | 2.83                     | 0.41              |
| 2:j:206:LEU:N   | 2:j:207:PRO:CD  | 2.83                     | 0.41              |
| 1:u:102:ALA:HA  | 1:u:103:PRO:HD3 | 1.92                     | 0.41              |
| 2:B:328:GLU:OE1 | 2:B:328:GLU:N   | 2.38                     | 0.41              |
| 2:N:206:LEU:N   | 2:N:207:PRO:CD  | 2.83                     | 0.41              |
| 2:V:206:LEU:N   | 2:V:207:PRO:CD  | 2.83                     | 0.41              |
| 2:p:206:LEU:N   | 2:p:207:PRO:CD  | 2.83                     | 0.41              |
| 2:z:295:CYS:N   | 2:z:296:PRO:CD  | 2.84                     | 0.41              |
| 2:2:206:LEU:N   | 2:2:207:PRO:CD  | 2.83                     | 0.41              |
| 2:Z:206:LEU:N   | 2:Z:207:PRO:CD  | 2.83                     | 0.41              |
| 2:b:206:LEU:N   | 2:b:207:PRO:CD  | 2.83                     | 0.41              |
| 2:h:206:LEU:N   | 2:h:207:PRO:CD  | 2.83                     | 0.41              |
| 2:n:295:CYS:N   | 2:n:296:PRO:CD  | 2.84                     | 0.41              |
| 2:r:328:GLU:OE1 | 2:r:328:GLU:N   | 2.38                     | 0.41              |
| 2:2:295:CYS:N   | 2:2:296:PRO:CD  | 2.84                     | 0.41              |
| 1:a:102:ALA:HA  | 1:a:103:PRO:HD3 | 1.92                     | 0.41              |
| 2:j:250:ASP:HA  | 2:j:251:PRO:HD3 | 1.95                     | 0.41              |
| 1:k:126:LEU:O   | 1:k:126:LEU:CG  | 2.61                     | 0.41              |
| 2:l:206:LEU:N   | 2:l:207:PRO:CD  | 2.83                     | 0.41              |
| 2:l:295:CYS:N   | 2:l:296:PRO:CD  | 2.84                     | 0.41              |
| 2:n:206:LEU:N   | 2:n:207:PRO:CD  | 2.83                     | 0.41              |
| 2:v:206:LEU:N   | 2:v:207:PRO:CD  | 2.83                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:x:206:LEU:N   | 2:x:207:PRO:CD  | 2.83                     | 0.41              |
| 2:z:206:LEU:N   | 2:z:207:PRO:CD  | 2.83                     | 0.41              |
| 1:E:61:ASN:OD1  | 1:E:61:ASN:C    | 2.64                     | 0.41              |
| 2:H:206:LEU:N   | 2:H:207:PRO:CD  | 2.83                     | 0.41              |
| 2:H:250:ASP:HA  | 2:H:251:PRO:HD3 | 1.95                     | 0.41              |
| 2:J:310:LEU:HA  | 2:J:311:PRO:HD3 | 1.94                     | 0.41              |
| 2:N:295:CYS:N   | 2:N:296:PRO:CD  | 2.84                     | 0.41              |
| 1:O:61:ASN:OD1  | 1:O:61:ASN:C    | 2.64                     | 0.41              |
| 2:Z:295:CYS:N   | 2:Z:296:PRO:CD  | 2.84                     | 0.41              |
| 2:b:295:CYS:N   | 2:b:296:PRO:CD  | 2.84                     | 0.41              |
| 1:c:126:LEU:O   | 1:c:126:LEU:CG  | 2.61                     | 0.41              |
| 2:d:377:LYS:HA  | 2:d:377:LYS:HD2 | 1.96                     | 0.41              |
| 2:p:295:CYS:N   | 2:p:296:PRO:CD  | 2.84                     | 0.41              |
| 2:v:377:LYS:HA  | 2:v:377:LYS:HD2 | 1.96                     | 0.41              |
| 2:x:295:CYS:N   | 2:x:296:PRO:CD  | 2.84                     | 0.41              |
| 1:1:61:ASN:OD1  | 1:1:61:ASN:C    | 2.64                     | 0.41              |
| 2:F:295:CYS:N   | 2:F:296:PRO:CD  | 2.84                     | 0.41              |
| 2:L:328:GLU:OE1 | 2:L:328:GLU:N   | 2.38                     | 0.41              |
| 2:T:295:CYS:N   | 2:T:296:PRO:CD  | 2.84                     | 0.41              |
| 1:a:61:ASN:OD1  | 1:a:61:ASN:C    | 2.64                     | 0.41              |
| 1:e:61:ASN:OD1  | 1:e:61:ASN:C    | 2.64                     | 0.41              |
| 2:f:295:CYS:N   | 2:f:296:PRO:CD  | 2.84                     | 0.41              |
| 2:B:295:CYS:N   | 2:B:296:PRO:CD  | 2.84                     | 0.40              |
| 2:J:206:LEU:N   | 2:J:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:V:250:ASP:HA  | 2:V:251:PRO:HD3 | 1.95                     | 0.40              |
| 2:X:295:CYS:N   | 2:X:296:PRO:CD  | 2.84                     | 0.40              |
| 2:j:206:LEU:N   | 2:j:207:PRO:HD2 | 2.36                     | 0.40              |
| 2:j:295:CYS:N   | 2:j:296:PRO:CD  | 2.84                     | 0.40              |
| 1:u:61:ASN:OD1  | 1:u:61:ASN:C    | 2.64                     | 0.40              |
| 1:5:61:ASN:OD1  | 1:5:61:ASN:C    | 2.64                     | 0.40              |
| 2:6:295:CYS:N   | 2:6:296:PRO:CD  | 2.84                     | 0.40              |
| 1:A:61:ASN:OD1  | 1:A:61:ASN:C    | 2.64                     | 0.40              |
| 1:A:89:LEU:HA   | 1:A:90:PRO:HD2  | 2.00                     | 0.40              |
| 2:B:284:ARG:NE  | 2:B:284:ARG:CA  | 2.84                     | 0.40              |
| 2:J:300:GLY:HA2 | 2:J:301:PRO:HD3 | 1.92                     | 0.40              |
| 1:K:102:ALA:HA  | 1:K:103:PRO:HD3 | 1.92                     | 0.40              |
| 2:L:295:CYS:N   | 2:L:296:PRO:CD  | 2.84                     | 0.40              |
| 2:T:206:LEU:N   | 2:T:207:PRO:HD2 | 2.36                     | 0.40              |
| 2:V:206:LEU:N   | 2:V:207:PRO:HD2 | 2.36                     | 0.40              |
| 2:X:206:LEU:N   | 2:X:207:PRO:HD2 | 2.37                     | 0.40              |
| 1:o:61:ASN:OD1  | 1:o:61:ASN:C    | 2.64                     | 0.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:q:61:ASN:OD1 | 1:q:61:ASN:C    | 2.64                     | 0.40              |
| 2:r:295:CYS:N  | 2:r:296:PRO:CD  | 2.84                     | 0.40              |
| 2:t:206:LEU:N  | 2:t:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:t:295:CYS:N  | 2:t:296:PRO:CD  | 2.84                     | 0.40              |
| 2:x:206:LEU:N  | 2:x:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:D:284:ARG:NE | 2:D:284:ARG:CA  | 2.84                     | 0.40              |
| 2:H:284:ARG:NE | 2:H:284:ARG:CA  | 2.84                     | 0.40              |
| 2:H:295:CYS:N  | 2:H:296:PRO:CD  | 2.84                     | 0.40              |
| 1:I:61:ASN:OD1 | 1:I:61:ASN:C    | 2.64                     | 0.40              |
| 2:L:206:LEU:N  | 2:L:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:P:284:ARG:NE | 2:P:284:ARG:CA  | 2.84                     | 0.40              |
| 2:P:295:CYS:N  | 2:P:296:PRO:CD  | 2.84                     | 0.40              |
| 2:R:295:CYS:N  | 2:R:296:PRO:CD  | 2.84                     | 0.40              |
| 2:Z:284:ARG:NE | 2:Z:284:ARG:CA  | 2.84                     | 0.40              |
| 2:b:284:ARG:NE | 2:b:284:ARG:CA  | 2.84                     | 0.40              |
| 2:l:206:LEU:N  | 2:l:207:PRO:HD2 | 2.37                     | 0.40              |
| 1:m:89:LEU:HA  | 1:m:90:PRO:HD2  | 2.00                     | 0.40              |
| 2:x:250:ASP:HA | 2:x:251:PRO:HD3 | 1.95                     | 0.40              |
| 1:y:61:ASN:C   | 1:y:61:ASN:OD1  | 2.64                     | 0.40              |
| 1:G:61:ASN:C   | 1:G:61:ASN:OD1  | 2.64                     | 0.40              |
| 2:H:206:LEU:N  | 2:H:207:PRO:HD2 | 2.36                     | 0.40              |
| 1:Q:126:LEU:O  | 1:Q:126:LEU:CG  | 2.61                     | 0.40              |
| 2:R:206:LEU:N  | 2:R:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:R:284:ARG:NE | 2:R:284:ARG:CA  | 2.84                     | 0.40              |
| 2:T:377:LYS:HA | 2:T:377:LYS:HD2 | 1.96                     | 0.40              |
| 1:U:61:ASN:OD1 | 1:U:61:ASN:C    | 2.64                     | 0.40              |
| 2:h:284:ARG:NE | 2:h:284:ARG:CA  | 2.84                     | 0.40              |
| 2:h:295:CYS:N  | 2:h:296:PRO:CD  | 2.84                     | 0.40              |
| 2:p:284:ARG:NE | 2:p:284:ARG:CA  | 2.84                     | 0.40              |
| 2:v:206:LEU:N  | 2:v:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:v:295:CYS:N  | 2:v:296:PRO:CD  | 2.84                     | 0.40              |
| 2:x:284:ARG:NE | 2:x:284:ARG:CA  | 2.84                     | 0.40              |
| 2:4:295:CYS:N  | 2:4:296:PRO:CD  | 2.84                     | 0.40              |
| 1:7:61:ASN:OD1 | 1:7:61:ASN:C    | 2.64                     | 0.40              |
| 2:N:284:ARG:NE | 2:N:284:ARG:CA  | 2.84                     | 0.40              |
| 1:Q:61:ASN:OD1 | 1:Q:61:ASN:C    | 2.64                     | 0.40              |
| 1:S:102:ALA:HA | 1:S:103:PRO:HD3 | 1.93                     | 0.40              |
| 2:Z:206:LEU:N  | 2:Z:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:d:284:ARG:NE | 2:d:284:ARG:CA  | 2.84                     | 0.40              |
| 2:h:206:LEU:N  | 2:h:207:PRO:HD2 | 2.37                     | 0.40              |
| 2:j:284:ARG:NE | 2:j:284:ARG:CA  | 2.84                     | 0.40              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 2:r:206:LEU:N | 2:r:207:PRO:HD2 | 2.37                     | 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   | 1     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | 3     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | 5     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | 7     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | A     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | C     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | E     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | G     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | I     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | K     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | M     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | O     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | Q     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | S     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | U     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | W     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | Y     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | a     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | c     | 123/125 (98%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | e     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | g     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | i     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | k     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | m     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | o     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | q     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | s     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | u     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | w     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | y     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 2   | 2     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | 4     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | 6     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | 8     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | B     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | D     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | F     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | H     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | J     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | L     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | N     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | P     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | R     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | T     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | V     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | X     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | Z     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | b     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | d     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |
| 2   | f     | 430/432 (100%) | 409 (95%) | 17 (4%) | 4 (1%)   | 14          | 47  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|----------|-------------|----|
| 2   | h     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | j     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | l     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | n     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | p     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | r     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | t     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | v     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | x     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 2   | z     | 430/432 (100%)    | 409 (95%)   | 17 (4%)  | 4 (1%)   | 14          | 47 |
| All | All   | 16590/16710 (99%) | 15870 (96%) | 600 (4%) | 120 (1%) | 20          | 51 |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 240 | ALA  |
| 2   | D     | 240 | ALA  |
| 2   | F     | 240 | ALA  |
| 2   | H     | 240 | ALA  |
| 2   | J     | 240 | ALA  |
| 2   | L     | 240 | ALA  |
| 2   | N     | 240 | ALA  |
| 2   | P     | 240 | ALA  |
| 2   | R     | 240 | ALA  |
| 2   | T     | 240 | ALA  |
| 2   | V     | 240 | ALA  |
| 2   | X     | 240 | ALA  |
| 2   | Z     | 240 | ALA  |
| 2   | b     | 240 | ALA  |
| 2   | d     | 240 | ALA  |
| 2   | f     | 240 | ALA  |
| 2   | h     | 240 | ALA  |
| 2   | j     | 240 | ALA  |
| 2   | l     | 240 | ALA  |
| 2   | n     | 240 | ALA  |
| 2   | p     | 240 | ALA  |
| 2   | r     | 240 | ALA  |
| 2   | t     | 240 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | v     | 240 | ALA  |
| 2   | x     | 240 | ALA  |
| 2   | z     | 240 | ALA  |
| 2   | 2     | 240 | ALA  |
| 2   | 4     | 240 | ALA  |
| 2   | 6     | 240 | ALA  |
| 2   | 8     | 240 | ALA  |
| 2   | H     | 258 | SER  |
| 2   | L     | 258 | SER  |
| 2   | X     | 258 | SER  |
| 2   | d     | 258 | SER  |
| 2   | v     | 258 | SER  |
| 2   | z     | 258 | SER  |
| 2   | 8     | 258 | SER  |
| 2   | B     | 258 | SER  |
| 2   | B     | 296 | PRO  |
| 2   | D     | 258 | SER  |
| 2   | D     | 296 | PRO  |
| 2   | F     | 258 | SER  |
| 2   | F     | 296 | PRO  |
| 2   | H     | 296 | PRO  |
| 2   | J     | 258 | SER  |
| 2   | J     | 296 | PRO  |
| 2   | L     | 296 | PRO  |
| 2   | N     | 258 | SER  |
| 2   | N     | 296 | PRO  |
| 2   | P     | 258 | SER  |
| 2   | P     | 296 | PRO  |
| 2   | R     | 258 | SER  |
| 2   | R     | 296 | PRO  |
| 2   | T     | 258 | SER  |
| 2   | T     | 296 | PRO  |
| 2   | V     | 258 | SER  |
| 2   | V     | 296 | PRO  |
| 2   | X     | 296 | PRO  |
| 2   | Z     | 258 | SER  |
| 2   | Z     | 296 | PRO  |
| 2   | b     | 258 | SER  |
| 2   | b     | 296 | PRO  |
| 2   | d     | 296 | PRO  |
| 2   | f     | 258 | SER  |
| 2   | f     | 296 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | h     | 258 | SER  |
| 2   | h     | 296 | PRO  |
| 2   | j     | 258 | SER  |
| 2   | j     | 296 | PRO  |
| 2   | l     | 258 | SER  |
| 2   | l     | 296 | PRO  |
| 2   | n     | 258 | SER  |
| 2   | n     | 296 | PRO  |
| 2   | p     | 258 | SER  |
| 2   | p     | 296 | PRO  |
| 2   | r     | 258 | SER  |
| 2   | r     | 296 | PRO  |
| 2   | t     | 258 | SER  |
| 2   | t     | 296 | PRO  |
| 2   | v     | 296 | PRO  |
| 2   | x     | 258 | SER  |
| 2   | x     | 296 | PRO  |
| 2   | z     | 296 | PRO  |
| 2   | 2     | 258 | SER  |
| 2   | 2     | 296 | PRO  |
| 2   | 4     | 258 | SER  |
| 2   | 4     | 296 | PRO  |
| 2   | 6     | 258 | SER  |
| 2   | 6     | 296 | PRO  |
| 2   | 8     | 296 | PRO  |
| 2   | B     | 309 | ASP  |
| 2   | D     | 309 | ASP  |
| 2   | F     | 309 | ASP  |
| 2   | H     | 309 | ASP  |
| 2   | J     | 309 | ASP  |
| 2   | L     | 309 | ASP  |
| 2   | N     | 309 | ASP  |
| 2   | P     | 309 | ASP  |
| 2   | R     | 309 | ASP  |
| 2   | T     | 309 | ASP  |
| 2   | V     | 309 | ASP  |
| 2   | X     | 309 | ASP  |
| 2   | Z     | 309 | ASP  |
| 2   | b     | 309 | ASP  |
| 2   | d     | 309 | ASP  |
| 2   | f     | 309 | ASP  |
| 2   | h     | 309 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | j     | 309 | ASP  |
| 2   | l     | 309 | ASP  |
| 2   | n     | 309 | ASP  |
| 2   | p     | 309 | ASP  |
| 2   | r     | 309 | ASP  |
| 2   | t     | 309 | ASP  |
| 2   | v     | 309 | ASP  |
| 2   | x     | 309 | ASP  |
| 2   | z     | 309 | ASP  |
| 2   | 2     | 309 | ASP  |
| 2   | 4     | 309 | ASP  |
| 2   | 6     | 309 | ASP  |
| 2   | 8     | 309 | ASP  |

