



## Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 12:18 AM EDT

PDB ID : 7UIT / pdb\_00007uit  
EMDB ID : EMD-26552  
Title : Cryo-EM of pH-controlled and self-assembled fibers, peptide 2  
Authors : Wang, F.; Grosvirt-Dramen, A.; Hochbaum, A.I.; Egelman, E.H.  
Deposited on : 2022-03-29  
Resolution : 3.90 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:

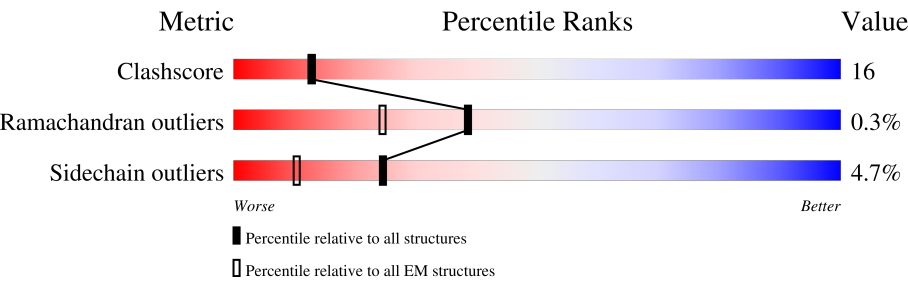
EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 0     | 30     | <div><div>90%</div><div><div></div><div></div><div></div><div></div></div><div>57%40%.</div></div>  |
| 1   | 1     | 30     | <div><div>83%</div><div><div></div><div></div><div></div><div></div></div><div>43%53%.</div></div>  |
| 1   | 2     | 30     | <div><div>73%</div><div><div></div><div></div><div></div><div></div></div><div>60%33%7%</div></div> |
| 1   | 3     | 30     | <div><div>80%</div><div><div></div><div></div><div></div><div></div></div><div>63%37%</div></div>   |
| 1   | 4     | 30     | <div><div>73%</div><div><div></div><div></div><div></div><div></div></div><div>60%37%. </div></div> |
| 1   | 5     | 30     | <div><div>77%</div><div><div></div><div></div><div></div><div></div></div><div>57%40%. </div></div> |
| 1   | 6     | 30     | <div><div>87%</div><div><div></div><div></div><div></div><div></div></div><div>60%37%. </div></div> |
| 1   | 7     | 30     | <div><div>83%</div><div><div></div><div></div><div></div><div></div></div><div>47%47%7%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 8     | 30     |                  |
| 1   | 9     | 30     |                  |
| 1   | A     | 30     |                  |
| 1   | AA    | 30     |                  |
| 1   | B     | 30     |                  |
| 1   | BA    | 30     |                  |
| 1   | C     | 30     |                  |
| 1   | CA    | 30     |                  |
| 1   | D     | 30     |                  |
| 1   | DA    | 30     |                  |
| 1   | E     | 30     |                  |
| 1   | EA    | 30     |                  |
| 1   | F     | 30     |                  |
| 1   | FA    | 30     |                  |
| 1   | G     | 30     |                  |
| 1   | GA    | 30     |                  |
| 1   | H     | 30     |                  |
| 1   | HA    | 30     |                  |
| 1   | I     | 30     |                  |
| 1   | IA    | 30     |                  |
| 1   | J     | 30     |                  |
| 1   | JA    | 30     |                  |
| 1   | K     | 30     |                  |
| 1   | L     | 30     |                  |
| 1   | M     | 30     |                  |

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| Mol | Chain | Length | Quality of chain                      |
|-----|-------|--------|---------------------------------------|
| 1   | N     | 30     | <div>53%</div> <div>63% 30% 7%</div>  |
| 1   | O     | 30     | <div>60%</div> <div>60% 37%</div>     |
| 1   | P     | 30     | <div>67%</div> <div>53% 47%</div>     |
| 1   | Q     | 30     | <div>53%</div> <div>63% 27% 10%</div> |
| 1   | R     | 30     | <div>57%</div> <div>57% 40%</div>     |
| 1   | S     | 30     | <div>50%</div> <div>57% 43%</div>     |
| 1   | T     | 30     | <div>67%</div> <div>57% 40%</div>     |
| 1   | U     | 30     | <div>90%</div> <div>63% 33%</div>     |
| 1   | V     | 30     | <div>77%</div> <div>57% 40%</div>     |
| 1   | W     | 30     | <div>80%</div> <div>57% 40%</div>     |
| 1   | X     | 30     | <div>70%</div> <div>70% 27%</div>     |
| 1   | Y     | 30     | <div>87%</div> <div>60% 37%</div>     |
| 1   | Z     | 30     | <div>13%</div> <div>60% 33% 7%</div>  |
| 1   | a     | 30     | <div>13%</div> <div>60% 40%</div>     |
| 1   | b     | 30     | <div>17%</div> <div>57% 37% 7%</div>  |
| 1   | c     | 30     | <div>13%</div> <div>63% 37%</div>     |
| 1   | d     | 30     | <div>10%</div> <div>63% 37%</div>     |
| 1   | e     | 30     | <div>13%</div> <div>63% 37%</div>     |
| 1   | f     | 30     | <div>20%</div> <div>60% 37%</div>     |
| 1   | g     | 30     | <div>20%</div> <div>67% 27% 7%</div>  |
| 1   | h     | 30     | <div>20%</div> <div>70% 30%</div>     |
| 1   | i     | 30     | <div>17%</div> <div>50% 50%</div>     |
| 1   | j     | 30     | <div>20%</div> <div>67% 30%</div>     |
| 1   | k     | 30     | <div>13%</div> <div>67% 27% 7%</div>  |
| 1   | l     | 30     | <div>37%</div> <div>60% 37%</div>     |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | m     | 30     |                  |
| 1   | n     | 30     |                  |
| 1   | o     | 30     |                  |
| 1   | p     | 30     |                  |
| 1   | q     | 30     |                  |
| 1   | r     | 30     |                  |
| 1   | s     | 30     |                  |
| 1   | t     | 30     |                  |
| 1   | u     | 30     |                  |
| 1   | v     | 30     |                  |
| 1   | w     | 30     |                  |
| 1   | x     | 30     |                  |
| 1   | y     | 30     |                  |
| 1   | z     | 30     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | PHI  | Q     | 5121 | -         | -        | X       | -                |
| 1   | PHI  | V     | 5621 | -         | -        | X       | -                |
| 1   | PHI  | z     | 3221 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17064 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 Peptide 2.

| Mol | Chain | Residues | Atoms |     |   |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|----|---------|-------|
| 1   | B     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | C     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | D     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | E     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | F     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | G     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | H     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | I     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | J     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | K     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | L     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | M     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | N     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | O     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | P     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | Q     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | R     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |

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| Mol | Chain | Residues | Atoms |     |   |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|----|---------|-------|
| 1   | S     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | T     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | U     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | V     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | W     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | X     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | Y     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | Z     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | a     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | b     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | c     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | d     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | e     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | f     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | g     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | h     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | i     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | j     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | k     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | l     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | m     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |

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| Mol | Chain | Residues | Atoms |     |   |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|----|---------|-------|
| 1   | n     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | o     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | p     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | q     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | r     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | s     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | t     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | u     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | v     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | w     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | x     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | y     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | z     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 0     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 1     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 2     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 3     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 4     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 5     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 6     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 7     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |

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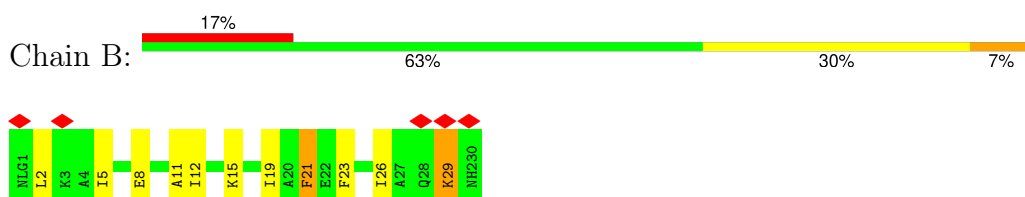
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| Mol | Chain | Residues | Atoms |     |   |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|----|---------|-------|
| 1   | 8     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | 9     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | AA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | BA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | CA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | DA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | EA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | FA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | A     | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | JA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | GA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | HA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |
| 1   | IA    | 30       | Total | C   | I | N  | O  | 0       | 1     |
|     |       |          | 237   | 159 | 1 | 39 | 38 |         |       |

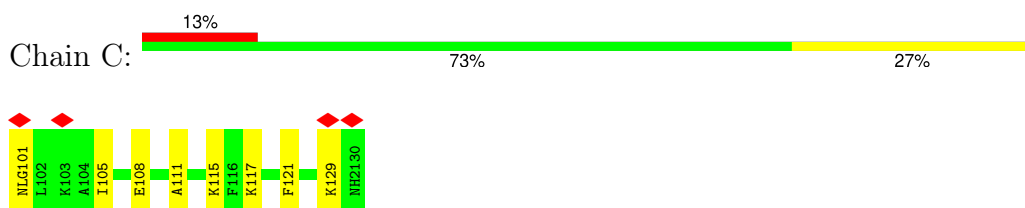
### 3 Residue-property plots [i](#)

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.

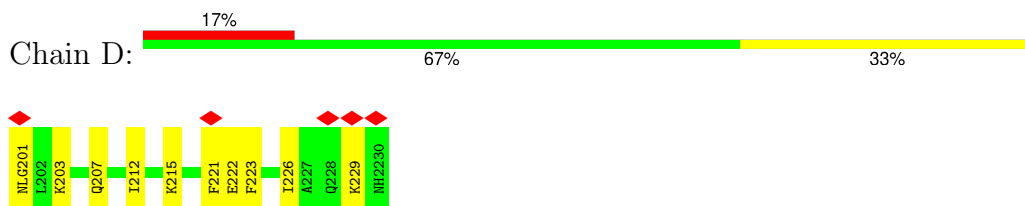
- Molecule 1: Peptide 2



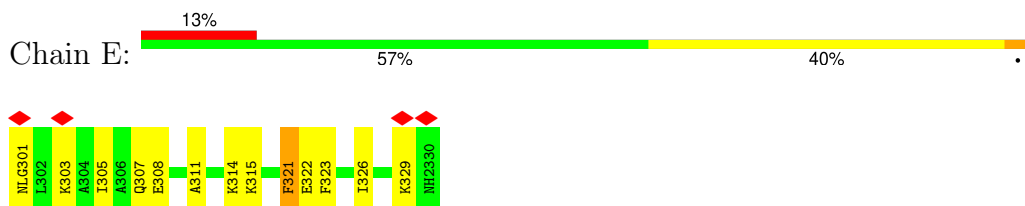
- Molecule 1: Peptide 2



- Molecule 1: Peptide 2

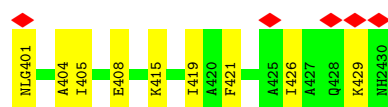


- Molecule 1: Peptide 2



- Molecule 1: Peptide 2

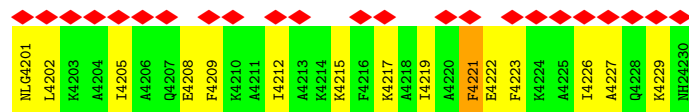
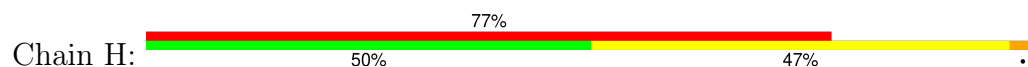




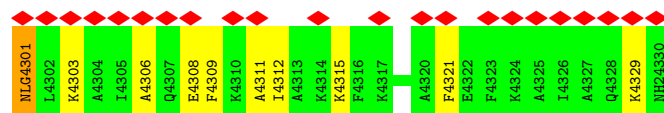
- Molecule 1: Peptide 2



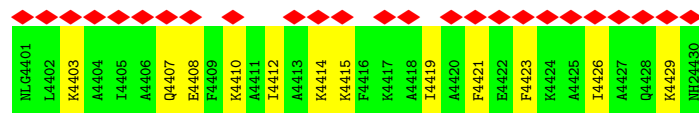
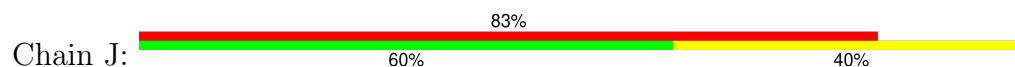
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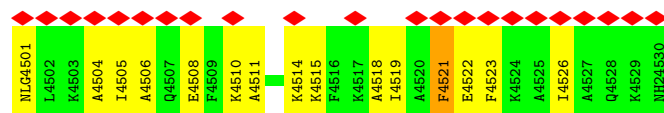
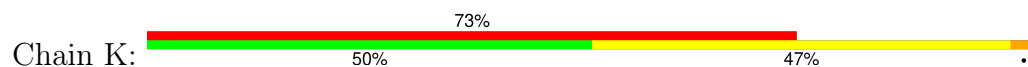
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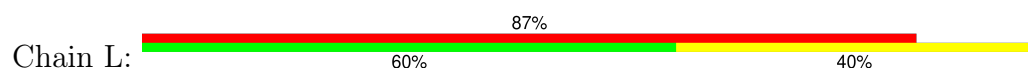
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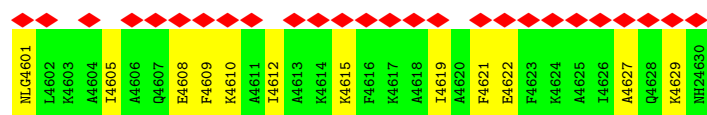


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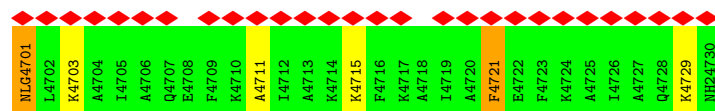
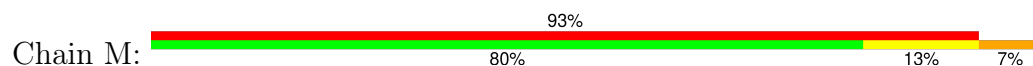


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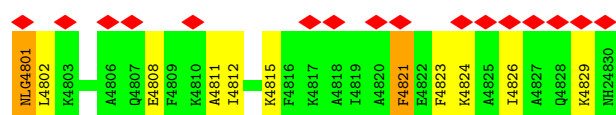




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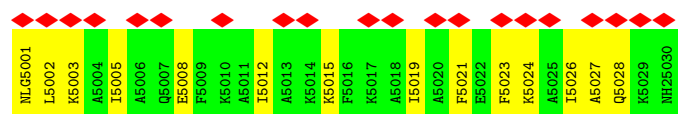
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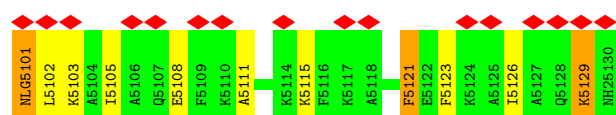
- Molecule 1: Peptide 2



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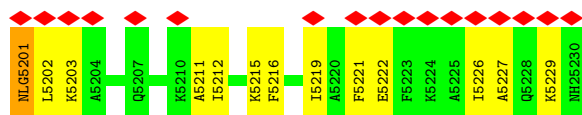


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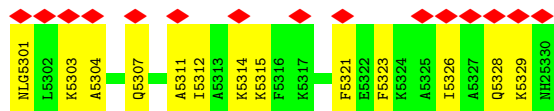


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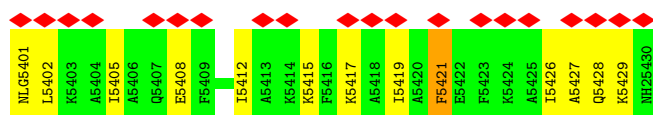




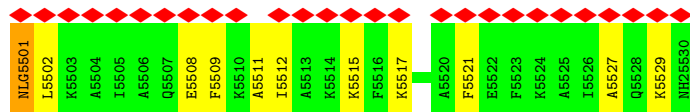
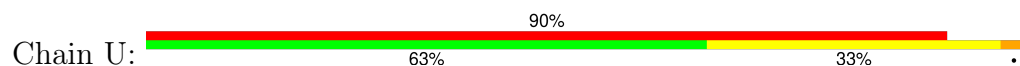
## ● Molecule 1: Peptide 2



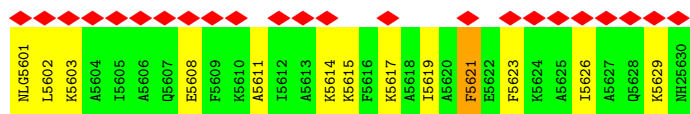
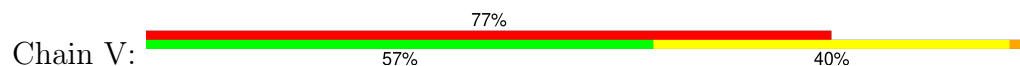
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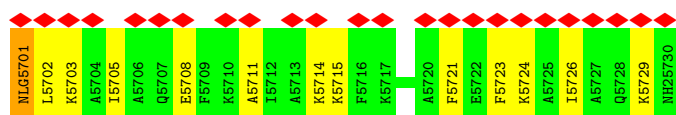
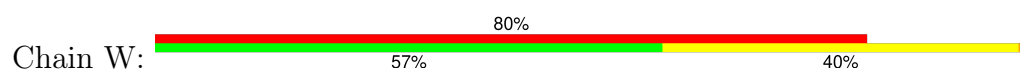
## ● Molecule 1: Peptide 2



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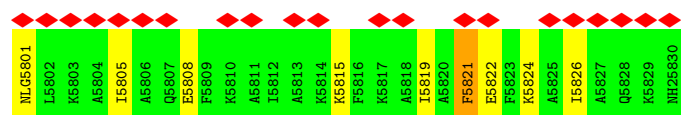


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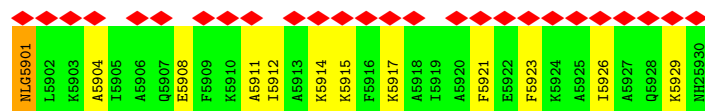
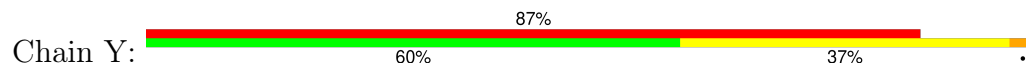


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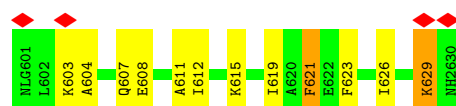




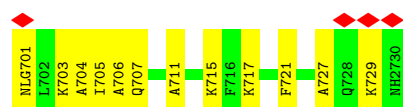
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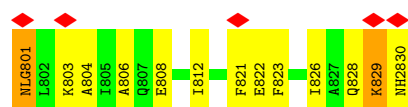
• Molecule 1: Peptide 2



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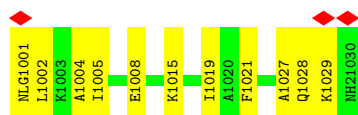


• Molecule 1: Peptide 2



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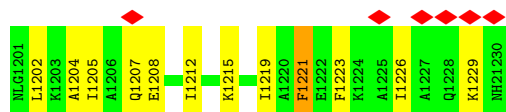




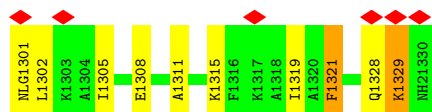
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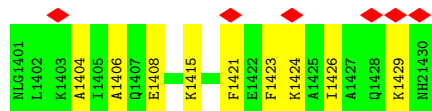
• Molecule 1: Peptide 2



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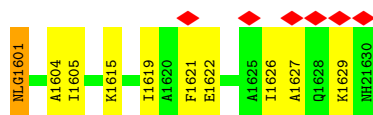


• Molecule 1: Peptide 2



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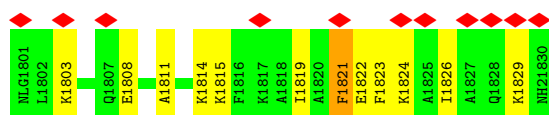