### 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   | 1     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | 3     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | 5     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | 7     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | A     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | C     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | E     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | G     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | I     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | K     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | M     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | O     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | Q     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | S     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | U     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | W     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | Y     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | a     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | c     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | e     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | g     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | i     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | k     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | m     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | o     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | q     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | s     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | u     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | w     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 1   | y     | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 2   | 2     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | 4     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | 6     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | 8     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | B     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | D     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | F     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | H     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | J     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | L     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | N     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | P     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | R     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | T     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |
| 2   | V     | 369/369 (100%) | 369 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed           | Rotameric    | Outliers | Percentiles |     |
|-----|-------|--------------------|--------------|----------|-------------|-----|
| 2   | X     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | Z     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | b     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | d     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | f     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | h     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | j     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | l     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | n     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | p     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | r     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | t     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | v     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | x     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| 2   | z     | 369/369 (100%)     | 369 (100%)   | 0        | 100         | 100 |
| All | All   | 14250/14250 (100%) | 14250 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 136 | GLN  |
| 2   | B     | 388 | GLN  |
| 2   | B     | 465 | GLN  |
| 2   | D     | 136 | GLN  |
| 2   | D     | 186 | HIS  |
| 2   | D     | 388 | GLN  |
| 2   | D     | 465 | GLN  |
| 2   | F     | 136 | GLN  |
| 2   | F     | 186 | HIS  |
| 2   | F     | 388 | GLN  |
| 2   | F     | 465 | GLN  |
| 2   | H     | 136 | GLN  |
| 2   | H     | 186 | HIS  |
| 2   | H     | 388 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 465 | GLN  |
| 2   | J     | 136 | GLN  |
| 2   | J     | 388 | GLN  |
| 2   | J     | 465 | GLN  |
| 2   | L     | 136 | GLN  |
| 2   | L     | 388 | GLN  |
| 2   | L     | 465 | GLN  |
| 2   | N     | 136 | GLN  |
| 2   | N     | 388 | GLN  |
| 2   | N     | 465 | GLN  |
| 2   | P     | 136 | GLN  |
| 2   | P     | 186 | HIS  |
| 2   | P     | 388 | GLN  |
| 2   | P     | 465 | GLN  |
| 2   | R     | 136 | GLN  |
| 2   | R     | 388 | GLN  |
| 2   | R     | 465 | GLN  |
| 2   | T     | 136 | GLN  |
| 2   | T     | 186 | HIS  |
| 2   | T     | 388 | GLN  |
| 2   | T     | 465 | GLN  |
| 2   | V     | 136 | GLN  |
| 2   | V     | 186 | HIS  |
| 2   | V     | 388 | GLN  |
| 2   | V     | 465 | GLN  |
| 2   | X     | 136 | GLN  |
| 2   | X     | 388 | GLN  |
| 2   | X     | 465 | GLN  |
| 2   | Z     | 136 | GLN  |
| 2   | Z     | 388 | GLN  |
| 2   | Z     | 465 | GLN  |
| 2   | b     | 136 | GLN  |
| 2   | b     | 186 | HIS  |
| 2   | b     | 388 | GLN  |
| 2   | b     | 465 | GLN  |
| 2   | d     | 136 | GLN  |
| 2   | d     | 186 | HIS  |
| 2   | d     | 388 | GLN  |
| 2   | d     | 465 | GLN  |
| 2   | f     | 136 | GLN  |
| 2   | f     | 186 | HIS  |
| 2   | f     | 388 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | f     | 465 | GLN  |
| 2   | h     | 136 | GLN  |
| 2   | h     | 186 | HIS  |
| 2   | h     | 388 | GLN  |
| 2   | h     | 465 | GLN  |
| 2   | j     | 136 | GLN  |
| 2   | j     | 388 | GLN  |
| 2   | j     | 465 | GLN  |
| 2   | l     | 388 | GLN  |
| 2   | l     | 465 | GLN  |
| 2   | n     | 388 | GLN  |
| 2   | n     | 465 | GLN  |
| 2   | p     | 136 | GLN  |
| 2   | p     | 388 | GLN  |
| 2   | p     | 465 | GLN  |
| 2   | r     | 388 | GLN  |
| 2   | r     | 465 | GLN  |
| 2   | t     | 136 | GLN  |
| 2   | t     | 186 | HIS  |
| 2   | t     | 388 | GLN  |
| 2   | t     | 465 | GLN  |
| 2   | v     | 136 | GLN  |
| 2   | v     | 186 | HIS  |
| 2   | v     | 388 | GLN  |
| 2   | v     | 465 | GLN  |
| 2   | x     | 388 | GLN  |
| 2   | z     | 388 | GLN  |
| 2   | 2     | 388 | GLN  |
| 2   | 4     | 388 | GLN  |
| 2   | 6     | 388 | GLN  |
| 2   | 8     | 388 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

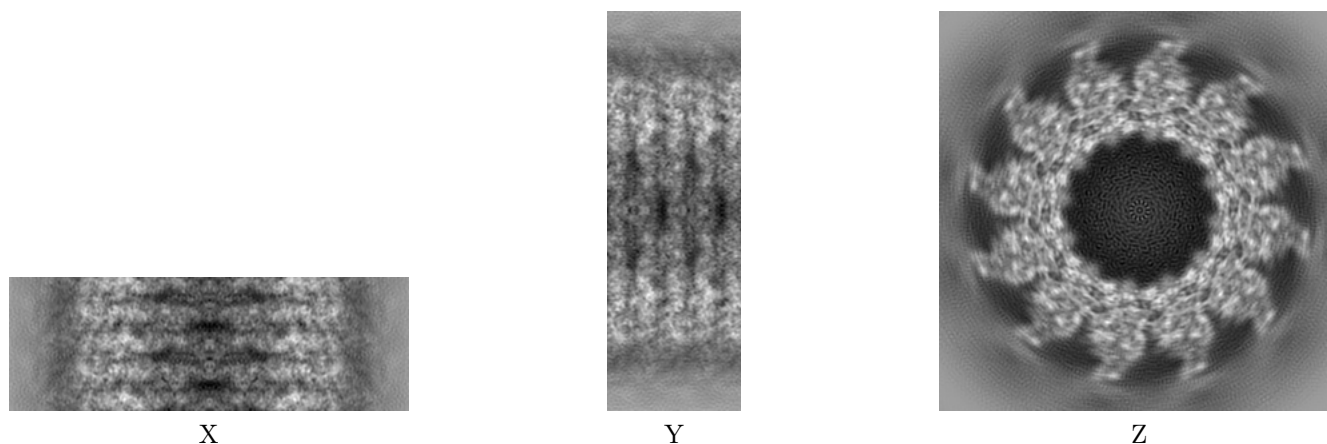
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2699. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