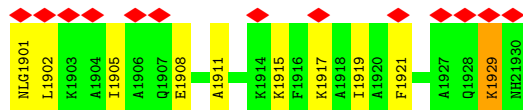
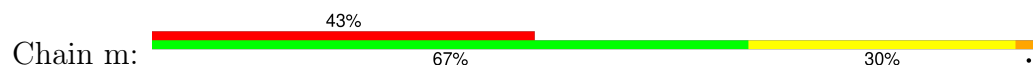
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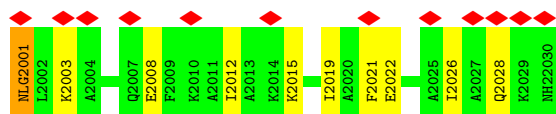
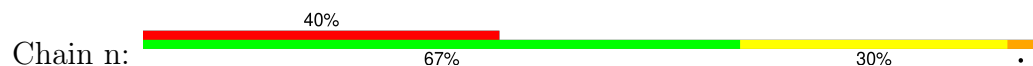
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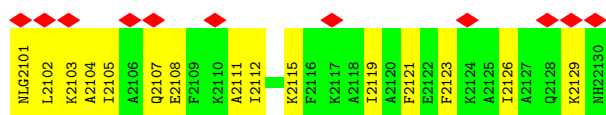
- Molecule 1: Peptide 2



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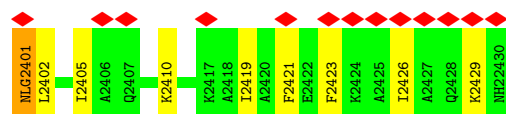
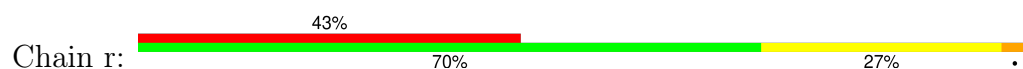




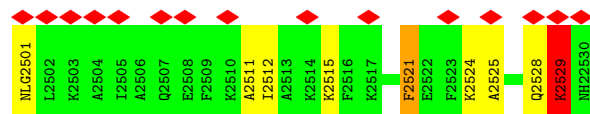
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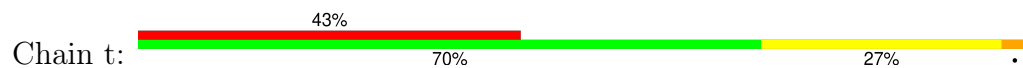
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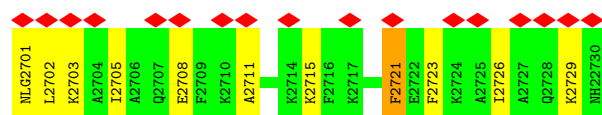
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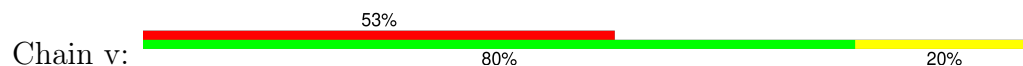
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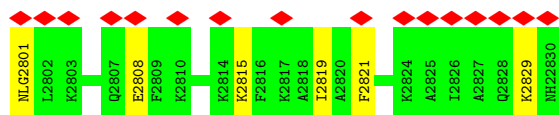


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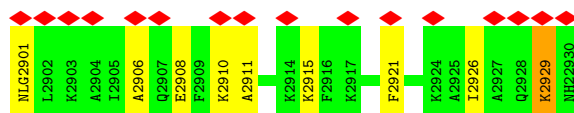


- Molecule 1: Peptide 2

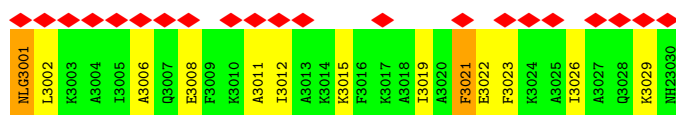




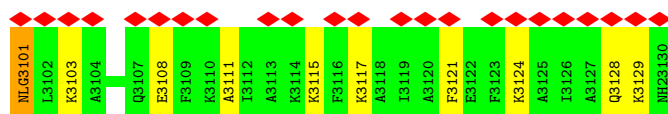
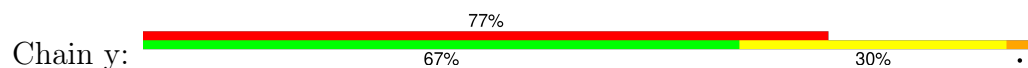
## ● Molecule 1: Peptide 2



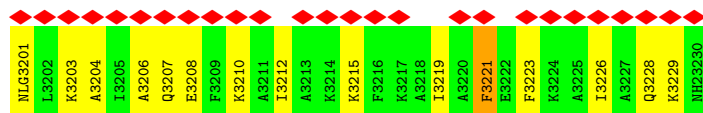
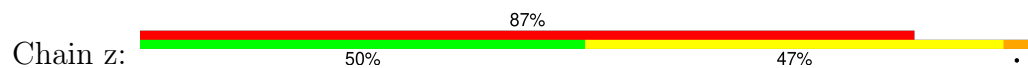
## ● Molecule 1: Peptide 2



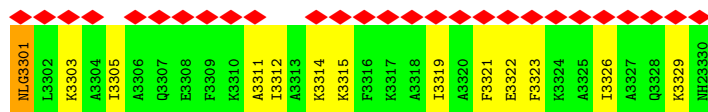
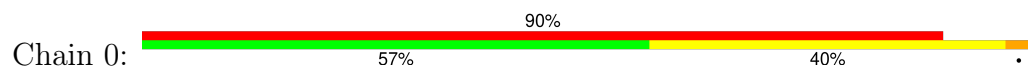
## ● Molecule 1: Peptide 2



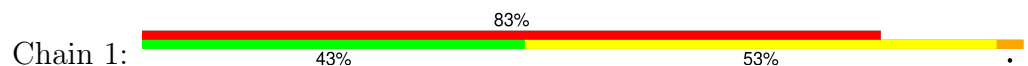
## ● Molecule 1: Peptide 2

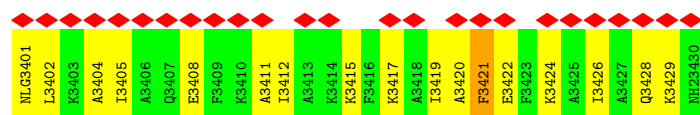


## ● Molecule 1: Peptide 2

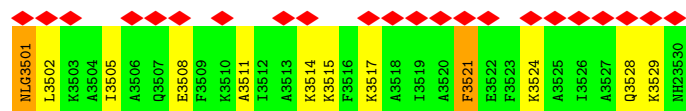
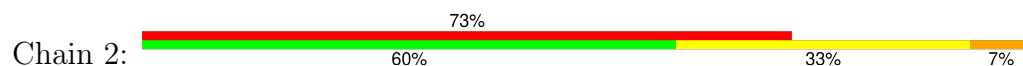


## ● Molecule 1: Peptide 2

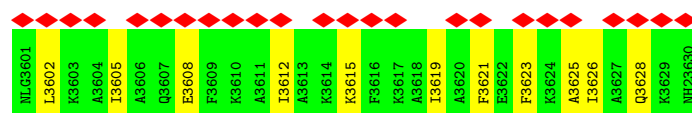
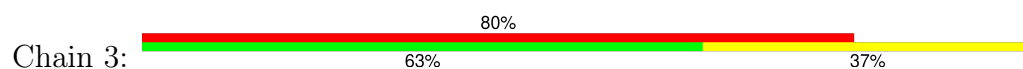




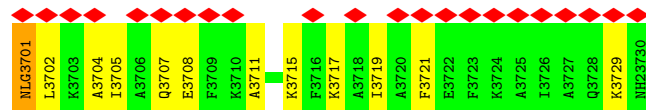
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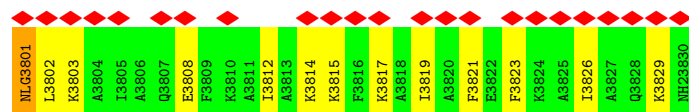
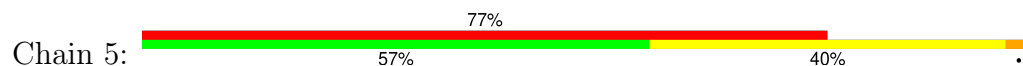
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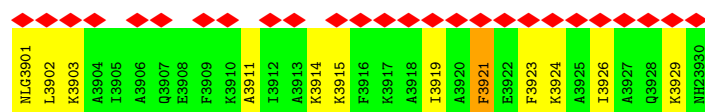
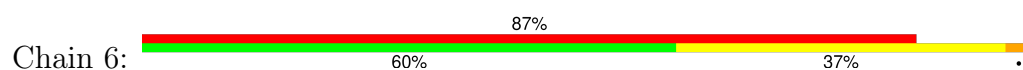
- Molecule 1: Peptide 2



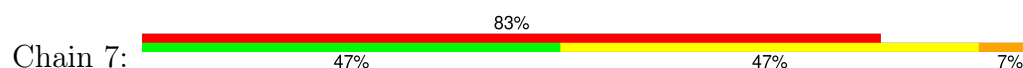
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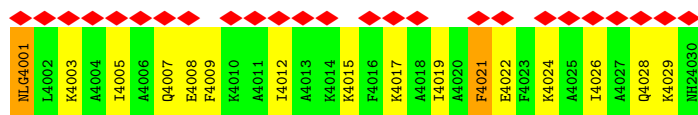


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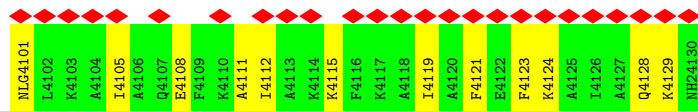
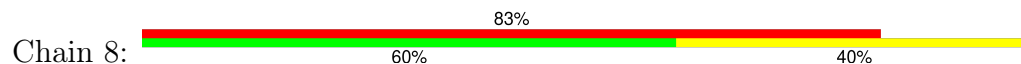


- Molecule 1: Peptide 2

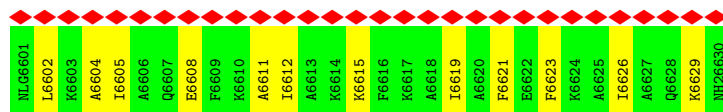




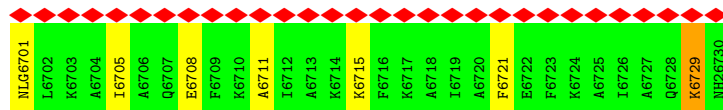
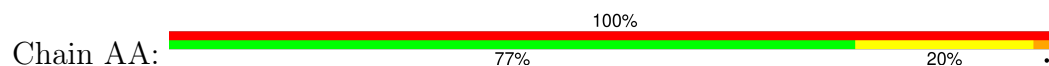
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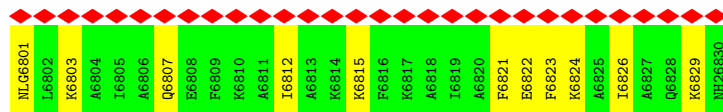
- Molecule 1: Peptide 2



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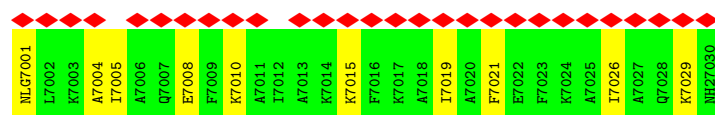


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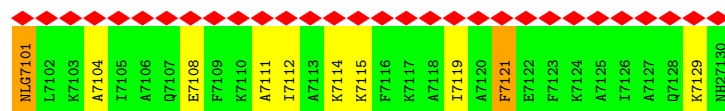


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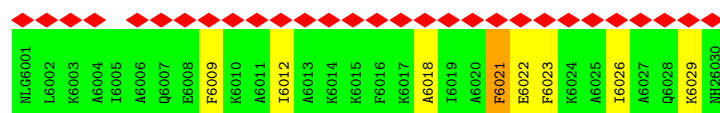
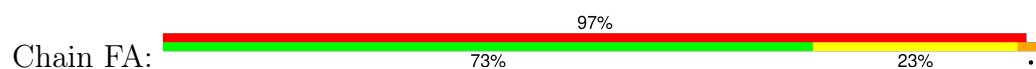




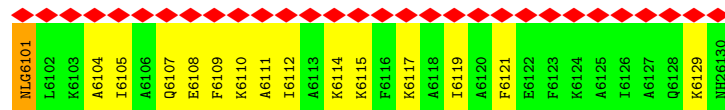
## ● Molecule 1: Peptide 2



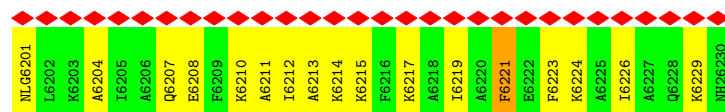
## ● Molecule 1: Peptide 2



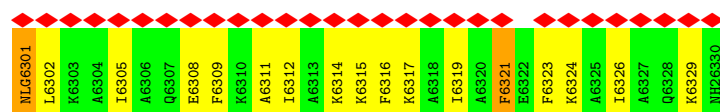
## ● Molecule 1: Peptide 2



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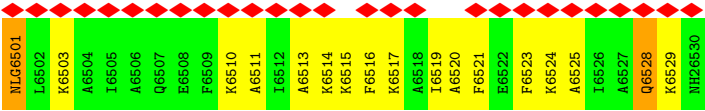
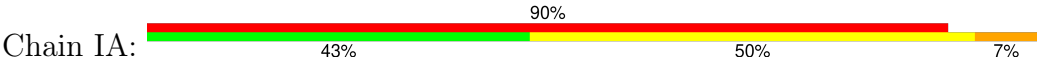


## ● Molecule 1: Peptide 2





● Molecule 1: Peptide 2



## 4 Experimental information

| Property                           | Value  | Source    |
|------------------------------------|--|-----------|
| EM reconstruction method           | HELICAL  | Depositor |
| Imposed symmetry                   | HELICAL, twist=-58.76°, rise=12.68 Å, axial sym=C1 | Depositor |
| Number of segments used            | 85453  | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                  | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION            | Depositor |
| Microscope                         | FEI TITAN KRIOS                                    | Depositor |
| Voltage (kV)                       | 300  | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 50   | Depositor |
| Minimum defocus (nm)               | 1000   | Depositor |
| Maximum defocus (nm)               | 2000   | Depositor |
| Magnification                      | Not provided                                       |           |
| Image detector                     | GATAN K3 (6k x 4k)                                 | Depositor |
| Maximum map value                  | 1.374  | Depositor |
| Minimum map value                  | -0.576   | Depositor |
| Average map value                  | 0.020  | Depositor |
| Map value standard deviation       | 0.078  | Depositor |
| Recommended contour level          | 0.4  | Depositor |
| Map size (Å)                       | 691.2, 691.2, 691.2                                | wwPDB     |
| Map dimensions                     | 640, 640, 640                                      | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                   | wwPDB     |
| Pixel spacing (Å)                  | 1.08, 1.08, 1.08                                   | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NLG, PHI, NH2