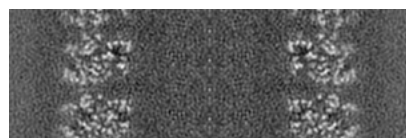
#### 6.1.1 Primary map



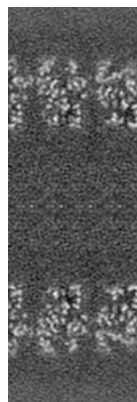
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

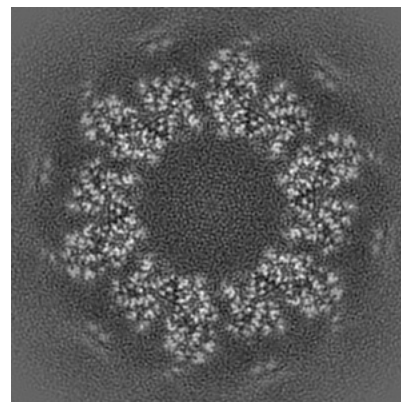
### 6.2.1 Primary map



X Index: 300



Y Index:  
300

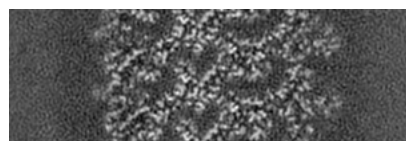


Z Index: 100

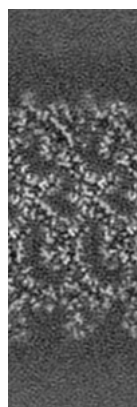
The images above show central slices of the map in three orthogonal directions.