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 0     | 0.25         | 0/213       | 0.39        | 0/278       |
| 1   | 1     | 0.25         | 0/213       | 0.42        | 0/278       |
| 1   | 2     | 0.23         | 0/213       | 0.44        | 0/278       |
| 1   | 3     | 0.24         | 0/213       | 0.31        | 0/278       |
| 1   | 4     | 0.24         | 0/213       | 0.45        | 0/278       |
| 1   | 5     | 0.23         | 0/213       | 0.35        | 0/278       |
| 1   | 6     | 0.22         | 0/213       | 0.39        | 0/278       |
| 1   | 7     | 0.22         | 0/213       | 0.34        | 0/278       |
| 1   | 8     | 0.24         | 0/213       | 0.37        | 0/278       |
| 1   | 9     | 0.31         | 0/213       | 0.39        | 0/278       |
| 1   | A     | 0.23         | 0/213       | 0.37        | 0/278       |
| 1   | AA    | 0.33         | 0/213       | 0.46        | 0/278       |
| 1   | B     | 0.31         | 0/213       | 0.39        | 0/278       |
| 1   | BA    | 0.32         | 0/213       | 0.46        | 0/278       |
| 1   | C     | 0.33         | 0/213       | 0.46        | 0/278       |
| 1   | CA    | 0.33         | 0/213       | 0.48        | 0/278       |
| 1   | D     | 0.31         | 0/213       | 0.45        | 0/278       |
| 1   | DA    | 0.31         | 0/213       | 0.37        | 0/278       |
| 1   | E     | 0.33         | 0/213       | 0.48        | 0/278       |
| 1   | EA    | 0.31         | 0/213       | 0.39        | 0/278       |
| 1   | F     | 0.30         | 0/213       | 0.37        | 0/278       |
| 1   | FA    | 0.26         | 0/213       | 0.43        | 0/278       |
| 1   | G     | 0.30         | 0/213       | 0.39        | 0/278       |
| 1   | GA    | 0.30         | 0/213       | 0.74        | 0/278       |
| 1   | H     | 0.23         | 0/213       | 0.37        | 0/278       |
| 1   | HA    | 0.33         | 0/213       | 0.73        | 0/278       |
| 1   | I     | 0.24         | 0/213       | 0.36        | 0/278       |
| 1   | IA    | 0.26         | 0/213       | 0.46        | 0/278       |
| 1   | J     | 0.24         | 0/213       | 0.34        | 0/278       |
| 1   | JA    | 0.25         | 0/213       | 0.55        | 0/278       |
| 1   | K     | 0.31         | 0/213       | 0.63        | 0/278       |
| 1   | L     | 0.23         | 0/213       | 0.33        | 0/278       |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | M     | 0.24         | 0/213   | 0.41        | 0/278   |
| 1   | N     | 0.25         | 0/213   | 0.37        | 0/278   |
| 1   | O     | 0.28         | 0/213   | 0.47        | 0/278   |
| 1   | P     | 0.25         | 0/213   | 0.37        | 0/278   |
| 1   | Q     | 0.27         | 0/213   | 0.45        | 0/278   |
| 1   | R     | 0.25         | 0/213   | 0.36        | 0/278   |
| 1   | S     | 0.25         | 0/213   | 0.38        | 0/278   |
| 1   | T     | 0.25         | 0/213   | 0.36        | 0/278   |
| 1   | U     | 0.25         | 0/213   | 0.39        | 0/278   |
| 1   | V     | 0.23         | 0/213   | 0.33        | 0/278   |
| 1   | W     | 0.22         | 0/213   | 0.30        | 0/278   |
| 1   | X     | 0.24         | 0/213   | 0.40        | 0/278   |
| 1   | Y     | 0.25         | 0/213   | 0.43        | 0/278   |
| 1   | Z     | 0.32         | 0/213   | 0.50        | 0/278   |
| 1   | a     | 0.31         | 0/213   | 0.51        | 0/278   |
| 1   | b     | 0.33         | 0/213   | 0.46        | 0/278   |
| 1   | c     | 0.32         | 0/213   | 0.47        | 0/278   |
| 1   | d     | 0.32         | 0/213   | 0.38        | 0/278   |
| 1   | e     | 0.31         | 0/213   | 0.37        | 0/278   |
| 1   | f     | 0.29         | 0/213   | 0.40        | 0/278   |
| 1   | g     | 0.32         | 0/213   | 0.45        | 0/278   |
| 1   | h     | 0.32         | 0/213   | 0.39        | 0/278   |
| 1   | i     | 0.32         | 0/213   | 0.49        | 0/278   |
| 1   | j     | 0.29         | 0/213   | 0.42        | 0/278   |
| 1   | k     | 0.29         | 0/213   | 0.39        | 0/278   |
| 1   | l     | 0.25         | 0/213   | 0.43        | 0/278   |
| 1   | m     | 0.29         | 0/213   | 0.38        | 0/278   |
| 1   | n     | 0.27         | 0/213   | 0.37        | 0/278   |
| 1   | o     | 0.31         | 0/213   | 0.58        | 0/278   |
| 1   | p     | 0.25         | 0/213   | 0.34        | 0/278   |
| 1   | q     | 0.26         | 0/213   | 0.40        | 0/278   |
| 1   | r     | 0.25         | 0/213   | 0.38        | 0/278   |
| 1   | s     | 0.24         | 0/213   | 0.31        | 0/278   |
| 1   | t     | 0.23         | 0/213   | 0.32        | 0/278   |
| 1   | u     | 0.24         | 0/213   | 0.33        | 0/278   |
| 1   | v     | 0.25         | 0/213   | 0.32        | 0/278   |
| 1   | w     | 0.25         | 0/213   | 0.37        | 0/278   |
| 1   | x     | 0.22         | 0/213   | 0.33        | 0/278   |
| 1   | y     | 0.22         | 0/213   | 0.32        | 0/278   |
| 1   | z     | 0.25         | 0/213   | 0.49        | 0/278   |
| All | All   | 0.27         | 0/15336 | 0.42        | 0/20016 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 0     | 0                   | 1                   |
| 1   | 2     | 0                   | 1                   |
| 1   | 4     | 0                   | 1                   |
| 1   | 5     | 0                   | 1                   |
| 1   | 7     | 0                   | 1                   |
| 1   | 8     | 0                   | 1                   |
| 1   | A     | 0                   | 1                   |
| 1   | AA    | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | DA    | 0                   | 1                   |
| 1   | EA    | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 1   | GA    | 0                   | 1                   |
| 1   | H     | 0                   | 1                   |
| 1   | HA    | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | IA    | 0                   | 1                   |
| 1   | JA    | 0                   | 1                   |
| 1   | K     | 0                   | 1                   |
| 1   | L     | 0                   | 1                   |
| 1   | M     | 0                   | 1                   |
| 1   | N     | 0                   | 1                   |
| 1   | O     | 0                   | 1                   |
| 1   | Q     | 0                   | 1                   |
| 1   | R     | 0                   | 1                   |
| 1   | S     | 0                   | 1                   |
| 1   | U     | 0                   | 1                   |
| 1   | W     | 0                   | 1                   |
| 1   | X     | 0                   | 1                   |
| 1   | Y     | 0                   | 1                   |
| 1   | a     | 0                   | 1                   |
| 1   | b     | 0                   | 1                   |
| 1   | c     | 0                   | 1                   |
| 1   | d     | 0                   | 1                   |
| 1   | g     | 0                   | 1                   |
| 1   | j     | 0                   | 1                   |
| 1   | k     | 0                   | 1                   |
| 1   | m     | 0                   | 1                   |
| 1   | n     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | p     | 0                   | 1                   |
| 1   | q     | 0                   | 1                   |
| 1   | r     | 0                   | 1                   |
| 1   | s     | 0                   | 1                   |
| 1   | v     | 0                   | 1                   |
| 1   | w     | 0                   | 1                   |
| 1   | x     | 0                   | 1                   |
| 1   | y     | 0                   | 1                   |
| All | All   | 0                   | 48                  |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | 0     | 3301 | NLG  | Mainchain |
| 1   | 2     | 3501 | NLG  | Mainchain |
| 1   | 4     | 3701 | NLG  | Mainchain |
| 1   | 5     | 3801 | NLG  | Mainchain |
| 1   | 7     | 4001 | NLG  | Mainchain |
| 1   | 8     | 4101 | NLG  | Mainchain |
| 1   | A     | 6101 | NLG  | Mainchain |
| 1   | AA    | 6701 | NLG  | Mainchain |
| 1   | C     | 101  | NLG  | Mainchain |
| 1   | DA    | 7001 | NLG  | Mainchain |
| 1   | EA    | 7101 | NLG  | Mainchain |
| 1   | F     | 401  | NLG  | Mainchain |
| 1   | G     | 501  | NLG  | Mainchain |
| 1   | GA    | 6301 | NLG  | Mainchain |
| 1   | H     | 4201 | NLG  | Mainchain |
| 1   | HA    | 6401 | NLG  | Mainchain |
| 1   | I     | 4301 | NLG  | Mainchain |
| 1   | IA    | 6501 | NLG  | Mainchain |
| 1   | JA    | 6201 | NLG  | Mainchain |
| 1   | K     | 4501 | NLG  | Mainchain |
| 1   | L     | 4601 | NLG  | Mainchain |
| 1   | M     | 4701 | NLG  | Mainchain |
| 1   | N     | 4801 | NLG  | Mainchain |
| 1   | O     | 4901 | NLG  | Mainchain |
| 1   | Q     | 5101 | NLG  | Mainchain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | R     | 5201 | NLG  | Mainchain |
| 1   | S     | 5301 | NLG  | Mainchain |
| 1   | U     | 5501 | NLG  | Mainchain |
| 1   | W     | 5701 | NLG  | Mainchain |
| 1   | X     | 5801 | NLG  | Mainchain |
| 1   | Y     | 5901 | NLG  | Mainchain |
| 1   | a     | 701  | NLG  | Mainchain |
| 1   | b     | 801  | NLG  | Mainchain |
| 1   | c     | 901  | NLG  | Mainchain |
| 1   | d     | 1001 | NLG  | Mainchain |
| 1   | g     | 1301 | NLG  | Mainchain |
| 1   | j     | 1601 | NLG  | Mainchain |
| 1   | k     | 1701 | NLG  | Mainchain |
| 1   | m     | 1901 | NLG  | Mainchain |
| 1   | n     | 2001 | NLG  | Mainchain |
| 1   | p     | 2201 | NLG  | Mainchain |
| 1   | q     | 2301 | NLG  | Mainchain |
| 1   | r     | 2401 | NLG  | Mainchain |
| 1   | s     | 2501 | NLG  | Mainchain |
| 1   | v     | 2801 | NLG  | Mainchain |
| 1   | w     | 2901 | NLG  | Mainchain |
| 1   | x     | 3001 | NLG  | Mainchain |
| 1   | y     | 3101 | NLG  | Mainchain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 237   | 0        | 258      | 13      | 0            |
| 1   | 1     | 237   | 0        | 258      | 26      | 0            |
| 1   | 2     | 237   | 0        | 258      | 11      | 0            |
| 1   | 3     | 237   | 0        | 258      | 26      | 0            |
| 1   | 4     | 237   | 0        | 258      | 10      | 0            |
| 1   | 5     | 237   | 0        | 258      | 10      | 0            |
| 1   | 6     | 237   | 0        | 258      | 11      | 0            |
| 1   | 7     | 237   | 0        | 258      | 16      | 0            |
| 1   | 8     | 237   | 0        | 258      | 11      | 0            |
| 1   | 9     | 237   | 0        | 258      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 237   | 0        | 258      | 14      | 0            |
| 1   | AA    | 237   | 0        | 258      | 5       | 0            |
| 1   | B     | 237   | 0        | 258      | 10      | 0            |
| 1   | BA    | 237   | 0        | 258      | 13      | 0            |
| 1   | C     | 237   | 0        | 258      | 5       | 0            |
| 1   | CA    | 237   | 0        | 258      | 10      | 0            |
| 1   | D     | 237   | 0        | 258      | 6       | 0            |
| 1   | DA    | 237   | 0        | 258      | 7       | 0            |
| 1   | E     | 237   | 0        | 258      | 13      | 0            |
| 1   | EA    | 237   | 0        | 258      | 9       | 0            |
| 1   | F     | 237   | 0        | 258      | 6       | 0            |
| 1   | FA    | 237   | 0        | 258      | 6       | 0            |
| 1   | G     | 237   | 0        | 258      | 7       | 0            |
| 1   | GA    | 237   | 0        | 258      | 16      | 0            |
| 1   | H     | 237   | 0        | 258      | 11      | 0            |
| 1   | HA    | 237   | 0        | 258      | 17      | 0            |
| 1   | I     | 237   | 0        | 258      | 10      | 0            |
| 1   | IA    | 237   | 0        | 258      | 16      | 0            |
| 1   | J     | 237   | 0        | 258      | 9       | 0            |
| 1   | JA    | 237   | 0        | 258      | 17      | 0            |
| 1   | K     | 237   | 0        | 258      | 11      | 0            |
| 1   | L     | 237   | 0        | 258      | 8       | 0            |
| 1   | M     | 237   | 0        | 258      | 5       | 0            |
| 1   | N     | 237   | 0        | 258      | 9       | 0            |
| 1   | O     | 237   | 0        | 258      | 13      | 0            |
| 1   | P     | 237   | 0        | 258      | 15      | 0            |
| 1   | Q     | 237   | 0        | 258      | 24      | 0            |
| 1   | R     | 237   | 0        | 258      | 13      | 0            |
| 1   | S     | 237   | 0        | 258      | 9       | 0            |
| 1   | T     | 237   | 0        | 258      | 14      | 0            |
| 1   | U     | 237   | 0        | 258      | 8       | 0            |
| 1   | V     | 237   | 0        | 258      | 16      | 0            |
| 1   | W     | 237   | 0        | 258      | 9       | 0            |
| 1   | X     | 237   | 0        | 258      | 8       | 0            |
| 1   | Y     | 237   | 0        | 258      | 10      | 0            |
| 1   | Z     | 237   | 0        | 258      | 13      | 0            |
| 1   | a     | 237   | 0        | 258      | 10      | 0            |
| 1   | b     | 237   | 0        | 258      | 12      | 0            |
| 1   | c     | 237   | 0        | 258      | 6       | 0            |
| 1   | d     | 237   | 0        | 258      | 5       | 0            |
| 1   | e     | 237   | 0        | 258      | 8       | 0            |
| 1   | f     | 237   | 0        | 258      | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | g     | 237   | 0        | 258      | 13      | 0            |
| 1   | h     | 237   | 0        | 258      | 10      | 0            |
| 1   | i     | 237   | 0        | 258      | 12      | 0            |
| 1   | j     | 237   | 0        | 258      | 7       | 0            |
| 1   | k     | 237   | 0        | 258      | 11      | 0            |
| 1   | l     | 237   | 0        | 258      | 9       | 0            |
| 1   | m     | 237   | 0        | 258      | 14      | 0            |
| 1   | n     | 237   | 0        | 258      | 7       | 0            |
| 1   | o     | 237   | 0        | 258      | 11      | 0            |
| 1   | p     | 237   | 0        | 258      | 13      | 0            |
| 1   | q     | 237   | 0        | 258      | 13      | 0            |
| 1   | r     | 237   | 0        | 258      | 7       | 0            |
| 1   | s     | 237   | 0        | 258      | 20      | 0            |
| 1   | t     | 237   | 0        | 258      | 7       | 0            |
| 1   | u     | 237   | 0        | 258      | 8       | 0            |
| 1   | v     | 237   | 0        | 258      | 4       | 0            |
| 1   | w     | 237   | 0        | 258      | 5       | 0            |
| 1   | x     | 237   | 0        | 258      | 14      | 0            |
| 1   | y     | 237   | 0        | 258      | 8       | 0            |
| 1   | z     | 237   | 0        | 258      | 26      | 0            |
| All | All   | 17064 | 0        | 18576    | 580     | 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 16.