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

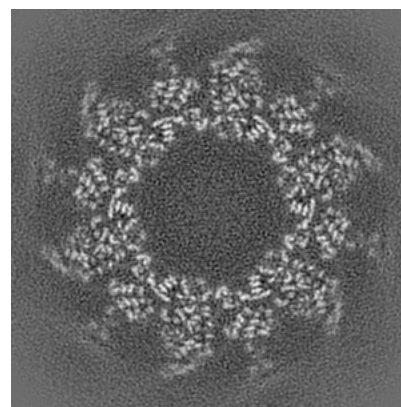
### 6.3.1 Primary map



X Index: 431



Y Index:  
431

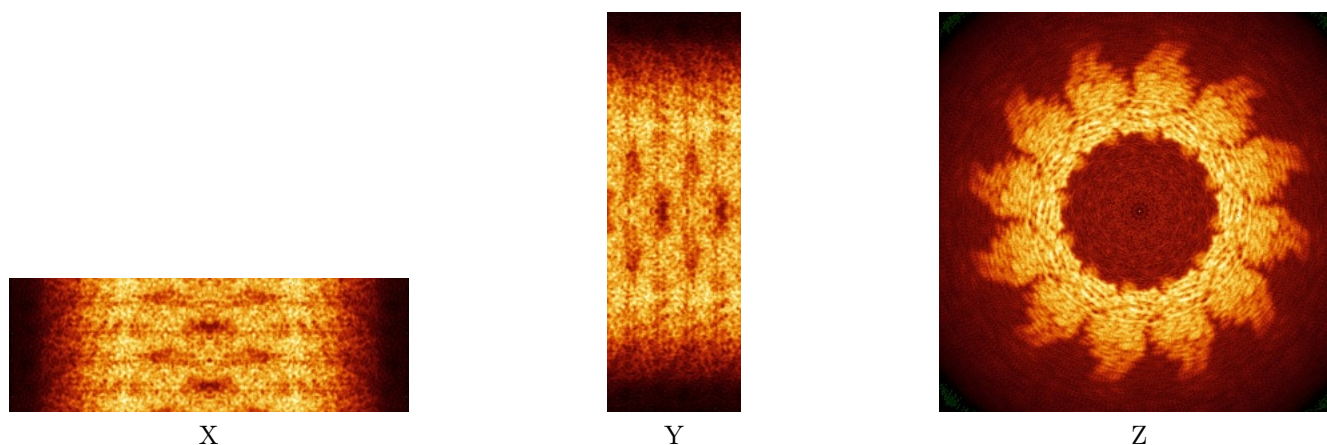


Z Index: 193

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

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

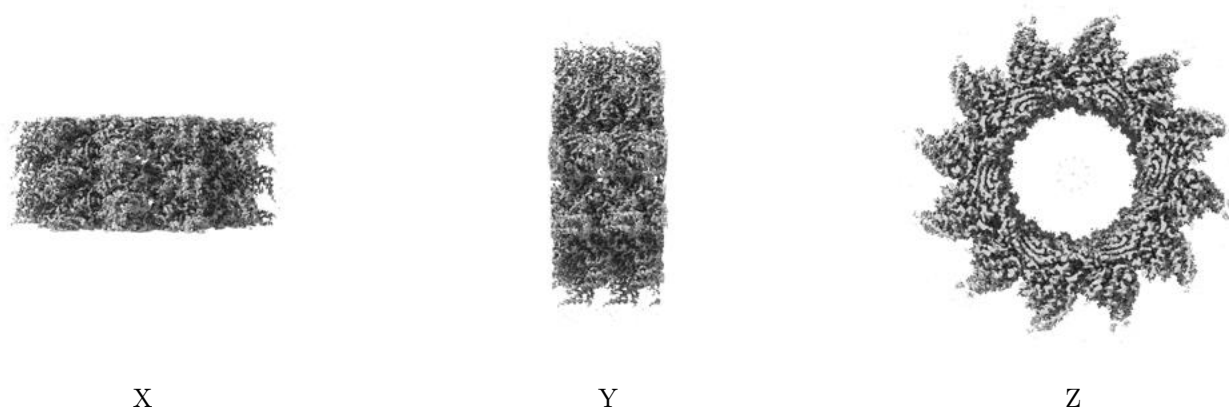
### 6.4.1 Primary map



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 120.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation

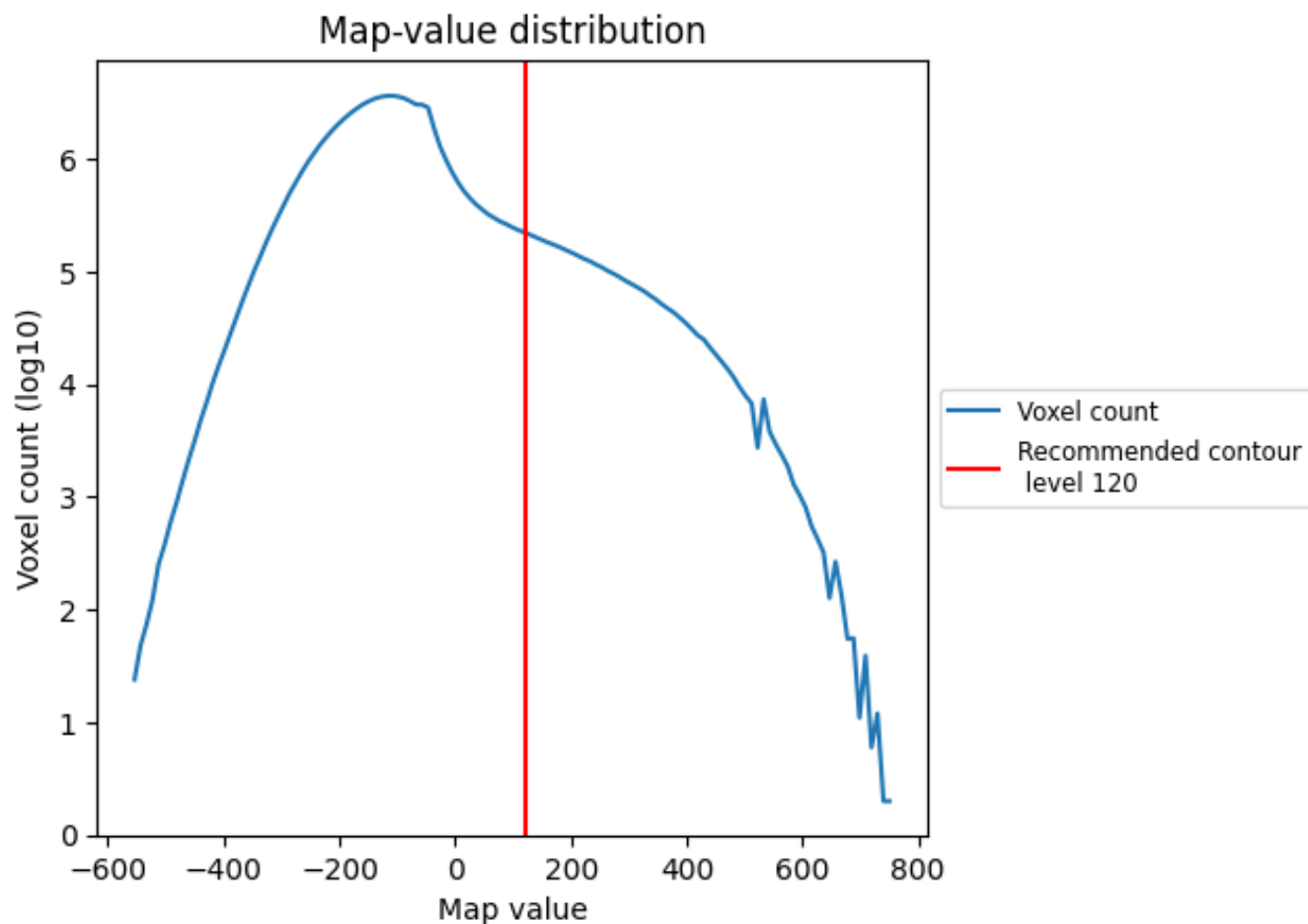
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

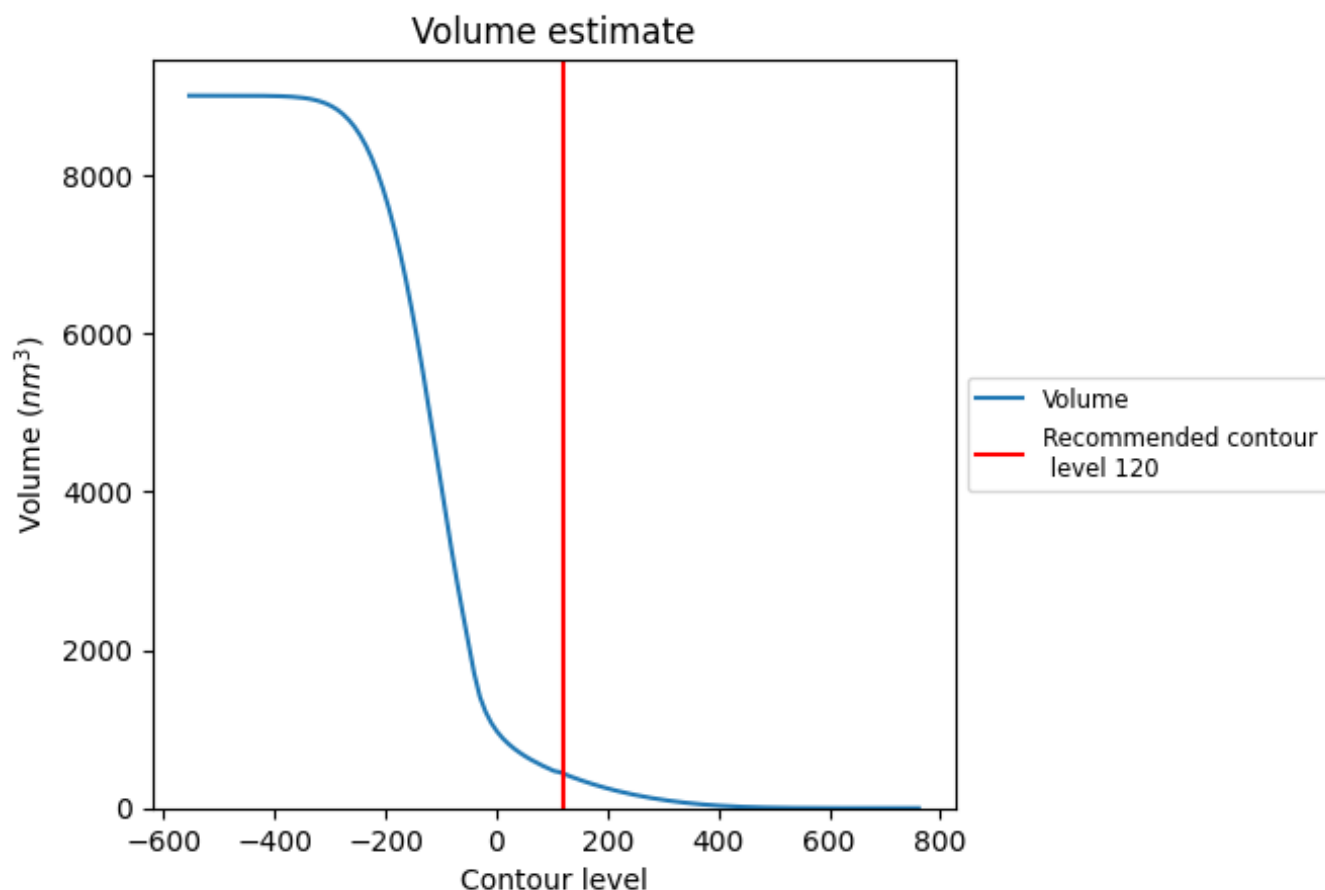
This section contains the results of statistical analysis of the map.