All (580) 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:Q:5121:PHI:I   | 1:s:2524:LYS:HD2 | 1.39                     | 1.93              |
| 1:z:3221:PHI:I   | 1:3:3625:ALA:HA  | 1.59                     | 1.70              |
| 1:Q:5121:PHI:I   | 1:s:2524:LYS:CD  | 2.32                     | 1.45              |
| 1:z:3221:PHI:I   | 1:3:3625:ALA:CA  | 2.30                     | 1.43              |
| 1:E:303:LYS:NZ   | 1:b:828:GLN:O    | 1.74                     | 1.21              |
| 1:x:3021:PHI:C   | 1:x:3021:PHI:HD2 | 1.74                     | 1.15              |
| 1:z:3221:PHI:I   | 1:3:3625:ALA:C   | 2.61                     | 1.11              |
| 1:R:5201:NLG:CD  | 1:R:5201:NLG:H2  | 1.66                     | 1.05              |
| 1:z:3221:PHI:I   | 1:3:3625:ALA:O   | 2.52                     | 0.98              |
| 1:V:5621:PHI:HE2 | 1:IA:6525:ALA:HA | 1.42                     | 0.97              |
| 1:V:5621:PHI:I   | 1:IA:6524:LYS:C  | 2.77                     | 0.97              |
| 1:Q:5121:PHI:HE1 | 1:r:2410:LYS:HE3 | 1.45                     | 0.95              |
| 1:z:3221:PHI:CE1 | 1:3:3628:GLN:CD  | 2.31                     | 0.94              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:x:3021:PHI:HD2  | 1:x:3021:PHI:O     | 1.67                     | 0.94              |
| 1:7:4017:LYS:O    | 1:7:4021:PHI:HD1   | 1.69                     | 0.93              |
| 1:x:3021:PHI:C    | 1:x:3021:PHI:CD2   | 2.45                     | 0.91              |
| 1:JA:6210:LYS:HG2 | 1:JA:6214:LYS:HZ3  | 1.39                     | 0.85              |
| 1:GA:6314:LYS:HA  | 1:GA:6317:LYS:HE2  | 1.58                     | 0.85              |
| 1:Q:5121:PHI:CE2  | 1:s:2524:LYS:NZ    | 2.42                     | 0.82              |
| 1:R:5201:NLG:CD   | 1:R:5201:NLG:N2    | 2.41                     | 0.81              |
| 1:Q:5121:PHI:I    | 1:s:2524:LYS:HB2   | 2.50                     | 0.81              |
| 1:Q:5121:PHI:HE1  | 1:r:2410:LYS:CE    | 2.11                     | 0.80              |
| 1:P:5023:PHE:HA   | 1:P:5026:ILE:HG12  | 1.64                     | 0.80              |
| 1:7:4017:LYS:HG2  | 1:7:4021:PHI:HE1   | 1.62                     | 0.80              |
| 1:z:3221:PHI:HE2  | 1:3:3625:ALA:HB1   | 1.62                     | 0.80              |
| 1:s:2525:ALA:O    | 1:s:2528:GLN:HG2   | 1.83                     | 0.79              |
| 1:q:2321:PHI:HD2  | 1:q:2321:PHI:O     | 1.81                     | 0.79              |
| 1:7:4017:LYS:CG   | 1:7:4021:PHI:HE1   | 2.16                     | 0.76              |
| 1:E:321:PHI:I     | 1:k:1721:PHI:HE2   | 2.56                     | 0.74              |
| 1:A:6107:GLN:NE2  | 1:A:6108:GLU:OE2   | 2.20                     | 0.74              |
| 1:2:3524:LYS:O    | 1:2:3528:GLN:NE2   | 2.21                     | 0.73              |
| 1:0:3326:ILE:HD13 | 1:1:3401:NLG:HGC2  | 1.71                     | 0.73              |
| 1:q:2321:PHI:O    | 1:q:2321:PHI:CD2   | 2.37                     | 0.72              |
| 1:R:5201:NLG:N2   | 1:R:5201:NLG:OE1   | 2.21                     | 0.72              |
| 1:1:3417:LYS:O    | 1:1:3421:PHI:HD1   | 1.87                     | 0.72              |
| 1:Q:5121:PHI:CE2  | 1:s:2524:LYS:HZ1   | 2.02                     | 0.72              |
| 1:1:3429:LYS:NZ   | 1:BA:6824:LYS:HE3  | 2.05                     | 0.72              |
| 1:K:4508:GLU:HB2  | 1:L:4619:ILE:HD11  | 1.71                     | 0.71              |
| 1:h:1423:PHE:HA   | 1:h:1426:ILE:HG22  | 1.71                     | 0.71              |
| 1:1:3429:LYS:HE3  | 1:BA:6824:LYS:HZ1  | 1.55                     | 0.71              |
| 1:7:4003:LYS:NZ   | 1:8:4128:GLN:OE1   | 2.24                     | 0.71              |
| 1:7:4024:LYS:CG   | 1:CA:6921:PHI:I    | 3.09                     | 0.71              |
| 1:Q:5121:PHI:I    | 1:s:2524:LYS:CG    | 3.09                     | 0.71              |
| 1:i:1523:PHE:HA   | 1:i:1526:ILE:HG22  | 1.74                     | 0.69              |
| 1:1:3401:NLG:HBC1 | 1:1:3402:LEU:HD22  | 1.75                     | 0.68              |
| 1:V:5623:PHE:HA   | 1:V:5626:ILE:HG22  | 1.76                     | 0.68              |
| 1:z:3221:PHI:CZ   | 1:3:3625:ALA:HA    | 2.24                     | 0.68              |
| 1:2:3511:ALA:O    | 1:2:3515:LYS:HG2   | 1.94                     | 0.68              |
| 1:g:1328:GLN:HG2  | 1:p:2221:PHI:I     | 2.63                     | 0.68              |
| 1:x:3021:PHI:O    | 1:x:3021:PHI:CD2   | 2.37                     | 0.67              |
| 1:7:4001:NLG:H8C2 | 1:7:4003:LYS:HG2   | 1.76                     | 0.67              |
| 1:CA:6923:PHE:HA  | 1:CA:6926:ILE:HG22 | 1.77                     | 0.67              |
| 1:1:3420:ALA:O    | 1:1:3424:LYS:HG3   | 1.94                     | 0.67              |
| 1:M:4711:ALA:O    | 1:M:4715:LYS:HG2   | 1.94                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:323:PHE:HA     | 1:E:326:ILE:HG22   | 1.76                     | 0.66              |
| 1:z:3221:PHI:CZ    | 1:3:3628:GLN:NE2   | 2.58                     | 0.66              |
| 1:t:2623:PHE:HA    | 1:t:2626:ILE:HG22  | 1.77                     | 0.66              |
| 1:T:5426:ILE:HD13  | 1:Y:5901:NLG:HGC2  | 1.78                     | 0.65              |
| 1:BA:6823:PHE:HA   | 1:BA:6826:ILE:HG22 | 1.79                     | 0.65              |
| 1:Q:5121:PHI:CE1   | 1:r:2410:LYS:HE3   | 2.24                     | 0.65              |
| 1:GA:6321:PHI:HA   | 1:GA:6324:LYS:HD2  | 1.79                     | 0.65              |
| 1:a:715:LYS:HB3    | 1:b:808:GLU:OE2    | 1.97                     | 0.64              |
| 1:0:3323:PHE:HA    | 1:0:3326:ILE:HG22  | 1.79                     | 0.64              |
| 1:7:4024:LYS:HG3   | 1:CA:6921:PHI:I    | 2.66                     | 0.64              |
| 1:Q:5121:PHI:I     | 1:s:2524:LYS:CB    | 3.15                     | 0.64              |
| 1:JA:6211:ALA:HA   | 1:JA:6214:LYS:HE2  | 1.78                     | 0.64              |
| 1:D:223:PHE:HA     | 1:D:226:ILE:HG22   | 1.79                     | 0.64              |
| 1:Q:5123:PHE:HA    | 1:Q:5126:ILE:HG22  | 1.80                     | 0.64              |
| 1:Q:5121:PHI:HE2   | 1:s:2524:LYS:CE    | 2.28                     | 0.64              |
| 1:k:1711:ALA:O     | 1:k:1715:LYS:HG2   | 1.97                     | 0.63              |
| 1:s:2515:LYS:HB2   | 1:t:2612:ILE:HD11  | 1.80                     | 0.63              |
| 1:P:5024:LYS:NZ    | 1:m:1929:LYS:HE2   | 2.13                     | 0.63              |
| 1:z:3201:NLG:H8C2  | 1:z:3203:LYS:HB2   | 1.80                     | 0.63              |
| 1:z:3223:PHE:HA    | 1:z:3226:ILE:HG22  | 1.79                     | 0.63              |
| 1:E:321:PHI:I      | 1:k:1724:LYS:HG3   | 2.68                     | 0.63              |
| 1:q:2311:ALA:O     | 1:q:2315:LYS:HG2   | 1.99                     | 0.63              |
| 1:p:2215:LYS:O     | 1:p:2219:ILE:HD12  | 1.99                     | 0.63              |
| 1:DA:7010:LYS:HE2  | 1:EA:7121:PHI:I    | 2.69                     | 0.63              |
| 1:g:1315:LYS:O     | 1:g:1319:ILE:HD12  | 1.98                     | 0.63              |
| 1:J:4403:LYS:O     | 1:J:4407:GLN:NE2   | 2.32                     | 0.63              |
| 1:T:5401:NLG:HBC2  | 1:T:5402:LEU:HD22  | 1.81                     | 0.63              |
| 1:z:3221:PHI:HE2   | 1:3:3625:ALA:CB    | 2.29                     | 0.62              |
| 1:GA:6323:PHE:HA   | 1:GA:6326:ILE:HG12 | 1.82                     | 0.62              |
| 1:q:2321:PHI:CD2   | 1:q:2321:PHI:C     | 2.74                     | 0.62              |
| 1:5:3823:PHE:HA    | 1:5:3826:ILE:HG22  | 1.82                     | 0.62              |
| 1:a:711:ALA:O      | 1:a:715:LYS:HG2    | 2.00                     | 0.62              |
| 1:GA:6312:ILE:HG22 | 1:GA:6316:PHE:HE2  | 1.63                     | 0.62              |
| 1:J:4423:PHE:HA    | 1:J:4426:ILE:HG22  | 1.82                     | 0.62              |
| 1:g:1315:LYS:HB3   | 1:h:1408:GLU:OE2   | 2.00                     | 0.62              |
| 1:IA:6516:PHE:HA   | 1:IA:6519:ILE:HD12 | 1.81                     | 0.62              |
| 1:q:2321:PHI:HD2   | 1:q:2321:PHI:C     | 2.29                     | 0.62              |
| 1:T:5419:ILE:HD11  | 1:Y:5908:GLU:HB3   | 1.82                     | 0.61              |
| 1:7:4017:LYS:HG2   | 1:7:4021:PHI:CE1   | 2.30                     | 0.61              |
| 1:z:3221:PHI:CE1   | 1:3:3628:GLN:NE2   | 2.62                     | 0.61              |
| 1:FA:6009:PHE:HA   | 1:FA:6012:ILE:HG12 | 1.81                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Q:5105:ILE:HD12  | 1:R:5219:ILE:HG13  | 1.83                     | 0.61              |
| 1:4:3711:ALA:O     | 1:4:3715:LYS:HG2   | 2.00                     | 0.61              |
| 1:N:4823:PHE:HA    | 1:N:4826:ILE:HG22  | 1.83                     | 0.60              |
| 1:S:5311:ALA:O     | 1:S:5315:LYS:HG2   | 2.00                     | 0.60              |
| 1:1:3429:LYS:HZ2   | 1:BA:6824:LYS:HE3  | 1.66                     | 0.60              |
| 1:A:6111:ALA:O     | 1:A:6115:LYS:HG2   | 2.01                     | 0.60              |
| 1:1:3429:LYS:CE    | 1:BA:6824:LYS:HZ1  | 2.13                     | 0.60              |
| 1:AA:6711:ALA:O    | 1:AA:6715:LYS:HG2  | 2.01                     | 0.60              |
| 1:JA:6213:ALA:HB1  | 1:GA:6317:LYS:HD3  | 1.83                     | 0.60              |
| 1:C:111:ALA:O      | 1:C:115:LYS:HG2    | 2.01                     | 0.60              |
| 1:w:2929:LYS:HZ3   | 1:w:2929:LYS:HA    | 1.67                     | 0.60              |
| 1:o:2123:PHE:HA    | 1:o:2126:ILE:HG22  | 1.83                     | 0.60              |
| 1:JA:6223:PHE:HA   | 1:JA:6226:ILE:HG22 | 1.82                     | 0.60              |
| 1:i:1501:NLG:H8C2  | 1:i:1503:LYS:HB2   | 1.82                     | 0.60              |
| 1:O:4911:ALA:O     | 1:O:4915:LYS:HG2   | 2.02                     | 0.60              |
| 1:s:2511:ALA:O     | 1:s:2515:LYS:HG2   | 2.02                     | 0.60              |
| 1:9:6608:GLU:O     | 1:9:6612:ILE:HD12  | 2.02                     | 0.60              |
| 1:H:4202:LEU:HD13  | 1:H:4205:ILE:HD12  | 1.83                     | 0.60              |
| 1:N:4808:GLU:O     | 1:N:4812:ILE:HD12  | 2.02                     | 0.60              |
| 1:FA:6023:PHE:HA   | 1:FA:6026:ILE:HG22 | 1.84                     | 0.60              |
| 1:A:6108:GLU:O     | 1:A:6112:ILE:HG12  | 2.01                     | 0.60              |
| 1:JA:6210:LYS:HG2  | 1:JA:6214:LYS:NZ   | 2.15                     | 0.59              |
| 1:Q:5111:ALA:O     | 1:Q:5115:LYS:HG2   | 2.02                     | 0.59              |
| 1:6:3921:PHI:HA    | 1:6:3924:LYS:HZ3   | 1.67                     | 0.59              |
| 1:IA:6511:ALA:O    | 1:IA:6515:LYS:HG2  | 2.01                     | 0.59              |
| 1:8:4111:ALA:O     | 1:8:4115:LYS:HG2   | 2.02                     | 0.59              |
| 1:I:4311:ALA:O     | 1:I:4315:LYS:HG2   | 2.02                     | 0.59              |
| 1:N:4821:PHI:I     | 1:T:5428:GLN:HG2   | 2.72                     | 0.59              |
| 1:9:6602:LEU:HD13  | 1:9:6605:ILE:HD12  | 1.85                     | 0.59              |
| 1:3:3602:LEU:HA    | 1:3:3605:ILE:HD12  | 1.84                     | 0.59              |
| 1:W:5723:PHE:HA    | 1:W:5726:ILE:HG22  | 1.84                     | 0.59              |
| 1:c:923:PHE:HA     | 1:c:926:ILE:HG22   | 1.83                     | 0.59              |
| 1:g:1311:ALA:O     | 1:g:1315:LYS:HG2   | 2.03                     | 0.59              |
| 1:g:1319:ILE:HD11  | 1:h:1408:GLU:OE1   | 2.03                     | 0.59              |
| 1:B:8:GLU:O        | 1:B:12:ILE:HD12    | 2.02                     | 0.58              |
| 1:r:2423:PHE:HA    | 1:r:2426:ILE:HG22  | 1.84                     | 0.58              |
| 1:GA:6312:ILE:HG22 | 1:GA:6316:PHE:CE2  | 2.38                     | 0.58              |
| 1:R:5201:NLG:HBC2  | 1:R:5202:LEU:HD22  | 1.85                     | 0.58              |
| 1:e:1111:ALA:O     | 1:e:1115:LYS:HG2   | 2.04                     | 0.58              |
| 1:w:2911:ALA:O     | 1:w:2915:LYS:HG2   | 2.02                     | 0.58              |
| 1:8:4124:LYS:O     | 1:8:4128:GLN:NE2   | 2.35                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Z:608:GLU:O      | 1:Z:612:ILE:HD12   | 2.04                     | 0.58              |
| 1:AA:6715:LYS:HB2  | 1:BA:6812:ILE:HD11 | 1.86                     | 0.58              |
| 1:B:2:LEU:HD13     | 1:B:5:ILE:HD12     | 1.85                     | 0.58              |
| 1:L:4610:LYS:HD3   | 1:X:5821:PHI:HE2   | 1.84                     | 0.58              |
| 1:O:4902:LEU:HD13  | 1:O:4905:ILE:HD13  | 1.84                     | 0.58              |
| 1:3:3608:GLU:O     | 1:3:3612:ILE:HD12  | 2.04                     | 0.58              |
| 1:6:3923:PHE:HA    | 1:6:3926:ILE:HG22  | 1.84                     | 0.58              |
| 1:GA:6305:ILE:HG23 | 1:GA:6309:PHE:HE2  | 1.69                     | 0.58              |
| 1:C:115:LYS:HB2    | 1:D:212:ILE:HD11   | 1.86                     | 0.57              |
| 1:A:6115:LYS:HB2   | 1:JA:6212:ILE:HD11 | 1.85                     | 0.57              |
| 1:g:1308:GLU:OE2   | 1:h:1415:LYS:HB3   | 2.05                     | 0.57              |
| 1:m:1908:GLU:OE2   | 1:n:2015:LYS:HB3   | 2.04                     | 0.57              |
| 1:B:19:ILE:HD11    | 1:G:508:GLU:HG2    | 1.86                     | 0.57              |
| 1:V:5621:PHI:I     | 1:IA:6528:GLN:HG2  | 2.74                     | 0.57              |
| 1:G:511:ALA:O      | 1:G:515:LYS:HG2    | 2.04                     | 0.57              |
| 1:l:1819:ILE:HD11  | 1:q:2308:GLU:HB2   | 1.87                     | 0.57              |
| 1:T:5402:LEU:HD13  | 1:T:5405:ILE:HD12  | 1.87                     | 0.57              |
| 1:b:804:ALA:O      | 1:b:808:GLU:HB2    | 2.04                     | 0.57              |
| 1:1:3429:LYS:NZ    | 1:BA:6824:LYS:CE   | 2.68                     | 0.57              |
| 1:Z:629:LYS:HZ3    | 1:Z:629:LYS:HA     | 1.70                     | 0.56              |
| 1:5:3815:LYS:O     | 1:5:3819:ILE:HG12  | 2.05                     | 0.56              |
| 1:K:4511:ALA:O     | 1:K:4515:LYS:HG2   | 2.04                     | 0.56              |
| 1:O:4915:LYS:HE2   | 1:P:5008:GLU:OE1   | 2.04                     | 0.56              |
| 1:c:911:ALA:O      | 1:c:915:LYS:HG2    | 2.05                     | 0.56              |
| 1:i:1504:ALA:O     | 1:i:1508:GLU:HG2   | 2.06                     | 0.56              |
| 1:k:1701:NLG:H8C2  | 1:k:1703:LYS:HB2   | 1.87                     | 0.56              |
| 1:EA:7111:ALA:O    | 1:EA:7115:LYS:HG2  | 2.04                     | 0.56              |
| 1:Q:5121:PHI:HE2   | 1:s:2524:LYS:HE3   | 1.86                     | 0.56              |
| 1:V:5621:PHI:CE2   | 1:IA:6525:ALA:HA   | 2.27                     | 0.56              |
| 1:Q:5121:PHI:HE2   | 1:s:2524:LYS:NZ    | 2.21                     | 0.56              |
| 1:u:2723:PHE:HA    | 1:u:2726:ILE:HG22  | 1.87                     | 0.56              |
| 1:y:3111:ALA:O     | 1:y:3115:LYS:HG2   | 2.05                     | 0.56              |
| 1:0:3315:LYS:HB2   | 1:1:3412:ILE:HD11  | 1.87                     | 0.56              |
| 1:GA:6308:GLU:OE2  | 1:HA:6419:ILE:HG13 | 2.06                     | 0.56              |
| 1:Z:619:ILE:HD11   | 1:e:1108:GLU:HB3   | 1.86                     | 0.56              |
| 1:J:4408:GLU:O     | 1:J:4412:ILE:HG12  | 2.05                     | 0.56              |
| 1:9:6619:ILE:HD11  | 1:EA:7108:GLU:HG2  | 1.86                     | 0.56              |
| 1:o:2115:LYS:O     | 1:o:2119:ILE:HD12  | 2.06                     | 0.56              |
| 1:6:3901:NLG:HBC1  | 1:6:3902:LEU:HD22  | 1.88                     | 0.56              |
| 1:H:4209:PHE:HA    | 1:H:4212:ILE:HG12  | 1.88                     | 0.56              |
| 1:H:4217:LYS:HD2   | 1:H:4221:PHI:I     | 2.76                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:4:3705:ILE:HD12  | 1:5:3819:ILE:HD12  | 1.88                     | 0.56              |
| 1:o:2108:GLU:O     | 1:o:2112:ILE:HD12  | 2.05                     | 0.55              |
| 1:2:3514:LYS:HA    | 1:2:3517:LYS:HE3   | 1.88                     | 0.55              |
| 1:U:5509:PHE:HA    | 1:U:5512:ILE:HG12  | 1.88                     | 0.55              |
| 1:u:2701:NLG:HBC1  | 1:u:2702:LEU:HD22  | 1.88                     | 0.55              |
| 1:E:307:GLN:NE2    | 1:b:830:NH2:N      | 2.54                     | 0.55              |
| 1:V:5601:NLG:H8C2  | 1:V:5603:LYS:HB2   | 1.88                     | 0.55              |
| 1:N:4801:NLG:HBC2  | 1:N:4802:LEU:HD22  | 1.88                     | 0.55              |
| 1:n:2001:NLG:H8C2  | 1:n:2003:LYS:HB2   | 1.89                     | 0.55              |
| 1:IA:6510:LYS:O    | 1:IA:6514:LYS:HG2  | 2.07                     | 0.55              |
| 1:P:5024:LYS:NZ    | 1:m:1929:LYS:CE    | 2.70                     | 0.55              |
| 1:T:5408:GLU:O     | 1:T:5412:ILE:HD12  | 2.06                     | 0.55              |
| 1:W:5705:ILE:HD12  | 1:X:5819:ILE:HG23  | 1.87                     | 0.55              |
| 1:W:5711:ALA:O     | 1:W:5715:LYS:HG2   | 2.06                     | 0.55              |
| 1:g:1321:PHI:HE1   | 1:p:2224:LYS:HD3   | 1.88                     | 0.55              |
| 1:m:1911:ALA:O     | 1:m:1915:LYS:HG2   | 2.07                     | 0.55              |
| 1:1:3429:LYS:HD2   | 1:1:3429:LYS:N     | 2.20                     | 0.55              |
| 1:7:4024:LYS:HG2   | 1:CA:6921:PHI:I    | 2.77                     | 0.55              |
| 1:B:23:PHE:HA      | 1:B:26:ILE:HG22    | 1.89                     | 0.55              |
| 1:3:3623:PHE:HE1   | 1:8:4105:ILE:HG12  | 1.72                     | 0.55              |
| 1:DA:7004:ALA:O    | 1:DA:7008:GLU:HG2  | 2.07                     | 0.55              |
| 1:9:6623:PHE:HA    | 1:9:6626:ILE:HG22  | 1.89                     | 0.54              |
| 1:O:4901:NLG:HBC1  | 1:O:4902:LEU:HD22  | 1.90                     | 0.54              |
| 1:r:2402:LEU:HD13  | 1:r:2405:ILE:HD12  | 1.88                     | 0.54              |
| 1:Q:5101:NLG:H8C2  | 1:Q:5103:LYS:HB2   | 1.89                     | 0.54              |
| 1:0:3315:LYS:HG3   | 1:1:3408:GLU:OE2   | 2.06                     | 0.54              |
| 1:K:4515:LYS:HD2   | 1:L:4608:GLU:OE2   | 2.06                     | 0.54              |
| 1:FA:6023:PHE:HE2  | 1:A:6109:PHE:HE2   | 1.54                     | 0.54              |
| 1:P:5024:LYS:HZ1   | 1:m:1929:LYS:HE2   | 1.72                     | 0.54              |
| 1:h:1404:ALA:O     | 1:h:1408:GLU:HB2   | 2.07                     | 0.54              |
| 1:1:3415:LYS:O     | 1:1:3419:ILE:HD12  | 2.08                     | 0.54              |
| 1:X:5815:LYS:O     | 1:X:5819:ILE:HD12  | 2.07                     | 0.54              |
| 1:HA:6415:LYS:O    | 1:HA:6419:ILE:HD12 | 2.08                     | 0.54              |
| 1:IA:6519:ILE:HG22 | 1:IA:6523:PHE:CE2  | 2.43                     | 0.54              |
| 1:B:15:LYS:HB2     | 1:G:512:ILE:HD11   | 1.90                     | 0.54              |
| 1:O:4902:LEU:HA    | 1:O:4905:ILE:HD13  | 1.90                     | 0.54              |
| 1:U:5511:ALA:O     | 1:U:5515:LYS:HG2   | 2.08                     | 0.54              |
| 1:9:6615:LYS:HB2   | 1:EA:7112:ILE:HD11 | 1.90                     | 0.54              |
| 1:F:404:ALA:O      | 1:F:408:GLU:HG2    | 2.07                     | 0.54              |
| 1:y:3108:GLU:HB2   | 1:z:3219:ILE:HD11  | 1.90                     | 0.54              |
| 1:O:4908:GLU:HG2   | 1:O:4909:PHE:N     | 2.23                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:j:1615:LYS:O    | 1:j:1619:ILE:HD12  | 2.08                     | 0.53              |
| 1:V:5611:ALA:O    | 1:V:5615:LYS:HG2   | 2.08                     | 0.53              |
| 1:n:2028:GLN:OE1  | 1:o:2103:LYS:NZ    | 2.25                     | 0.53              |
| 1:T:5408:GLU:OE2  | 1:Y:5915:LYS:HE2   | 2.07                     | 0.53              |
| 1:V:5621:PHI:HE2  | 1:IA:6525:ALA:CA   | 2.29                     | 0.53              |
| 1:t:2601:NLG:H8C2 | 1:t:2603:LYS:HB2   | 1.91                     | 0.53              |
| 1:O:4905:ILE:HA   | 1:O:4908:GLU:OE1   | 2.08                     | 0.53              |
| 1:h:1424:LYS:HD2  | 1:i:1503:LYS:HZ1   | 1.73                     | 0.53              |
| 1:u:2715:LYS:HD2  | 1:v:2808:GLU:OE2   | 2.08                     | 0.53              |
| 1:K:4514:LYS:HE2  | 1:K:4514:LYS:HA    | 1.91                     | 0.53              |
| 1:I:4308:GLU:O    | 1:I:4312:ILE:HG12  | 2.09                     | 0.53              |
| 1:u:2711:ALA:O    | 1:u:2715:LYS:HG2   | 2.09                     | 0.53              |
| 1:4:3715:LYS:HB2  | 1:5:3812:ILE:HD11  | 1.90                     | 0.53              |
| 1:HA:6409:PHE:HA  | 1:HA:6412:ILE:HD12 | 1.91                     | 0.53              |
| 1:m:1915:LYS:HB2  | 1:n:2012:ILE:HD11  | 1.91                     | 0.53              |
| 1:B:11:ALA:O      | 1:B:15:LYS:HG3     | 2.09                     | 0.53              |
| 1:F:415:LYS:O     | 1:F:419:ILE:HD12   | 2.09                     | 0.53              |
| 1:f:1202:LEU:HD13 | 1:f:1205:ILE:HD12  | 1.90                     | 0.53              |
| 1:f:1223:PHE:HA   | 1:f:1226:ILE:HG22  | 1.90                     | 0.53              |
| 1:g:1302:LEU:HD13 | 1:g:1305:ILE:HD13  | 1.90                     | 0.53              |
| 1:i:1512:ILE:HD11 | 1:j:1615:LYS:HB2   | 1.91                     | 0.53              |
| 1:E:311:ALA:O     | 1:E:315:LYS:HG2    | 2.09                     | 0.52              |
| 1:b:801:NLG:H8C2  | 1:b:803:LYS:HB2    | 1.90                     | 0.52              |
| 1:z:3221:PHI:HE2  | 1:3:3625:ALA:CA    | 2.39                     | 0.52              |
| 1:K:4523:PHE:HA   | 1:K:4526:ILE:HG22  | 1.91                     | 0.52              |
| 1:Z:615:LYS:HB2   | 1:e:1112:ILE:HD11  | 1.92                     | 0.52              |
| 1:6:3911:ALA:O    | 1:6:3915:LYS:HG2   | 2.10                     | 0.52              |
| 1:DA:7015:LYS:O   | 1:DA:7019:ILE:HD12 | 2.09                     | 0.52              |
| 1:I:4315:LYS:HB2  | 1:J:4412:ILE:HD11  | 1.90                     | 0.52              |
| 1:R:5203:LYS:NZ   | 1:S:5328:GLN:OE1   | 2.41                     | 0.52              |
| 1:4:3704:ALA:HA   | 1:4:3707:GLN:NE2   | 2.25                     | 0.52              |
| 1:7:4009:PHE:HD1  | 1:7:4012:ILE:HD12  | 1.75                     | 0.52              |
| 1:W:5708:GLU:HB3  | 1:X:5819:ILE:HD11  | 1.92                     | 0.52              |
| 1:0:3323:PHE:HE1  | 1:1:3405:ILE:HG12  | 1.74                     | 0.52              |
| 1:1:3429:LYS:HZ1  | 1:BA:6824:LYS:HE3  | 1.74                     | 0.52              |
| 1:d:1015:LYS:O    | 1:d:1019:ILE:HD12  | 2.08                     | 0.52              |
| 1:o:2111:ALA:O    | 1:o:2115:LYS:HG2   | 2.09                     | 0.52              |
| 1:W:5701:NLG:H8C1 | 1:W:5703:LYS:HE2   | 1.91                     | 0.52              |
| 1:7:4007:GLN:NE2  | 1:7:4008:GLU:OE1   | 2.41                     | 0.52              |
| 1:o:2104:ALA:HA   | 1:o:2107:GLN:NE2   | 2.25                     | 0.52              |
| 1:D:201:NLG:H8C2  | 1:D:203:LYS:HB2    | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:9:6611:ALA:O     | 1:9:6615:LYS:HG3   | 2.09                     | 0.51              |
| 1:HA:6405:ILE:O    | 1:HA:6409:PHE:HD1  | 1.94                     | 0.51              |
| 1:HA:6412:ILE:HG22 | 1:HA:6416:PHE:CE2  | 2.45                     | 0.51              |
| 1:HA:6416:PHE:HA   | 1:HA:6419:ILE:HD13 | 1.92                     | 0.51              |
| 1:IA:6520:ALA:O    | 1:IA:6524:LYS:HG3  | 2.10                     | 0.51              |
| 1:H:4215:LYS:O     | 1:H:4219:ILE:HG12  | 2.10                     | 0.51              |
| 1:r:2419:ILE:HD11  | 1:w:2908:GLU:HB3   | 1.92                     | 0.51              |
| 1:CA:6911:ALA:O    | 1:CA:6915:LYS:HG2  | 2.09                     | 0.51              |
| 1:T:5417:LYS:HD2   | 1:T:5421:PHI:I     | 2.80                     | 0.51              |
| 1:f:1208:GLU:OE2   | 1:k:1715:LYS:HB3   | 2.11                     | 0.51              |
| 1:P:5024:LYS:HZ2   | 1:m:1929:LYS:HE3   | 1.75                     | 0.51              |
| 1:Q:5121:PHI:CE2   | 1:s:2524:LYS:HZ2   | 2.24                     | 0.51              |
| 1:5:3801:NLG:H8C2  | 1:5:3803:LYS:HB2   | 1.93                     | 0.51              |
| 1:l:1811:ALA:O     | 1:l:1814:LYS:HG2   | 2.10                     | 0.51              |
| 1:v:2815:LYS:O     | 1:v:2819:ILE:HD12  | 2.09                     | 0.51              |
| 1:m:1919:ILE:HD11  | 1:n:2008:GLU:OE1   | 2.11                     | 0.51              |
| 1:o:2115:LYS:HD2   | 1:p:2208:GLU:OE2   | 2.11                     | 0.51              |
| 1:t:2601:NLG:HBC1  | 1:t:2602:LEU:HD22  | 1.92                     | 0.51              |
| 1:CA:6908:GLU:HB3  | 1:DA:7019:ILE:HD11 | 1.93                     | 0.51              |
| 1:a:715:LYS:HB2    | 1:b:812:ILE:HD11   | 1.93                     | 0.51              |
| 1:C:108:GLU:OE1    | 1:D:215:LYS:HD2    | 2.12                     | 0.50              |
| 1:E:308:GLU:HB3    | 1:F:419:ILE:HD11   | 1.93                     | 0.50              |
| 1:j:1627:ALA:HB1   | 1:k:1703:LYS:HZ2   | 1.77                     | 0.50              |
| 1:u:2705:ILE:HD12  | 1:v:2819:ILE:HG23  | 1.92                     | 0.50              |
| 1:x:3019:ILE:HD11  | 1:2:3508:GLU:HB3   | 1.94                     | 0.50              |
| 1:V:5603:LYS:HZ3   | 1:W:5724:LYS:HG2   | 1.76                     | 0.50              |
| 1:o:2105:ILE:HD12  | 1:p:2219:ILE:HG23  | 1.94                     | 0.50              |
| 1:BA:6801:NLG:H8C2 | 1:BA:6803:LYS:HB2  | 1.92                     | 0.50              |
| 1:m:1902:LEU:HA    | 1:m:1905:ILE:HD13  | 1.92                     | 0.50              |
| 1:4:3715:LYS:HE2   | 1:5:3808:GLU:OE1   | 2.11                     | 0.50              |
| 1:N:4815:LYS:HB2   | 1:S:5312:ILE:HD11  | 1.93                     | 0.50              |
| 1:R:5216:PHE:HA    | 1:R:5219:ILE:HG22  | 1.93                     | 0.50              |
| 1:V:5601:NLG:HBC1  | 1:V:5602:LEU:HD22  | 1.93                     | 0.50              |
| 1:GA:6305:ILE:HG23 | 1:GA:6309:PHE:CE2  | 2.47                     | 0.50              |
| 1:HA:6416:PHE:HB2  | 1:IA:6513:ALA:HB2  | 1.93                     | 0.50              |
| 1:O:4915:LYS:HB2   | 1:P:5012:ILE:HD11  | 1.94                     | 0.49              |
| 1:U:5501:NLG:HBC1  | 1:U:5502:LEU:HD12  | 1.94                     | 0.49              |
| 1:0:3311:ALA:HB1   | 1:0:3315:LYS:NZ    | 2.27                     | 0.49              |
| 1:A:6101:NLG:HGC2  | 1:JA:6226:ILE:HB   | 1.93                     | 0.49              |
| 1:IA:6501:NLG:H8C2 | 1:IA:6503:LYS:HD2  | 1.95                     | 0.49              |
| 1:4:3719:ILE:HD11  | 1:5:3808:GLU:HB2   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6:3921:PHI:HD1   | 1:6:3924:LYS:NZ    | 2.27                     | 0.49              |
| 1:W:5715:LYS:HB3   | 1:X:5808:GLU:OE2   | 2.13                     | 0.49              |
| 1:d:1002:LEU:HD13  | 1:d:1005:ILE:HD13  | 1.93                     | 0.49              |
| 1:GA:6311:ALA:O    | 1:GA:6314:LYS:HG2  | 2.12                     | 0.49              |
| 1:l:1815:LYS:HB2   | 1:q:2312:ILE:HD11  | 1.94                     | 0.49              |
| 1:u:2721:PHI:I     | 1:x:3006:ALA:HB1   | 2.83                     | 0.49              |
| 1:H:4226:ILE:HD13  | 1:M:4701:NLG:HGC2  | 1.95                     | 0.49              |
| 1:3:3623:PHE:HA    | 1:3:3626:ILE:HG22  | 1.95                     | 0.49              |
| 1:AA:6708:GLU:OE1  | 1:BA:6815:LYS:HD2  | 2.12                     | 0.49              |
| 1:3:3605:ILE:HD13  | 1:8:4123:PHE:HE1   | 1.77                     | 0.49              |
| 1:A:6110:LYS:HE2   | 1:A:6114:LYS:NZ    | 2.27                     | 0.49              |
| 1:Y:5923:PHE:HA    | 1:Y:5926:ILE:HG22  | 1.95                     | 0.48              |
| 1:f:1219:ILE:HG23  | 1:k:1705:ILE:HD12  | 1.94                     | 0.48              |
| 1:M:4721:PHI:I     | 1:X:5824:LYS:HB3   | 2.84                     | 0.48              |
| 1:z:3208:GLU:O     | 1:z:3212:ILE:HG12  | 2.13                     | 0.48              |
| 1:HA:6412:ILE:HG22 | 1:HA:6416:PHE:HE2  | 1.78                     | 0.48              |
| 1:K:4518:ALA:O     | 1:K:4521:PHI:HB2   | 2.13                     | 0.48              |
| 1:s:2515:LYS:HE2   | 1:t:2608:GLU:OE1   | 2.14                     | 0.48              |
| 1:y:3124:LYS:HG2   | 1:y:3128:GLN:HE22  | 1.77                     | 0.48              |
| 1:3:3619:ILE:HD11  | 1:8:4108:GLU:HB3   | 1.95                     | 0.48              |
| 1:N:4812:ILE:HG23  | 1:S:5312:ILE:HD12  | 1.95                     | 0.48              |
| 1:T:5415:LYS:HB2   | 1:Y:5912:ILE:HD11  | 1.96                     | 0.48              |
| 1:d:1004:ALA:O     | 1:d:1008:GLU:HG2   | 2.13                     | 0.48              |
| 1:y:3124:LYS:O     | 1:y:3128:GLN:NE2   | 2.47                     | 0.48              |
| 1:I:4315:LYS:HE2   | 1:J:4408:GLU:OE1   | 2.13                     | 0.48              |
| 1:x:3001:NLG:HBC2  | 1:x:3002:LEU:HD22  | 1.95                     | 0.48              |
| 1:GA:6315:LYS:O    | 1:GA:6319:ILE:HG13 | 2.14                     | 0.48              |
| 1:w:2906:ALA:O     | 1:w:2910:LYS:HG2   | 2.14                     | 0.48              |
| 1:z:3215:LYS:O     | 1:z:3219:ILE:HG12  | 2.14                     | 0.48              |
| 1:GA:6315:LYS:HD3  | 1:HA:6415:LYS:HZ3  | 1.78                     | 0.48              |
| 1:b:822:GLU:O      | 1:b:826:ILE:HD12   | 2.13                     | 0.48              |
| 1:HA:6414:LYS:O    | 1:HA:6417:LYS:HG2  | 2.14                     | 0.48              |
| 1:i:1522:GLU:OE1   | 1:j:1605:ILE:HD11  | 2.14                     | 0.48              |
| 1:o:2101:NLG:H8C2  | 1:o:2103:LYS:HB2   | 1.96                     | 0.48              |
| 1:p:2203:LYS:HD2   | 1:q:2327:ALA:HB1   | 1.96                     | 0.47              |
| 1:6:3901:NLG:H8C2  | 1:6:3903:LYS:HB3   | 1.96                     | 0.47              |
| 1:1:3428:GLN:C     | 1:1:3429:LYS:HD2   | 2.39                     | 0.47              |
| 1:Z:604:ALA:HA     | 1:Z:607:GLN:NE2    | 2.30                     | 0.47              |
| 1:0:3301:NLG:H8C2  | 1:0:3303:LYS:HB3   | 1.96                     | 0.47              |
| 1:7:4024:LYS:HD3   | 1:CA:6921:PHI:HE2  | 1.95                     | 0.47              |
| 1:D:207:GLN:HA     | 1:D:207:GLN:OE1    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:H:4223:PHE:HB3  | 1:I:4306:ALA:HB2   | 1.97                     | 0.47              |
| 1:K:4506:ALA:O    | 1:K:4510:LYS:HG2   | 2.15                     | 0.47              |
| 1:Y:5901:NLG:O    | 1:Y:5904:ALA:N     | 2.47                     | 0.47              |
| 1:Y:5914:LYS:HG3  | 1:Y:5917:LYS:NZ    | 2.29                     | 0.47              |
| 1:c:908:GLU:HB3   | 1:d:1019:ILE:HD11  | 1.95                     | 0.47              |
| 1:y:3115:LYS:HB2  | 1:z:3212:ILE:HD11  | 1.95                     | 0.47              |
| 1:O:3305:ILE:HD12 | 1:1:3419:ILE:HG23  | 1.97                     | 0.47              |
| 1:BA:6807:GLN:HA  | 1:BA:6807:GLN:OE1  | 2.15                     | 0.47              |
| 1:Y:5911:ALA:O    | 1:Y:5915:LYS:HG2   | 2.15                     | 0.47              |
| 1:6:3921:PHI:HA   | 1:6:3924:LYS:NZ    | 2.28                     | 0.47              |
| 1:a:705:ILE:HD12  | 1:a:705:ILE:H      | 1.79                     | 0.47              |
| 1:u:2708:GLU:HB3  | 1:v:2819:ILE:HD11  | 1.96                     | 0.47              |
| 1:4:3704:ALA:HA   | 1:4:3707:GLN:CD    | 2.40                     | 0.47              |
| 1:t:2621:PHI:HA   | 1:t:2621:PHI:HD2   | 1.59                     | 0.47              |
| 1:i:1529:LYS:HD2  | 1:i:1529:LYS:HA    | 1.59                     | 0.46              |
| 1:h:1424:LYS:HD2  | 1:i:1503:LYS:NZ    | 2.31                     | 0.46              |
| 1:x:3023:PHE:HA   | 1:x:3026:ILE:HG22  | 1.96                     | 0.46              |
| 1:2:3521:PHI:HA   | 1:2:3524:LYS:HZ2   | 1.79                     | 0.46              |
| 1:z:3204:ALA:HA   | 1:z:3207:GLN:NE2   | 2.31                     | 0.46              |
| 1:3:3608:GLU:HG2  | 1:8:4119:ILE:HD11  | 1.97                     | 0.46              |
| 1:O:4923:PHE:HE1  | 1:P:5005:ILE:HG13  | 1.81                     | 0.46              |
| 1:f:1204:ALA:HA   | 1:f:1207:GLN:NE2   | 2.30                     | 0.46              |
| 1:J:4410:LYS:O    | 1:J:4414:LYS:HG2   | 2.14                     | 0.46              |
| 1:Z:603:LYS:HD2   | 1:a:727:ALA:HB1    | 1.97                     | 0.46              |
| 1:P:5015:LYS:O    | 1:P:5019:ILE:HG12  | 2.16                     | 0.46              |
| 1:z:3221:PHI:HE1  | 1:3:3628:GLN:CD    | 2.35                     | 0.46              |
| 1:O:3312:ILE:HG23 | 1:1:3412:ILE:HD12  | 1.97                     | 0.46              |
| 1:O:3319:ILE:HD11 | 1:1:3408:GLU:HG2   | 1.97                     | 0.46              |
| 1:JA:6221:PHI:HA  | 1:JA:6224:LYS:NZ   | 2.31                     | 0.46              |
| 1:I:4312:ILE:HD11 | 1:J:4415:LYS:HB2   | 1.98                     | 0.46              |
| 1:V:5621:PHI:I    | 1:IA:6524:LYS:HB3  | 2.85                     | 0.46              |
| 1:p:2210:LYS:HB3  | 1:p:2210:LYS:HE3   | 1.77                     | 0.46              |
| 1:A:6109:PHE:HE1  | 1:JA:6219:ILE:HD13 | 1.81                     | 0.46              |
| 1:GA:6323:PHE:CD1 | 1:GA:6326:ILE:HD11 | 2.51                     | 0.46              |
| 1:E:322:GLU:OE1   | 1:F:405:ILE:HD11   | 2.16                     | 0.46              |
| 1:Z:621:PHI:HA    | 1:Z:621:PHI:HD2    | 1.57                     | 0.46              |
| 1:h:1406:ALA:HB1  | 1:i:1524:LYS:HG3   | 1.96                     | 0.46              |
| 1:l:1808:GLU:OE2  | 1:q:2315:LYS:HE3   | 2.15                     | 0.46              |
| 1:O:4912:ILE:HG23 | 1:P:5012:ILE:HD12  | 1.97                     | 0.46              |
| 1:P:5024:LYS:HZ2  | 1:m:1929:LYS:CE    | 2.28                     | 0.46              |
| 1:P:5027:ALA:HA   | 1:Q:5102:LEU:HD12  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:g:1315:LYS:HE2   | 1:h:1408:GLU:OE2  | 2.16                     | 0.46              |
| 1:x:3012:ILE:HD11  | 1:2:3515:LYS:HB2  | 1.98                     | 0.46              |
| 1:z:3207:GLN:HB2   | 1:z:3210:LYS:HE3  | 1.97                     | 0.46              |
| 1:H:4208:GLU:OE2   | 1:M:4715:LYS:HE3  | 2.16                     | 0.46              |
| 1:s:2512:ILE:HG23  | 1:t:2612:ILE:HD12 | 1.98                     | 0.46              |
| 1:L:4615:LYS:O     | 1:L:4619:ILE:HG12 | 2.16                     | 0.45              |
| 1:V:5621:PHI:I     | 1:IA:6528:GLN:CG  | 3.34                     | 0.45              |
| 1:f:1215:LYS:HB2   | 1:k:1712:ILE:HD11 | 1.97                     | 0.45              |
| 1:n:2022:GLU:O     | 1:n:2026:ILE:HD12 | 2.15                     | 0.45              |
| 1:A:6115:LYS:HE2   | 1:JA:6208:GLU:OE1 | 2.17                     | 0.45              |
| 1:i:1501:NLG:HBC1  | 1:i:1502:LEU:HD22 | 1.98                     | 0.45              |
| 1:p:2201:NLG:H8C2  | 1:p:2203:LYS:HD3  | 1.98                     | 0.45              |
| 1:JA:6204:ALA:O    | 1:JA:6208:GLU:HG2 | 2.16                     | 0.45              |
| 1:JA:6217:LYS:O    | 1:JA:6221:PHI:HD1 | 2.17                     | 0.45              |
| 1:H:4227:ALA:HB1   | 1:I:4303:LYS:HD2  | 1.98                     | 0.45              |
| 1:N:4808:GLU:OE2   | 1:S:5315:LYS:HE3  | 2.17                     | 0.45              |
| 1:k:1721:PHI:HA    | 1:k:1721:PHI:HD2  | 1.63                     | 0.45              |
| 1:2:3501:NLG:HBC1  | 1:2:3502:LEU:HD12 | 1.99                     | 0.45              |
| 1:6:3914:LYS:HE2   | 1:6:3914:LYS:HB2  | 1.80                     | 0.45              |
| 1:E:307:GLN:HE22   | 1:b:829:LYS:C     | 2.25                     | 0.45              |
| 1:H:4223:PHE:HA    | 1:H:4226:ILE:HG22 | 1.98                     | 0.45              |
| 1:E:303:LYS:CE     | 1:b:829:LYS:HZ3   | 2.30                     | 0.45              |
| 1:X:5805:ILE:H     | 1:X:5805:ILE:HD12 | 1.82                     | 0.45              |
| 1:a:703:LYS:O      | 1:a:706:ALA:N     | 2.50                     | 0.45              |
| 1:x:3021:PHI:HD2   | 1:x:3022:GLU:N    | 2.28                     | 0.45              |
| 1:1:3422:GLU:O     | 1:1:3426:ILE:HG12 | 2.16                     | 0.45              |
| 1:6:3926:ILE:HD13  | 1:7:4001:NLG:HGC2 | 1.99                     | 0.45              |
| 1:G:501:NLG:O      | 1:G:504:ALA:N     | 2.50                     | 0.45              |
| 1:N:4824:LYS:HD2   | 1:O:4903:LYS:HZ3  | 1.81                     | 0.45              |
| 1:d:1027:ALA:HB1   | 1:e:1103:LYS:NZ   | 2.31                     | 0.45              |
| 1:4:3708:GLU:HB3   | 1:5:3819:ILE:HD11 | 1.98                     | 0.45              |
| 1:5:3801:NLG:HBC1  | 1:5:3802:LEU:HD22 | 1.98                     | 0.45              |
| 1:7:4015:LYS:O     | 1:7:4019:ILE:HG12 | 2.16                     | 0.45              |
| 1:HA:6401:NLG:H8C2 | 1:HA:6403:LYS:HB3 | 1.99                     | 0.45              |
| 1:D:222:GLU:HA     | 1:D:222:GLU:OE1   | 2.17                     | 0.44              |
| 1:L:4627:ALA:HB1   | 1:M:4703:LYS:HD3  | 1.98                     | 0.44              |
| 1:P:5001:NLG:H8C2  | 1:P:5003:LYS:HB2  | 1.98                     | 0.44              |
| 1:S:5323:PHE:HA    | 1:S:5326:ILE:HG22 | 1.98                     | 0.44              |
| 1:l:1823:PHE:HA    | 1:l:1826:ILE:HG22 | 1.99                     | 0.44              |
| 1:GA:6305:ILE:HD13 | 1:GA:6308:GLU:OE2 | 2.17                     | 0.44              |
| 1:x:3023:PHE:HE1   | 1:2:3505:ILE:HG12 | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:y:3101:NLG:H8C2  | 1:y:3103:LYS:HB2   | 2.00                     | 0.44              |
| 1:CA:6922:GLU:OE1  | 1:DA:7005:ILE:HD11 | 2.16                     | 0.44              |
| 1:Q:5121:PHI:CE2   | 1:s:2524:LYS:CE    | 2.93                     | 0.44              |
| 1:m:1908:GLU:HG2   | 1:n:2019:ILE:HG12  | 1.98                     | 0.44              |
| 1:FA:6018:ALA:HA   | 1:FA:6021:PHI:HD1  | 2.00                     | 0.44              |
| 1:IA:6515:LYS:O    | 1:IA:6519:ILE:HG13 | 2.18                     | 0.44              |
| 1:z:3221:PHI:CE2   | 1:3:3625:ALA:HA    | 2.47                     | 0.44              |
| 1:FA:6018:ALA:O    | 1:FA:6021:PHI:HB3  | 2.18                     | 0.44              |
| 1:o:2101:NLG:HBC1  | 1:o:2102:LEU:HD22  | 1.98                     | 0.44              |
| 1:BA:6822:GLU:HA   | 1:BA:6822:GLU:OE1  | 2.17                     | 0.44              |
| 1:GA:6301:NLG:HBC1 | 1:GA:6302:LEU:HD22 | 1.99                     | 0.44              |
| 1:E:305:ILE:HD12   | 1:F:419:ILE:HG23   | 2.00                     | 0.44              |
| 1:L:4605:ILE:H     | 1:L:4605:ILE:HD12  | 1.83                     | 0.44              |
| 1:f:1212:ILE:HG23  | 1:k:1712:ILE:HD12  | 1.99                     | 0.44              |
| 1:j:1601:NLG:O     | 1:j:1604:ALA:N     | 2.44                     | 0.44              |
| 1:S:5314:LYS:HE2   | 1:S:5314:LYS:HB2   | 1.81                     | 0.44              |
| 1:a:704:ALA:HA     | 1:a:707:GLN:NE2    | 2.33                     | 0.44              |
| 1:p:2217:LYS:HE2   | 1:q:2310:LYS:NZ    | 2.33                     | 0.44              |
| 1:4:3717:LYS:HB2   | 1:4:3717:LYS:HE3   | 1.80                     | 0.44              |
| 1:N:4811:ALA:O     | 1:N:4815:LYS:HG3   | 2.18                     | 0.43              |
| 1:4:3701:NLG:HBC2  | 1:4:3702:LEU:HD12  | 2.00                     | 0.43              |
| 1:CA:6905:ILE:HD12 | 1:DA:7019:ILE:HG23 | 2.00                     | 0.43              |
| 1:W:5701:NLG:HBC1  | 1:W:5702:LEU:HD22  | 2.00                     | 0.43              |
| 1:u:2701:NLG:H8C2  | 1:u:2703:LYS:HB3   | 2.00                     | 0.43              |
| 1:y:3115:LYS:HE2   | 1:z:3208:GLU:OE1   | 2.18                     | 0.43              |
| 1:2:3505:ILE:H     | 1:2:3505:ILE:HD12  | 1.83                     | 0.43              |
| 1:EA:7101:NLG:O    | 1:EA:7104:ALA:N    | 2.50                     | 0.43              |
| 1:A:6104:ALA:O     | 1:A:6108:GLU:HG2   | 2.19                     | 0.43              |
| 1:GA:6311:ALA:C    | 1:GA:6315:LYS:HZ3  | 2.25                     | 0.43              |
| 1:E:314:LYS:HB2    | 1:E:314:LYS:HE2    | 1.86                     | 0.43              |
| 1:Q:5121:PHI:I     | 1:s:2524:LYS:HD3   | 2.67                     | 0.43              |
| 1:3:3608:GLU:OE2   | 1:8:4115:LYS:HE3   | 2.18                     | 0.43              |
| 1:W:5714:LYS:HB2   | 1:W:5714:LYS:HE2   | 1.79                     | 0.43              |
| 1:H:4221:PHI:HD2   | 1:H:4221:PHI:HA    | 1.73                     | 0.43              |
| 1:b:806:ALA:HB1    | 1:c:924:LYS:HG3    | 1.99                     | 0.43              |
| 1:m:1917:LYS:HE3   | 1:m:1917:LYS:HB2   | 1.82                     | 0.43              |
| 1:p:2205:ILE:HD12  | 1:p:2205:ILE:H     | 1.82                     | 0.43              |
| 1:G:521:PHI:HA     | 1:G:521:PHI:HD2    | 1.56                     | 0.43              |
| 1:U:5515:LYS:HE2   | 1:V:5608:GLU:OE1   | 2.17                     | 0.43              |
| 1:i:1511:ALA:O     | 1:i:1515:LYS:HG2   | 2.18                     | 0.43              |
| 1:x:3008:GLU:O     | 1:x:3012:ILE:HG12  | 2.17                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:3404:ALA:O    | 1:1:3408:GLU:HB2   | 2.19                     | 0.43              |
| 1:EA:7121:PHI:HD2 | 1:EA:7121:PHI:HA   | 1.55                     | 0.43              |
| 1:A:6105:ILE:HG12 | 1:JA:6223:PHE:CE1  | 2.52                     | 0.43              |
| 1:V:5615:LYS:O    | 1:V:5619:ILE:HG12  | 2.19                     | 0.43              |
| 1:i:1505:ILE:HD12 | 1:j:1619:ILE:HG23  | 2.01                     | 0.43              |
| 1:p:2206:ALA:HB2  | 1:q:2323:PHE:HB3   | 1.99                     | 0.43              |
| 1:K:4518:ALA:O    | 1:K:4522:GLU:OE1   | 2.37                     | 0.43              |
| 1:g:1305:ILE:H    | 1:g:1305:ILE:HD12  | 1.84                     | 0.43              |
| 1:a:717:LYS:HB2   | 1:a:717:LYS:HE3    | 1.74                     | 0.43              |
| 1:5:3814:LYS:O    | 1:5:3817:LYS:HG2   | 2.18                     | 0.43              |
| 1:Q:5129:LYS:HD3  | 1:s:2521:PHI:HE1   | 2.00                     | 0.43              |
| 1:9:6608:GLU:HB2  | 1:EA:7119:ILE:HD11 | 2.01                     | 0.43              |
| 1:R:5216:PHE:O    | 1:R:5219:ILE:HG22  | 2.19                     | 0.42              |
| 1:R:5222:GLU:O    | 1:R:5226:ILE:HG12  | 2.19                     | 0.42              |
| 1:g:1302:LEU:HA   | 1:g:1305:ILE:HD13  | 2.01                     | 0.42              |
| 1:g:1329:LYS:HD2  | 1:g:1329:LYS:HA    | 1.77                     | 0.42              |
| 1:r:2401:NLG:HGC2 | 1:w:2926:ILE:HD11  | 2.01                     | 0.42              |
| 1:JA:6204:ALA:O   | 1:JA:6207:GLN:HG3  | 2.19                     | 0.42              |
| 1:HA:6404:ALA:O   | 1:HA:6408:GLU:OE1  | 2.37                     | 0.42              |
| 1:p:2221:PHI:HA   | 1:p:2221:PHI:HD2   | 1.58                     | 0.42              |
| 1:z:3221:PHI:CE2  | 1:3:3628:GLN:NE2   | 2.82                     | 0.42              |
| 1:A:6117:LYS:HE3  | 1:A:6117:LYS:HB2   | 1.80                     | 0.42              |
| 1:HA:6414:LYS:HA  | 1:HA:6417:LYS:HZ3  | 1.84                     | 0.42              |
| 1:Q:5108:GLU:OE2  | 1:R:5215:LYS:HD2   | 2.19                     | 0.42              |
| 1:6:3915:LYS:O    | 1:6:3919:ILE:HG12  | 2.19                     | 0.42              |
| 1:7:4022:GLU:O    | 1:7:4026:ILE:HG12  | 2.18                     | 0.42              |
| 1:EA:7114:LYS:HE2 | 1:EA:7114:LYS:HB2  | 1.79                     | 0.42              |
| 1:Z:612:ILE:HG23  | 1:e:1112:ILE:HD12  | 2.01                     | 0.42              |
| 1:Z:623:PHE:HA    | 1:Z:626:ILE:HG22   | 2.00                     | 0.42              |
| 1:o:2115:LYS:HB2  | 1:p:2212:ILE:HD11  | 2.01                     | 0.42              |
| 1:1:3408:GLU:O    | 1:1:3412:ILE:HG12  | 2.18                     | 0.42              |
| 1:3:3602:LEU:HD13 | 1:3:3605:ILE:HD12  | 2.00                     | 0.42              |
| 1:R:5227:ALA:HB1  | 1:S:5303:LYS:NZ    | 2.34                     | 0.42              |
| 1:T:5408:GLU:CD   | 1:Y:5915:LYS:HE2   | 2.45                     | 0.42              |
| 1:U:5508:GLU:HB3  | 1:V:5619:ILE:HD11  | 2.02                     | 0.42              |
| 1:c:914:LYS:HB2   | 1:c:914:LYS:HE2    | 1.73                     | 0.42              |
| 1:B:21:PHI:HD2    | 1:B:21:PHI:HA      | 1.54                     | 0.42              |
| 1:P:5001:NLG:HBC1 | 1:P:5002:LEU:HD22  | 2.01                     | 0.42              |
| 1:e:1101:NLG:HBC1 | 1:e:1102:LEU:HD22  | 2.01                     | 0.42              |
| 1:3:3612:ILE:HG23 | 1:8:4112:ILE:HD12  | 2.01                     | 0.42              |
| 1:8:4105:ILE:H    | 1:8:4105:ILE:HD12  | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K:4504:ALA:O     | 1:K:4508:GLU:OE1   | 2.38                     | 0.42              |
| 1:T:5402:LEU:HB3   | 1:U:5527:ALA:HB2   | 2.02                     | 0.42              |
| 1:9:6619:ILE:HD11  | 1:EA:7108:GLU:CG   | 2.50                     | 0.42              |
| 1:CA:6901:NLG:HGC1 | 1:DA:7026:ILE:HD11 | 2.02                     | 0.42              |
| 1:B:19:ILE:HD11    | 1:G:508:GLU:CG     | 2.50                     | 0.42              |
| 1:I:4309:PHE:CZ    | 1:J:4419:ILE:HD13  | 2.55                     | 0.42              |
| 1:T:5401:NLG:O     | 1:T:5405:ILE:HG13  | 2.20                     | 0.42              |
| 1:Y:5914:LYS:HB2   | 1:Y:5914:LYS:HE2   | 1.82                     | 0.42              |
| 1:l:1821:PHI:HA    | 1:l:1824:LYS:HZ2   | 1.84                     | 0.42              |
| 1:q:2314:LYS:HB2   | 1:q:2314:LYS:HE2   | 1.88                     | 0.42              |
| 1:C:117:LYS:HE3    | 1:C:117:LYS:HB2    | 1.76                     | 0.41              |
| 1:Z:611:ALA:O      | 1:Z:615:LYS:HG3    | 2.20                     | 0.41              |
| 1:g:1319:ILE:HD11  | 1:h:1408:GLU:CD    | 2.44                     | 0.41              |
| 1:E:301:NLG:HGC1   | 1:F:426:ILE:HD11   | 2.02                     | 0.41              |
| 1:I:4301:NLG:H8C2  | 1:I:4303:LYS:HD3   | 2.01                     | 0.41              |
| 1:l:1803:LYS:HB3   | 1:l:1803:LYS:HE3   | 1.86                     | 0.41              |
| 1:x:3011:ALA:O     | 1:x:3015:LYS:HG3   | 2.20                     | 0.41              |
| 1:FA:6018:ALA:O    | 1:FA:6022:GLU:OE1  | 2.38                     | 0.41              |
| 1:HA:6414:LYS:HG3  | 1:HA:6417:LYS:HZ1  | 1.85                     | 0.41              |
| 1:B:8:GLU:HB2      | 1:G:519:ILE:HD11   | 2.01                     | 0.41              |
| 1:K:4505:ILE:HD11  | 1:L:4622:GLU:HB2   | 2.02                     | 0.41              |
| 1:K:4519:ILE:HG22  | 1:K:4523:PHE:CE2   | 2.55                     | 0.41              |
| 1:l:1822:GLU:HB3   | 1:q:2305:ILE:HD11  | 2.02                     | 0.41              |
| 1:m:1905:ILE:HD12  | 1:m:1905:ILE:H     | 1.86                     | 0.41              |
| 1:O:4905:ILE:HD12  | 1:O:4905:ILE:H     | 1.86                     | 0.41              |
| 1:Q:5115:LYS:HB2   | 1:R:5212:ILE:HD11  | 2.02                     | 0.41              |
| 1:b:822:GLU:HA     | 1:b:822:GLU:OE1    | 2.21                     | 0.41              |
| 1:f:1221:PHI:HD2   | 1:f:1221:PHI:HA    | 1.51                     | 0.41              |
| 1:0:3322:GLU:OE2   | 1:1:3401:NLG:HGC1  | 2.20                     | 0.41              |
| 1:1:3429:LYS:HZ1   | 1:BA:6824:LYS:CE   | 2.32                     | 0.41              |
| 1:9:6604:ALA:O     | 1:9:6608:GLU:HG2   | 2.21                     | 0.41              |
| 1:A:6109:PHE:CE1   | 1:JA:6219:ILE:HD13 | 2.55                     | 0.41              |
| 1:H:4222:GLU:OE2   | 1:H:4223:PHE:HD1   | 2.02                     | 0.41              |
| 1:IA:6514:LYS:O    | 1:IA:6517:LYS:HG2  | 2.21                     | 0.41              |
| 1:2:3511:ALA:HA    | 1:2:3514:LYS:HG2   | 2.01                     | 0.41              |
| 1:e:1114:LYS:HE2   | 1:e:1114:LYS:HB2   | 1.82                     | 0.41              |
| 1:3:3615:LYS:HB2   | 1:8:4112:ILE:HD11  | 2.03                     | 0.41              |
| 1:AA:6705:ILE:HD12 | 1:AA:6705:ILE:H    | 1.85                     | 0.41              |
| 1:C:105:ILE:HD12   | 1:C:105:ILE:H      | 1.85                     | 0.41              |
| 1:S:5304:ALA:HA    | 1:S:5307:GLN:HE21  | 1.84                     | 0.41              |
| 1:y:3117:LYS:HE3   | 1:y:3117:LYS:HB2   | 1.83                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:6729:LYS:HD2 | 1:AA:6729:LYS:HA   | 1.82                     | 0.41              |
| 1:T:5427:ALA:HA   | 1:U:5502:LEU:HD22  | 2.03                     | 0.41              |
| 1:Z:603:LYS:NZ    | 1:a:727:ALA:O      | 2.51                     | 0.41              |
| 1:j:1622:GLU:O    | 1:j:1626:ILE:HG12  | 2.20                     | 0.41              |
| 1:s:2529:LYS:HA   | 1:s:2529:LYS:HD2   | 1.80                     | 0.41              |
| 1:x:3008:GLU:OE2  | 1:2:3515:LYS:HE3   | 2.21                     | 0.41              |
| 1:0:3314:LYS:HB2  | 1:0:3314:LYS:HE2   | 1.86                     | 0.41              |
| 1:0:3315:LYS:CB   | 1:1:3412:ILE:HD11  | 2.50                     | 0.41              |
| 1:JA:6215:LYS:O   | 1:JA:6219:ILE:HG13 | 2.21                     | 0.41              |
| 1:HA:6411:ALA:O   | 1:HA:6414:LYS:HB3  | 2.21                     | 0.41              |
| 1:Z:623:PHE:O     | 1:Z:626:ILE:HG22   | 2.21                     | 0.41              |
| 1:c:904:ALA:O     | 1:c:908:GLU:HG2    | 2.21                     | 0.41              |
| 1:k:1714:LYS:HE2  | 1:k:1714:LYS:HB2   | 1.83                     | 0.41              |
| 1:z:3203:LYS:O    | 1:z:3206:ALA:N     | 2.54                     | 0.41              |
| 1:z:3204:ALA:O    | 1:z:3208:GLU:HG2   | 2.21                     | 0.41              |
| 1:A:6119:ILE:HD11 | 1:JA:6208:GLU:HB3  | 2.03                     | 0.41              |
| 1:HA:6404:ALA:O   | 1:HA:6407:GLN:HB3  | 2.21                     | 0.41              |
| 1:HA:6422:GLU:O   | 1:HA:6426:ILE:HG12 | 2.21                     | 0.41              |
| 1:U:5517:LYS:HE3  | 1:U:5517:LYS:HB2   | 1.77                     | 0.40              |
| 1:V:5614:LYS:O    | 1:V:5617:LYS:HG2   | 2.21                     | 0.40              |
| 1:X:5822:GLU:O    | 1:X:5826:ILE:HG12  | 2.22                     | 0.40              |
| 1:B:29:LYS:HD2    | 1:B:29:LYS:HA      | 1.84                     | 0.40              |
| 1:O:4915:LYS:HB3  | 1:P:5008:GLU:CD    | 2.46                     | 0.40              |
| 1:R:5211:ALA:O    | 1:R:5215:LYS:HG2   | 2.21                     | 0.40              |
| 1:T:5421:PHI:HD2  | 1:T:5421:PHI:HA    | 1.73                     | 0.40              |
| 1:l:1815:LYS:O    | 1:l:1819:ILE:HG12  | 2.21                     | 0.40              |
| 1:m:1929:LYS:HD2  | 1:m:1929:LYS:HA    | 1.84                     | 0.40              |
| 1:1:3411:ALA:O    | 1:1:3415:LYS:HG2   | 2.21                     | 0.40              |
| 1:I:4312:ILE:HD11 | 1:J:4415:LYS:CB    | 2.52                     | 0.40              |
| 1:L:4609:PHE:HA   | 1:L:4612:ILE:HD12  | 2.02                     | 0.40              |
| 1:a:705:ILE:HG12  | 1:b:823:PHE:CE1    | 2.57                     | 0.40              |
| 1:z:3221:PHI:CE2  | 1:3:3628:GLN:HE21  | 2.33                     | 0.40              |
| 1:6:3923:PHE:HE1  | 1:7:4005:ILE:HG21  | 1.86                     | 0.40              |
| 1:Z:619:ILE:HG23  | 1:e:1105:ILE:HD12  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 1   | 0     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 1     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 2     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 3     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 4     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 5     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 6     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 7     | 27/30 (90%) | 26 (96%)  | 0       | 1 (4%)   | 2           | 23  |
| 1   | 8     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | 9     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | A     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | AA    | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | B     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | BA    | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | C     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | CA    | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | D     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | DA    | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | E     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | EA    | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | F     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | FA    | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | G     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | GA    | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | H     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 1   | HA    | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | I     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | IA    | 27/30 (90%) | 26 (96%)  | 0       | 1 (4%)   | 2           | 23  |
| 1   | J     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | JA    | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | K     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | L     | 27/30 (90%) | 25 (93%)  | 2 (7%)  | 0        | 100         | 100 |
| 1   | M     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | N     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | O     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | P     | 27/30 (90%) | 26 (96%)  | 0       | 1 (4%)   | 2           | 23  |
| 1   | Q     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | R     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | S     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | T     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | U     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | V     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | W     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | X     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | Y     | 27/30 (90%) | 25 (93%)  | 2 (7%)  | 0        | 100         | 100 |
| 1   | Z     | 27/30 (90%) | 27 (100%) | 0       | 0        | 100         | 100 |
| 1   | a     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | b     | 27/30 (90%) | 25 (93%)  | 2 (7%)  | 0        | 100         | 100 |
| 1   | c     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | d     | 27/30 (90%) | 26 (96%)  | 0       | 1 (4%)   | 2           | 23  |
| 1   | e     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | f     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | g     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | h     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | i     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 1   | j     | 27/30 (90%) | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | k     | 27/30 (90%)     | 25 (93%)   | 2 (7%)  | 0        | 100         | 100 |
| 1   | l     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | m     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | n     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | o     | 27/30 (90%)     | 27 (100%)  | 0       | 0        | 100         | 100 |
| 1   | p     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | q     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | r     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | s     | 27/30 (90%)     | 26 (96%)   | 0       | 1 (4%)   | 2           | 23  |
| 1   | t     | 27/30 (90%)     | 27 (100%)  | 0       | 0        | 100         | 100 |
| 1   | u     | 27/30 (90%)     | 27 (100%)  | 0       | 0        | 100         | 100 |
| 1   | v     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | w     | 27/30 (90%)     | 27 (100%)  | 0       | 0        | 100         | 100 |
| 1   | x     | 27/30 (90%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 1   | y     | 27/30 (90%)     | 25 (93%)   | 2 (7%)  | 0        | 100         | 100 |
| 1   | z     | 27/30 (90%)     | 26 (96%)   | 0       | 1 (4%)   | 2           | 23  |
| All | All   | 1944/2160 (90%) | 1883 (97%) | 55 (3%) | 6 (0%)   | 38          | 70  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | P     | 5028 | GLN  |
| 1   | d     | 1028 | GLN  |
| 1   | s     | 2529 | LYS  |
| 1   | z     | 3228 | GLN  |
| 1   | 7     | 4028 | GLN  |
| 1   | IA    | 6528 | GLN  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | 0     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 1     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | 2     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 3     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | 4     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 5     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 6     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 7     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 8     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | 9     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | A     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | AA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | B     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | BA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | C     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | CA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | D     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | DA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | E     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | EA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | F     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | FA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | G     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | GA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | H     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | HA    | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | I     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | IA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | J     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | JA    | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | K     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | L     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | M     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | N     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | O     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | P     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | Q     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | R     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | S     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | T     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | U     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | V     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | W     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | X     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | Y     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | Z     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | a     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | b     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | c     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | d     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | e     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | f     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | g     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | h     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | i     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | j     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | k     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | l     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | m     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | n     | 19/19 (100%) | 19 (100%) | 0        | 100         | 100 |
| 1   | o     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | p     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |
| 1   | q     | 19/19 (100%) | 18 (95%)  | 1 (5%)   | 19          | 44  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | r     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | s     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | t     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | u     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | v     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | w     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | x     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | y     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| 1   | z     | 19/19 (100%)     | 18 (95%)   | 1 (5%)   | 19          | 44 |
| All | All   | 1368/1368 (100%) | 1304 (95%) | 64 (5%)  | 24          | 47 |

All (64) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 29   | LYS  |
| 1   | C     | 129  | LYS  |
| 1   | D     | 229  | LYS  |
| 1   | E     | 329  | LYS  |
| 1   | F     | 429  | LYS  |
| 1   | G     | 529  | LYS  |
| 1   | H     | 4229 | LYS  |
| 1   | I     | 4329 | LYS  |
| 1   | J     | 4429 | LYS  |
| 1   | L     | 4629 | LYS  |
| 1   | M     | 4729 | LYS  |
| 1   | N     | 4829 | LYS  |
| 1   | O     | 4929 | LYS  |
| 1   | Q     | 5129 | LYS  |
| 1   | R     | 5229 | LYS  |
| 1   | S     | 5329 | LYS  |
| 1   | T     | 5429 | LYS  |
| 1   | U     | 5529 | LYS  |
| 1   | V     | 5629 | LYS  |
| 1   | W     | 5729 | LYS  |
| 1   | Y     | 5929 | LYS  |
| 1   | Z     | 629  | LYS  |
| 1   | a     | 729  | LYS  |
| 1   | b     | 829  | LYS  |
| 1   | c     | 929  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | d     | 1029 | LYS  |
| 1   | e     | 1129 | LYS  |
| 1   | f     | 1229 | LYS  |
| 1   | g     | 1329 | LYS  |
| 1   | h     | 1429 | LYS  |
| 1   | j     | 1629 | LYS  |
| 1   | k     | 1729 | LYS  |
| 1   | l     | 1829 | LYS  |
| 1   | m     | 1929 | LYS  |
| 1   | o     | 2129 | LYS  |
| 1   | p     | 2229 | LYS  |
| 1   | q     | 2329 | LYS  |
| 1   | r     | 2429 | LYS  |
| 1   | s     | 2529 | LYS  |
| 1   | t     | 2629 | LYS  |
| 1   | u     | 2729 | LYS  |
| 1   | v     | 2829 | LYS  |
| 1   | w     | 2929 | LYS  |
| 1   | x     | 3029 | LYS  |
| 1   | y     | 3129 | LYS  |
| 1   | z     | 3229 | LYS  |
| 1   | 0     | 3329 | LYS  |
| 1   | 2     | 3529 | LYS  |
| 1   | 4     | 3729 | LYS  |
| 1   | 5     | 3829 | LYS  |
| 1   | 6     | 3929 | LYS  |
| 1   | 7     | 4029 | LYS  |
| 1   | 8     | 4129 | LYS  |
| 1   | 9     | 6629 | LYS  |
| 1   | AA    | 6729 | LYS  |
| 1   | BA    | 6829 | LYS  |
| 1   | CA    | 6929 | LYS  |
| 1   | DA    | 7029 | LYS  |
| 1   | EA    | 7129 | LYS  |
| 1   | FA    | 6029 | LYS  |
| 1   | A     | 6129 | LYS  |
| 1   | JA    | 6229 | LYS  |
| 1   | GA    | 6329 | LYS  |
| 1   | IA    | 6529 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 428  | GLN  |
| 1   | J     | 4407 | GLN  |
| 1   | J     | 4428 | GLN  |
| 1   | W     | 5707 | GLN  |
| 1   | X     | 5828 | GLN  |
| 1   | b     | 828  | GLN  |
| 1   | d     | 1028 | GLN  |
| 1   | y     | 3128 | GLN  |
| 1   | 0     | 3328 | GLN  |
| 1   | 1     | 3428 | GLN  |
| 1   | 5     | 3828 | GLN  |
| 1   | 7     | 4028 | GLN  |
| 1   | BA    | 6828 | GLN  |
| 1   | DA    | 7028 | GLN  |
| 1   | JA    | 6228 | GLN  |
| 1   | HA    | 6428 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