### 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 437 nm<sup>3</sup>; this corresponds to an approximate mass of 395 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

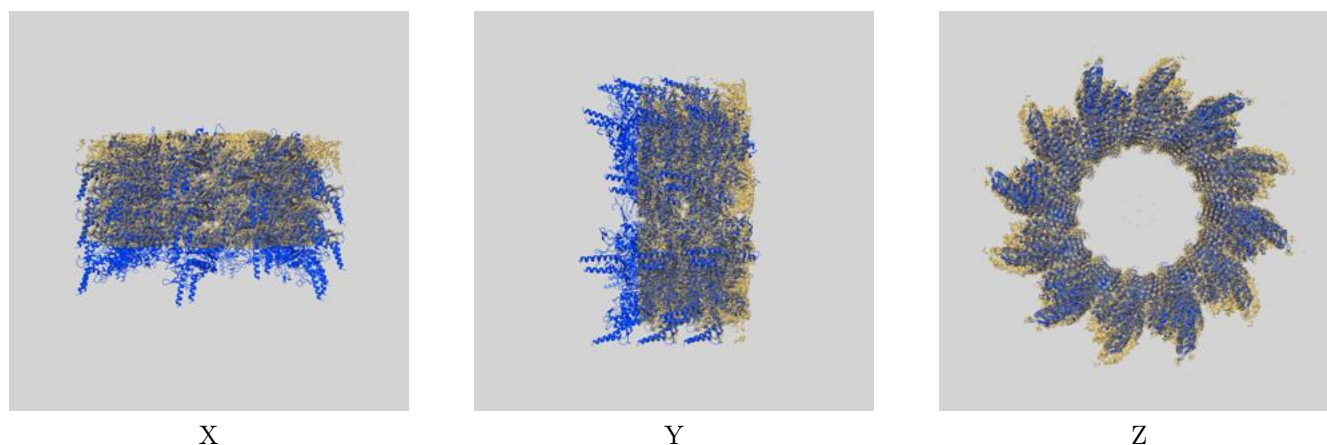
## 8 Fourier-Shell correlation ⓘ

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

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

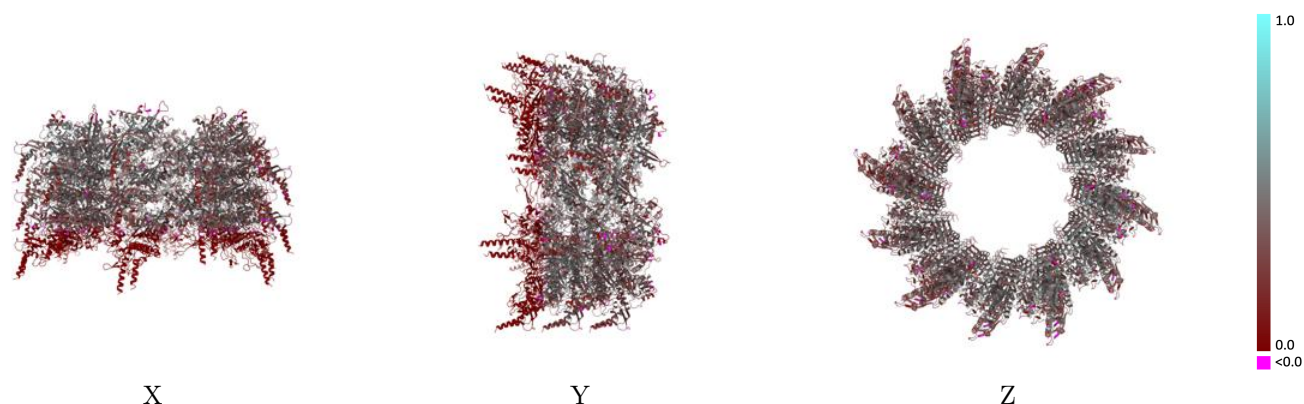
This section contains information regarding the fit between EMDB map EMD-2699 and PDB model 3J9G. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

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



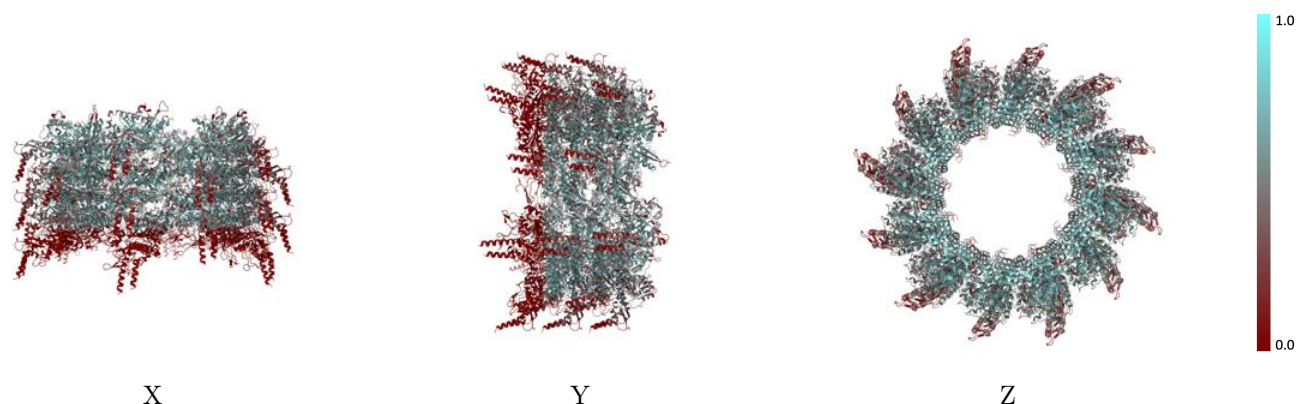
The images above show the 3D surface view of the map at the recommended contour level 120.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