72 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | PHI  | t     | 2621 | 1    | 11,12,13     | 1.15 | 1 (9%)      | 10,15,17    | 0.46 | 0           |
| 1   | PHI  | p     | 2221 | 1    | 11,12,13     | 1.18 | 1 (9%)      | 10,15,17    | 0.45 | 0           |
| 1   | PHI  | JA    | 6221 | 1    | 11,12,13     | 1.17 | 1 (9%)      | 10,15,17    | 0.48 | 0           |
| 1   | PHI  | M     | 4721 | 1    | 11,12,13     | 1.18 | 1 (9%)      | 10,15,17    | 0.53 | 0           |
| 1   | PHI  | 2     | 3521 | 1    | 11,12,13     | 1.17 | 1 (9%)      | 10,15,17    | 0.47 | 0           |
| 1   | PHI  | 6     | 3921 | 1    | 11,12,13     | 1.18 | 1 (9%)      | 10,15,17    | 0.40 | 0           |
| 1   | PHI  | Y     | 5921 | 1    | 11,12,13     | 1.20 | 1 (9%)      | 10,15,17    | 0.51 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PHI  | e     | 1121 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.49 | 0        |
| 1   | PHI  | N     | 4821 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | AA    | 6721 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | EA    | 7121 | 1    | 11,12,13     | 1.14 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | G     | 521  | 1    | 11,12,13     | 1.14 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | 8     | 4121 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.56 | 0        |
| 1   | PHI  | i     | 1521 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.44 | 0        |
| 1   | PHI  | CA    | 6921 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.52 | 0        |
| 1   | PHI  | q     | 2321 | 1    | 11,12,13     | 1.15 | 1 (9%)   | 10,15,17    | 0.44 | 0        |
| 1   | PHI  | 5     | 3821 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.52 | 0        |
| 1   | PHI  | Q     | 5121 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.45 | 0        |
| 1   | PHI  | IA    | 6521 | 1    | 11,12,13     | 1.19 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | O     | 4921 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.46 | 0        |
| 1   | PHI  | f     | 1221 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.49 | 0        |
| 1   | PHI  | R     | 5221 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.50 | 0        |
| 1   | PHI  | m     | 1921 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.44 | 0        |
| 1   | PHI  | A     | 6121 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.51 | 0        |
| 1   | PHI  | L     | 4621 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.46 | 0        |
| 1   | PHI  | 9     | 6621 | 1    | 11,12,13     | 1.15 | 1 (9%)   | 10,15,17    | 0.45 | 0        |
| 1   | PHI  | 3     | 3621 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.46 | 0        |
| 1   | PHI  | c     | 921  | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | n     | 2021 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.51 | 0        |
| 1   | PHI  | W     | 5721 | 1    | 11,12,13     | 1.19 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | V     | 5621 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.45 | 0        |
| 1   | PHI  | w     | 2921 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | r     | 2421 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.46 | 0        |
| 1   | PHI  | 4     | 3721 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.45 | 0        |
| 1   | PHI  | s     | 2521 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.46 | 0        |
| 1   | PHI  | I     | 4321 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.50 | 0        |
| 1   | PHI  | DA    | 7021 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.54 | 0        |
| 1   | PHI  | HA    | 6421 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | P     | 5021 | 1    | 11,12,13     | 1.14 | 1 (9%)   | 10,15,17    | 0.54 | 0        |
| 1   | PHI  | GA    | 6321 | 1    | 11,12,13     | 1.20 | 1 (9%)   | 10,15,17    | 0.49 | 0        |
| 1   | PHI  | S     | 5321 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.53 | 0        |
| 1   | PHI  | J     | 4421 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.48 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PHI  | U     | 5521 | 1    | 11,12,13     | 1.19 | 1 (9%)   | 10,15,17    | 0.52 | 0        |
| 1   | PHI  | E     | 321  | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.49 | 0        |
| 1   | PHI  | X     | 5821 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.50 | 0        |
| 1   | PHI  | h     | 1421 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | 0     | 3321 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.45 | 0        |
| 1   | PHI  | 7     | 4021 | 1    | 11,12,13     | 1.14 | 1 (9%)   | 10,15,17    | 0.46 | 0        |
| 1   | PHI  | a     | 721  | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.52 | 0        |
| 1   | PHI  | o     | 2121 | 1    | 11,12,13     | 1.19 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | C     | 121  | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.43 | 0        |
| 1   | PHI  | D     | 221  | 1    | 11,12,13     | 1.15 | 1 (9%)   | 10,15,17    | 0.49 | 0        |
| 1   | PHI  | j     | 1621 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.56 | 0        |
| 1   | PHI  | BA    | 6821 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.52 | 0        |
| 1   | PHI  | d     | 1021 | 1    | 11,12,13     | 1.19 | 1 (9%)   | 10,15,17    | 0.64 | 0        |
| 1   | PHI  | g     | 1321 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.65 | 0        |
| 1   | PHI  | l     | 3421 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.50 | 0        |
| 1   | PHI  | K     | 4521 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.56 | 0        |
| 1   | PHI  | v     | 2821 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | k     | 1721 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.51 | 0        |
| 1   | PHI  | F     | 421  | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.54 | 0        |
| 1   | PHI  | H     | 4221 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.49 | 0        |
| 1   | PHI  | x     | 3021 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | u     | 2721 | 1    | 11,12,13     | 1.20 | 1 (9%)   | 10,15,17    | 0.47 | 0        |
| 1   | PHI  | y     | 3121 | 1    | 11,12,13     | 1.17 | 1 (9%)   | 10,15,17    | 0.44 | 0        |
| 1   | PHI  | z     | 3221 | 1    | 11,12,13     | 1.16 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | FA    | 6021 | 1    | 11,12,13     | 1.19 | 1 (9%)   | 10,15,17    | 0.50 | 0        |
| 1   | PHI  | Z     | 621  | 1    | 11,12,13     | 1.12 | 1 (9%)   | 10,15,17    | 0.51 | 0        |
| 1   | PHI  | b     | 821  | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.50 | 0        |
| 1   | PHI  | T     | 5421 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | l     | 1821 | 1    | 11,12,13     | 1.18 | 1 (9%)   | 10,15,17    | 0.48 | 0        |
| 1   | PHI  | B     | 21   | 1    | 11,12,13     | 1.14 | 1 (9%)   | 10,15,17    | 0.48 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 1   | PHI  | t     | 2621 | 1    | -       | 4/5/6/8  | 0/1/1/1 |
| 1   | PHI  | p     | 2221 | 1    | -       | 5/5/6/8  | 0/1/1/1 |
| 1   | PHI  | JA    | 6221 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | M     | 4721 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 2     | 3521 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 6     | 3921 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | Y     | 5921 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | e     | 1121 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | N     | 4821 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | AA    | 6721 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | EA    | 7121 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | G     | 521  | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 8     | 4121 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | i     | 1521 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | CA    | 6921 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | q     | 2321 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 5     | 3821 | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | Q     | 5121 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | IA    | 6521 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | O     | 4921 | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | f     | 1221 | 1    | -       | 5/5/6/8  | 0/1/1/1 |
| 1   | PHI  | R     | 5221 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | m     | 1921 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | A     | 6121 | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | L     | 4621 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 9     | 6621 | 1    | -       | 5/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 3     | 3621 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | c     | 921  | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | n     | 2021 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | W     | 5721 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | V     | 5621 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | w     | 2921 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | r     | 2421 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 4     | 3721 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | s     | 2521 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | I     | 4321 | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | DA    | 7021 | 1    | -       | 2/5/6/8  | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 1   | PHI  | HA    | 6421 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | P     | 5021 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | GA    | 6321 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | S     | 5321 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | J     | 4421 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | U     | 5521 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | E     | 321  | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | X     | 5821 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | h     | 1421 | 1    | -       | 4/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 0     | 3321 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | 7     | 4021 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | a     | 721  | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | o     | 2121 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | C     | 121  | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | D     | 221  | 1    | -       | 4/5/6/8  | 0/1/1/1 |
| 1   | PHI  | j     | 1621 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | BA    | 6821 | 1    | -       | 4/5/6/8  | 0/1/1/1 |
| 1   | PHI  | d     | 1021 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | g     | 1321 | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | l     | 3421 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | K     | 4521 | 1    | -       | 1/5/6/8  | 0/1/1/1 |
| 1   | PHI  | v     | 2821 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | k     | 1721 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | F     | 421  | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | H     | 4221 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | x     | 3021 | 1    | -       | 3/5/6/8  | 0/1/1/1 |
| 1   | PHI  | u     | 2721 | 1    | -       | 0/5/6/8  | 0/1/1/1 |
| 1   | PHI  | y     | 3121 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | z     | 3221 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | FA    | 6021 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | Z     | 621  | 1    | -       | 4/5/6/8  | 0/1/1/1 |
| 1   | PHI  | b     | 821  | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | T     | 5421 | 1    | -       | 2/5/6/8  | 0/1/1/1 |
| 1   | PHI  | l     | 1821 | 1    | -       | 4/5/6/8  | 0/1/1/1 |
| 1   | PHI  | B     | 21   | 1    | -       | 4/5/6/8  | 0/1/1/1 |