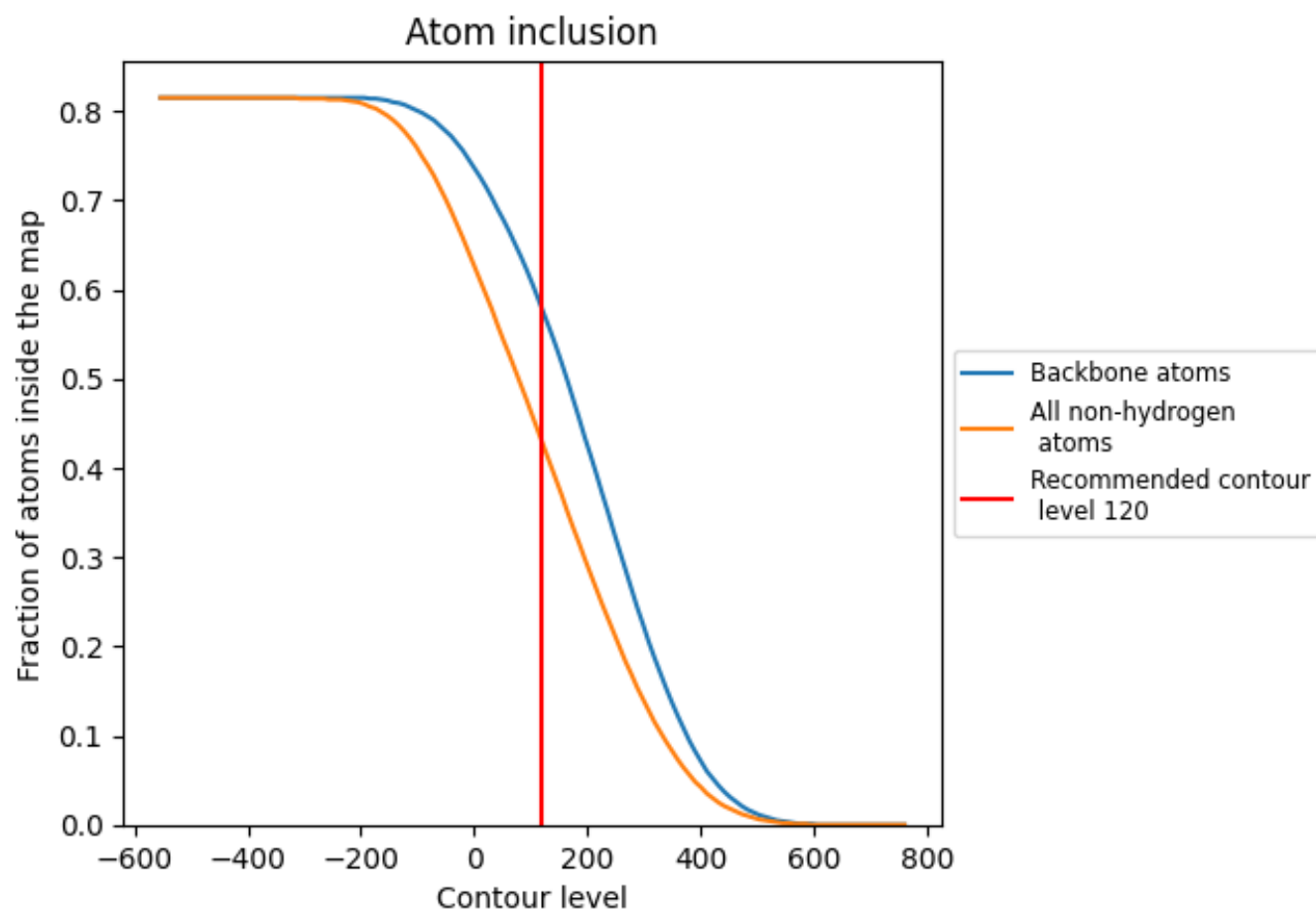
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (120).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 43% 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 (120) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.4300         | 0.3070  |
| 1     | 0.3290         | 0.2790  |
| 2     | 0.4770         | 0.3080  |
| 3     | 0.3340         | 0.2950  |
| 4     | 0.4790         | 0.3130  |
| 5     | 0.3520         | 0.3070  |
| 6     | 0.5140         | 0.3490  |
| 7     | 0.4160         | 0.3670  |
| 8     | 0.5560         | 0.4080  |
| A     | 0.0290         | 0.0250  |
| B     | 0.2180         | 0.1520  |
| C     | 0.0310         | 0.0290  |
| D     | 0.2120         | 0.1500  |
| E     | 0.0260         | 0.0260  |
| F     | 0.1970         | 0.1320  |
| G     | 0.0270         | 0.0270  |
| H     | 0.1820         | 0.1230  |
| I     | 0.0220         | 0.0250  |
| J     | 0.1840         | 0.1170  |
| K     | 0.0270         | 0.0220  |
| L     | 0.2030         | 0.1330  |
| M     | 0.3390         | 0.2840  |
| N     | 0.5280         | 0.3570  |
| O     | 0.3700         | 0.3080  |
| P     | 0.5430         | 0.3710  |
| Q     | 0.3560         | 0.2920  |
| R     | 0.5090         | 0.3440  |
| S     | 0.3280         | 0.2690  |
| T     | 0.4880         | 0.3250  |
| U     | 0.3530         | 0.2800  |
| V     | 0.4900         | 0.3180  |
| W     | 0.3680         | 0.2750  |
| X     | 0.4990         | 0.3300  |
| Y     | 0.3850         | 0.3210  |
| Z     | 0.5600         | 0.3890  |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.3700   |  0.3230   |
| b     |  0.5620   |  0.3900   |
| c     |  0.3760   |  0.3340   |
| d     |  0.5530   |  0.3840   |
| e     |  0.3640   |  0.3130   |
| f     |  0.5370   |  0.3720   |
| g     |  0.3910   |  0.3410   |
| h     |  0.5440   |  0.3890   |
| i     |  0.3980   |  0.3430   |
| j     |  0.5610   |  0.3920   |
| k     |  0.3950   |  0.3440   |
| l     |  0.5640   |  0.4010   |
| m     |  0.3570   |  0.3060   |
| n     |  0.5440   |  0.3690   |
| o     |  0.3470   |  0.3120   |
| p     |  0.5310   |  0.3620   |
| q     |  0.3510   |  0.3110   |
| r     |  0.5360   |  0.3650   |
| s     |  0.3960   |  0.3350   |
| t     |  0.5590  |  0.3990  |
| u     |  0.4150 |  0.3720 |
| v     |  0.5820 |  0.4220 |
| w     |  0.4090 |  0.3730 |
| x     |  0.5520 |  0.4070 |
| y     |  0.3550 |  0.3080 |
| z     |  0.5160 |  0.3500 |