All (72) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | CA    | 6921 | PHI  | CZ-I  | -3.09 | 2.02        | 2.10     |
| 1   | p     | 2221 | PHI  | CZ-I  | -3.08 | 2.02        | 2.10     |
| 1   | E     | 321  | PHI  | CZ-I  | -3.08 | 2.02        | 2.10     |
| 1   | i     | 1521 | PHI  | CZ-I  | -3.06 | 2.02        | 2.10     |
| 1   | GA    | 6321 | PHI  | CZ-I  | -3.05 | 2.02        | 2.10     |
| 1   | AA    | 6721 | PHI  | CZ-I  | -3.04 | 2.02        | 2.10     |
| 1   | C     | 121  | PHI  | CZ-I  | -3.04 | 2.02        | 2.10     |
| 1   | u     | 2721 | PHI  | CZ-I  | -3.04 | 2.02        | 2.10     |
| 1   | Q     | 5121 | PHI  | CZ-I  | -3.03 | 2.02        | 2.10     |
| 1   | Y     | 5921 | PHI  | CZ-I  | -3.03 | 2.02        | 2.10     |
| 1   | d     | 1021 | PHI  | CZ-I  | -3.02 | 2.02        | 2.10     |
| 1   | B     | 21   | PHI  | CZ-I  | -3.02 | 2.02        | 2.10     |
| 1   | DA    | 7021 | PHI  | CZ-I  | -3.02 | 2.02        | 2.10     |
| 1   | 5     | 3821 | PHI  | CZ-I  | -3.02 | 2.02        | 2.10     |
| 1   | b     | 821  | PHI  | CZ-I  | -3.02 | 2.02        | 2.10     |
| 1   | k     | 1721 | PHI  | CZ-I  | -3.01 | 2.02        | 2.10     |
| 1   | G     | 521  | PHI  | CZ-I  | -3.01 | 2.02        | 2.10     |
| 1   | g     | 1321 | PHI  | CZ-I  | -3.01 | 2.02        | 2.10     |
| 1   | JA    | 6221 | PHI  | CZ-I  | -3.00 | 2.02        | 2.10     |
| 1   | e     | 1121 | PHI  | CZ-I  | -3.00 | 2.02        | 2.10     |
| 1   | x     | 3021 | PHI  | CZ-I  | -3.00 | 2.02        | 2.10     |
| 1   | 9     | 6621 | PHI  | CZ-I  | -3.00 | 2.02        | 2.10     |
| 1   | W     | 5721 | PHI  | CZ-I  | -3.00 | 2.02        | 2.10     |
| 1   | N     | 4821 | PHI  | CZ-I  | -3.00 | 2.02        | 2.10     |
| 1   | I     | 4321 | PHI  | CZ-I  | -2.99 | 2.02        | 2.10     |
| 1   | U     | 5521 | PHI  | CZ-I  | -2.99 | 2.02        | 2.10     |
| 1   | m     | 1921 | PHI  | CZ-I  | -2.99 | 2.02        | 2.10     |
| 1   | F     | 421  | PHI  | CZ-I  | -2.99 | 2.02        | 2.10     |
| 1   | O     | 4921 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | IA    | 6521 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | h     | 1421 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | l     | 1821 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | y     | 3121 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | EA    | 7121 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | A     | 6121 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | c     | 921  | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | V     | 5621 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | Z     | 621  | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | a     | 721  | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | M     | 4721 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | f     | 1221 | PHI  | CZ-I  | -2.98 | 2.02        | 2.10     |
| 1   | 0     | 3321 | PHI  | CZ-I  | -2.97 | 2.02        | 2.10     |
| 1   | j     | 1621 | PHI  | CZ-I  | -2.97 | 2.02        | 2.10     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | l     | 3421 | PHI  | CZ-I  | -2.97 | 2.02        | 2.10     |
| 1   | o     | 2121 | PHI  | CZ-I  | -2.97 | 2.02        | 2.10     |
| 1   | v     | 2821 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | X     | 5821 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | n     | 2021 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | H     | 4221 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | BA    | 6821 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | S     | 5321 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | w     | 2921 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | T     | 5421 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | 3     | 3621 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | 8     | 4121 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | R     | 5221 | PHI  | CZ-I  | -2.96 | 2.02        | 2.10     |
| 1   | r     | 2421 | PHI  | CZ-I  | -2.95 | 2.02        | 2.10     |
| 1   | J     | 4421 | PHI  | CZ-I  | -2.95 | 2.02        | 2.10     |
| 1   | P     | 5021 | PHI  | CZ-I  | -2.95 | 2.02        | 2.10     |
| 1   | 4     | 3721 | PHI  | CZ-I  | -2.95 | 2.02        | 2.10     |
| 1   | D     | 221  | PHI  | CZ-I  | -2.95 | 2.02        | 2.10     |
| 1   | 6     | 3921 | PHI  | CZ-I  | -2.95 | 2.02        | 2.10     |
| 1   | FA    | 6021 | PHI  | CZ-I  | -2.94 | 2.02        | 2.10     |
| 1   | t     | 2621 | PHI  | CZ-I  | -2.94 | 2.02        | 2.10     |
| 1   | z     | 3221 | PHI  | CZ-I  | -2.94 | 2.02        | 2.10     |
| 1   | q     | 2321 | PHI  | CZ-I  | -2.94 | 2.02        | 2.10     |
| 1   | s     | 2521 | PHI  | CZ-I  | -2.93 | 2.02        | 2.10     |
| 1   | HA    | 6421 | PHI  | CZ-I  | -2.93 | 2.02        | 2.10     |
| 1   | K     | 4521 | PHI  | CZ-I  | -2.92 | 2.02        | 2.10     |
| 1   | L     | 4621 | PHI  | CZ-I  | -2.91 | 2.02        | 2.10     |
| 1   | 2     | 3521 | PHI  | CZ-I  | -2.91 | 2.02        | 2.10     |
| 1   | 7     | 4021 | PHI  | CZ-I  | -2.85 | 2.02        | 2.10     |

There are no bond angle outliers.

There are no chirality outliers.

All (147) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | B     | 21   | PHI  | C-CA-CB-CG |
| 1   | D     | 221  | PHI  | C-CA-CB-CG |
| 1   | E     | 321  | PHI  | C-CA-CB-CG |
| 1   | F     | 421  | PHI  | N-CA-CB-CG |
| 1   | F     | 421  | PHI  | C-CA-CB-CG |
| 1   | J     | 4421 | PHI  | C-CA-CB-CG |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | L     | 4621 | PHI  | N-CA-CB-CG |
| 1   | L     | 4621 | PHI  | C-CA-CB-CG |
| 1   | M     | 4721 | PHI  | C-CA-CB-CG |
| 1   | M     | 4721 | PHI  | O-C-CA-CB  |
| 1   | N     | 4821 | PHI  | O-C-CA-CB  |
| 1   | P     | 5021 | PHI  | C-CA-CB-CG |
| 1   | Q     | 5121 | PHI  | C-CA-CB-CG |
| 1   | R     | 5221 | PHI  | N-CA-CB-CG |
| 1   | R     | 5221 | PHI  | C-CA-CB-CG |
| 1   | U     | 5521 | PHI  | O-C-CA-CB  |
| 1   | V     | 5621 | PHI  | C-CA-CB-CG |
| 1   | W     | 5721 | PHI  | C-CA-CB-CG |
| 1   | X     | 5821 | PHI  | C-CA-CB-CG |
| 1   | Z     | 621  | PHI  | O-C-CA-CB  |
| 1   | b     | 821  | PHI  | C-CA-CB-CG |
| 1   | c     | 921  | PHI  | N-CA-CB-CG |
| 1   | c     | 921  | PHI  | C-CA-CB-CG |
| 1   | d     | 1021 | PHI  | C-CA-CB-CG |
| 1   | f     | 1221 | PHI  | C-CA-CB-CG |
| 1   | f     | 1221 | PHI  | O-C-CA-CB  |
| 1   | h     | 1421 | PHI  | C-CA-CB-CG |
| 1   | i     | 1521 | PHI  | C-CA-CB-CG |
| 1   | j     | 1621 | PHI  | N-CA-CB-CG |
| 1   | j     | 1621 | PHI  | C-CA-CB-CG |
| 1   | l     | 1821 | PHI  | C-CA-CB-CG |
| 1   | n     | 2021 | PHI  | C-CA-CB-CG |
| 1   | o     | 2121 | PHI  | C-CA-CB-CG |
| 1   | p     | 2221 | PHI  | O-C-CA-CB  |
| 1   | r     | 2421 | PHI  | C-CA-CB-CG |
| 1   | t     | 2621 | PHI  | C-CA-CB-CG |
| 1   | v     | 2821 | PHI  | N-CA-CB-CG |
| 1   | v     | 2821 | PHI  | C-CA-CB-CG |
| 1   | w     | 2921 | PHI  | C-CA-CB-CG |
| 1   | w     | 2921 | PHI  | O-C-CA-CB  |
| 1   | z     | 3221 | PHI  | C-CA-CB-CG |
| 1   | 0     | 3321 | PHI  | C-CA-CB-CG |
| 1   | 1     | 3421 | PHI  | C-CA-CB-CG |
| 1   | 2     | 3521 | PHI  | O-C-CA-CB  |
| 1   | 3     | 3621 | PHI  | C-CA-CB-CG |
| 1   | 7     | 4021 | PHI  | C-CA-CB-CG |
| 1   | 9     | 6621 | PHI  | C-CA-CB-CG |
| 1   | 9     | 6621 | PHI  | O-C-CA-CB  |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | BA    | 6821 | PHI  | C-CA-CB-CG   |
| 1   | DA    | 7021 | PHI  | N-CA-CB-CG   |
| 1   | DA    | 7021 | PHI  | C-CA-CB-CG   |
| 1   | JA    | 6221 | PHI  | C-CA-CB-CG   |
| 1   | HA    | 6421 | PHI  | C-CA-CB-CG   |
| 1   | IA    | 6521 | PHI  | C-CA-CB-CG   |
| 1   | q     | 2321 | PHI  | CA-CB-CG-CD2 |
| 1   | f     | 1221 | PHI  | CA-CB-CG-CD2 |
| 1   | Z     | 621  | PHI  | CA-CB-CG-CD2 |
| 1   | q     | 2321 | PHI  | CA-CB-CG-CD1 |
| 1   | B     | 21   | PHI  | N-CA-CB-CG   |
| 1   | D     | 221  | PHI  | N-CA-CB-CG   |
| 1   | J     | 4421 | PHI  | N-CA-CB-CG   |
| 1   | M     | 4721 | PHI  | N-CA-CB-CG   |
| 1   | P     | 5021 | PHI  | N-CA-CB-CG   |
| 1   | Y     | 5921 | PHI  | N-CA-CB-CG   |
| 1   | b     | 821  | PHI  | N-CA-CB-CG   |
| 1   | d     | 1021 | PHI  | N-CA-CB-CG   |
| 1   | f     | 1221 | PHI  | N-CA-CB-CG   |
| 1   | h     | 1421 | PHI  | N-CA-CB-CG   |
| 1   | n     | 2021 | PHI  | N-CA-CB-CG   |
| 1   | p     | 2221 | PHI  | N-CA-CB-CG   |
| 1   | y     | 3121 | PHI  | N-CA-CB-CG   |
| 1   | z     | 3221 | PHI  | N-CA-CB-CG   |
| 1   | 1     | 3421 | PHI  | N-CA-CB-CG   |
| 1   | 3     | 3621 | PHI  | N-CA-CB-CG   |
| 1   | 7     | 4021 | PHI  | N-CA-CB-CG   |
| 1   | 9     | 6621 | PHI  | N-CA-CB-CG   |
| 1   | BA    | 6821 | PHI  | N-CA-CB-CG   |
| 1   | HA    | 6421 | PHI  | N-CA-CB-CG   |
| 1   | IA    | 6521 | PHI  | N-CA-CB-CG   |
| 1   | f     | 1221 | PHI  | CA-CB-CG-CD1 |
| 1   | Z     | 621  | PHI  | CA-CB-CG-CD1 |
| 1   | B     | 21   | PHI  | CA-CB-CG-CD2 |
| 1   | 9     | 6621 | PHI  | CA-CB-CG-CD2 |
| 1   | p     | 2221 | PHI  | CA-CB-CG-CD2 |
| 1   | l     | 1821 | PHI  | CA-CB-CG-CD2 |
| 1   | B     | 21   | PHI  | CA-CB-CG-CD1 |
| 1   | 2     | 3521 | PHI  | CA-CB-CG-CD2 |
| 1   | G     | 521  | PHI  | CA-CB-CG-CD2 |
| 1   | 9     | 6621 | PHI  | CA-CB-CG-CD1 |
| 1   | EA    | 7121 | PHI  | CA-CB-CG-CD2 |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | p     | 2221 | PHI  | CA-CB-CG-CD1 |
| 1   | 2     | 3521 | PHI  | CA-CB-CG-CD1 |
| 1   | G     | 521  | PHI  | CA-CB-CG-CD1 |
| 1   | t     | 2621 | PHI  | CA-CB-CG-CD2 |
| 1   | EA    | 7121 | PHI  | CA-CB-CG-CD1 |
| 1   | l     | 1821 | PHI  | CA-CB-CG-CD1 |
| 1   | T     | 5421 | PHI  | CA-CB-CG-CD2 |
| 1   | t     | 2621 | PHI  | CA-CB-CG-CD1 |
| 1   | T     | 5421 | PHI  | CA-CB-CG-CD1 |
| 1   | k     | 1721 | PHI  | CA-CB-CG-CD1 |
| 1   | H     | 4221 | PHI  | CA-CB-CG-CD2 |
| 1   | e     | 1121 | PHI  | CA-CB-CG-CD1 |
| 1   | k     | 1721 | PHI  | CA-CB-CG-CD2 |
| 1   | e     | 1121 | PHI  | CA-CB-CG-CD2 |
| 1   | H     | 4221 | PHI  | CA-CB-CG-CD1 |
| 1   | h     | 1421 | PHI  | CA-CB-CG-CD2 |
| 1   | h     | 1421 | PHI  | CA-CB-CG-CD1 |
| 1   | G     | 521  | PHI  | C-CA-CB-CG   |
| 1   | K     | 4521 | PHI  | C-CA-CB-CG   |
| 1   | V     | 5621 | PHI  | N-CA-CB-CG   |
| 1   | X     | 5821 | PHI  | N-CA-CB-CG   |
| 1   | Y     | 5921 | PHI  | C-CA-CB-CG   |
| 1   | Z     | 621  | PHI  | C-CA-CB-CG   |
| 1   | l     | 1821 | PHI  | N-CA-CB-CG   |
| 1   | m     | 1921 | PHI  | C-CA-CB-CG   |
| 1   | p     | 2221 | PHI  | C-CA-CB-CG   |
| 1   | r     | 2421 | PHI  | N-CA-CB-CG   |
| 1   | s     | 2521 | PHI  | C-CA-CB-CG   |
| 1   | t     | 2621 | PHI  | N-CA-CB-CG   |
| 1   | w     | 2921 | PHI  | N-CA-CB-CG   |
| 1   | y     | 3121 | PHI  | C-CA-CB-CG   |
| 1   | 4     | 3721 | PHI  | C-CA-CB-CG   |
| 1   | 6     | 3921 | PHI  | C-CA-CB-CG   |
| 1   | 8     | 4121 | PHI  | C-CA-CB-CG   |
| 1   | EA    | 7121 | PHI  | C-CA-CB-CG   |
| 1   | FA    | 6021 | PHI  | N-CA-CB-CG   |
| 1   | FA    | 6021 | PHI  | C-CA-CB-CG   |
| 1   | JA    | 6221 | PHI  | N-CA-CB-CG   |
| 1   | x     | 3021 | PHI  | CA-CB-CG-CD2 |
| 1   | 8     | 4121 | PHI  | CA-CB-CG-CD2 |
| 1   | x     | 3021 | PHI  | CA-CB-CG-CD1 |
| 1   | 8     | 4121 | PHI  | CA-CB-CG-CD1 |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | N     | 4821 | PHI  | CA-CB-CG-CD2 |
| 1   | BA    | 6821 | PHI  | CA-CB-CG-CD2 |
| 1   | D     | 221  | PHI  | CA-CB-CG-CD2 |
| 1   | N     | 4821 | PHI  | CA-CB-CG-CD1 |
| 1   | D     | 221  | PHI  | CA-CB-CG-CD1 |
| 1   | BA    | 6821 | PHI  | CA-CB-CG-CD1 |
| 1   | C     | 121  | PHI  | C-CA-CB-CG   |
| 1   | Q     | 5121 | PHI  | N-CA-CB-CG   |
| 1   | e     | 1121 | PHI  | C-CA-CB-CG   |
| 1   | k     | 1721 | PHI  | C-CA-CB-CG   |
| 1   | x     | 3021 | PHI  | C-CA-CB-CG   |
| 1   | AA    | 6721 | PHI  | C-CA-CB-CG   |
| 1   | CA    | 6921 | PHI  | C-CA-CB-CG   |
| 1   | GA    | 6321 | PHI  | C-CA-CB-CG   |
| 1   | S     | 5321 | PHI  | CA-CB-CG-CD2 |

There are no ring outliers.

32 monomers are involved in 89 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | t     | 2621 | PHI  | 1       | 0            |
| 1   | p     | 2221 | PHI  | 2       | 0            |
| 1   | JA    | 6221 | PHI  | 2       | 0            |
| 1   | M     | 4721 | PHI  | 1       | 0            |
| 1   | 2     | 3521 | PHI  | 1       | 0            |
| 1   | 6     | 3921 | PHI  | 3       | 0            |
| 1   | N     | 4821 | PHI  | 1       | 0            |
| 1   | EA    | 7121 | PHI  | 2       | 0            |
| 1   | G     | 521  | PHI  | 1       | 0            |
| 1   | CA    | 6921 | PHI  | 4       | 0            |
| 1   | q     | 2321 | PHI  | 4       | 0            |
| 1   | Q     | 5121 | PHI  | 16      | 0            |
| 1   | f     | 1221 | PHI  | 1       | 0            |
| 1   | V     | 5621 | PHI  | 7       | 0            |
| 1   | s     | 2521 | PHI  | 1       | 0            |
| 1   | GA    | 6321 | PHI  | 1       | 0            |
| 1   | E     | 321  | PHI  | 2       | 0            |
| 1   | X     | 5821 | PHI  | 1       | 0            |
| 1   | 7     | 4021 | PHI  | 4       | 0            |
| 1   | g     | 1321 | PHI  | 1       | 0            |
| 1   | 1     | 3421 | PHI  | 1       | 0            |
| 1   | K     | 4521 | PHI  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | k     | 1721 | PHI  | 2       | 0            |
| 1   | H     | 4221 | PHI  | 2       | 0            |
| 1   | x     | 3021 | PHI  | 5       | 0            |
| 1   | u     | 2721 | PHI  | 1       | 0            |
| 1   | z     | 3221 | PHI  | 15      | 0            |
| 1   | FA    | 6021 | PHI  | 2       | 0            |
| 1   | Z     | 621  | PHI  | 1       | 0            |
| 1   | T     | 5421 | PHI  | 2       | 0            |
| 1   | l     | 1821 | PHI  | 1       | 0            |
| 1   | B     | 21   | PHI  | 1       | 0            |

## 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.

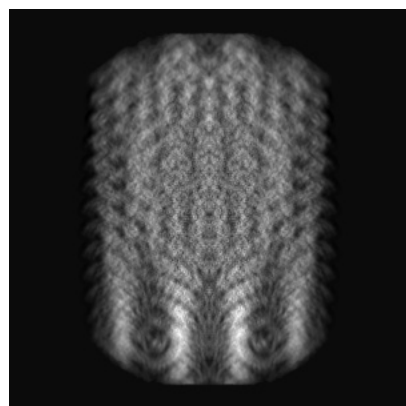
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26552. These allow visual inspection of the internal detail of the map and identification of artifacts.

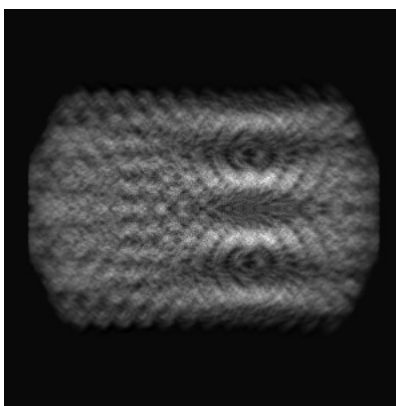
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

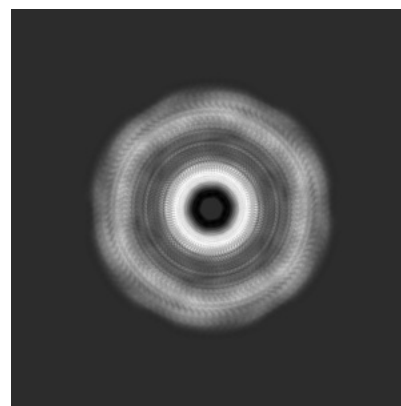
#### 6.1.1 Primary map



X

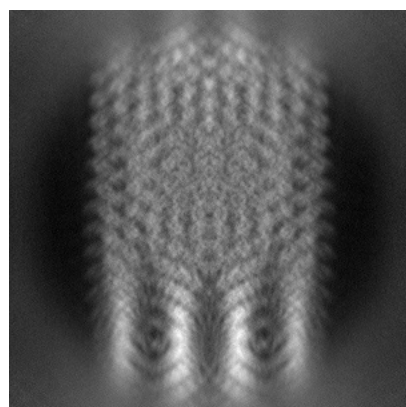


Y

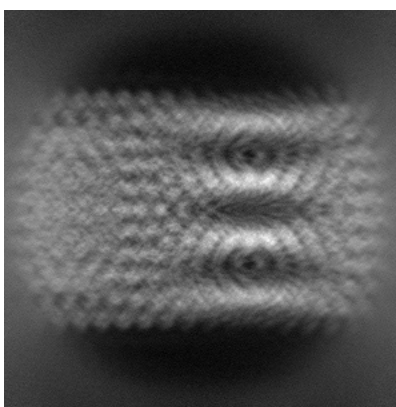


Z

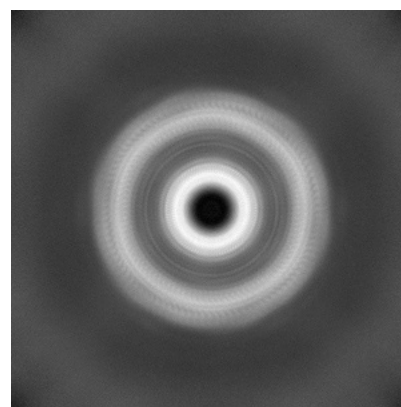
#### 6.1.2 Raw map



X



Y

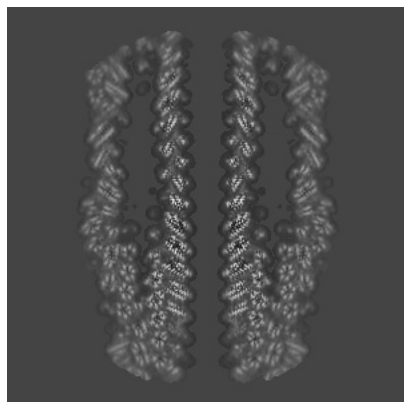


Z

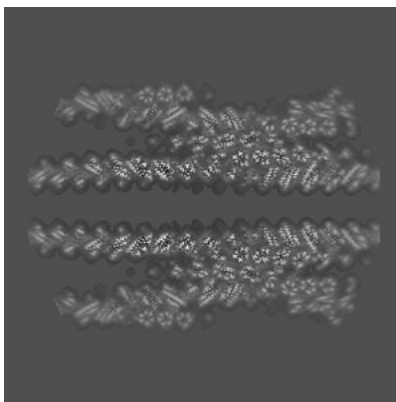
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

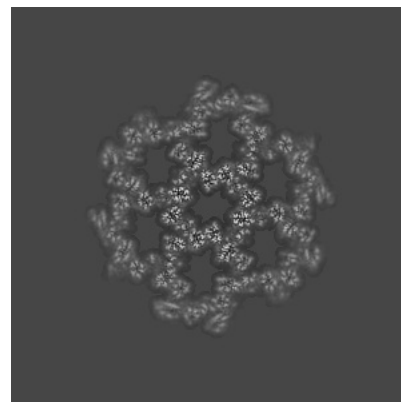
### 6.2.1 Primary map



X Index: 320

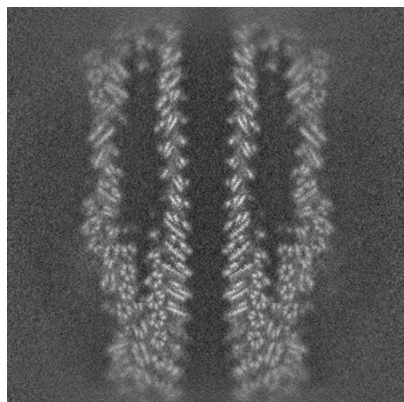


Y Index: 320

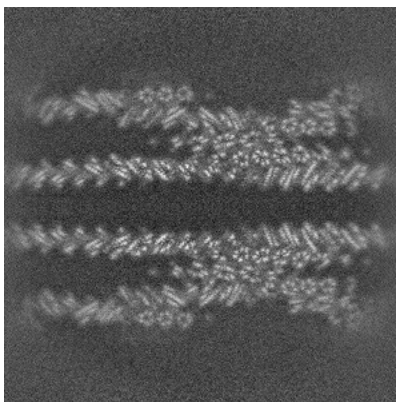


Z Index: 320

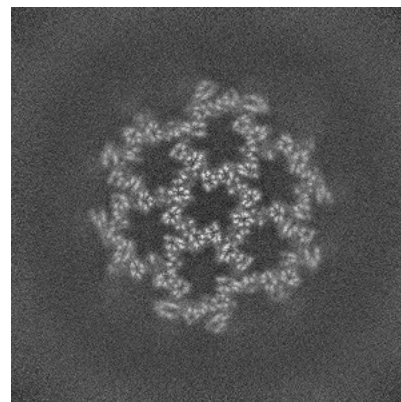
### 6.2.2 Raw map



X Index: 320



Y Index: 320

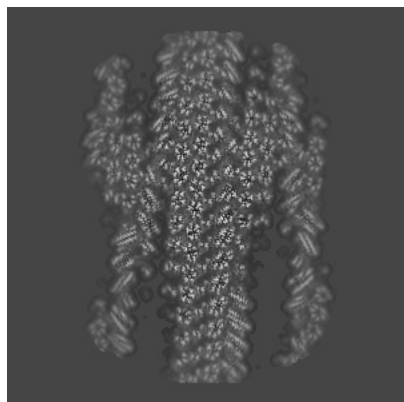


Z Index: 320

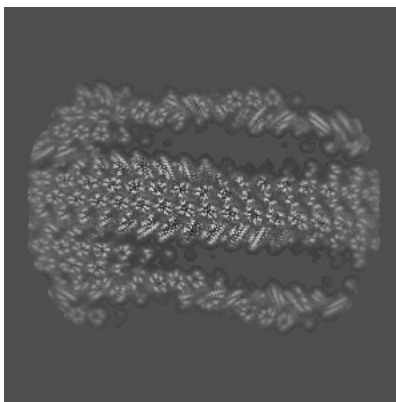
The images above show central slices of the map in three orthogonal directions.

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

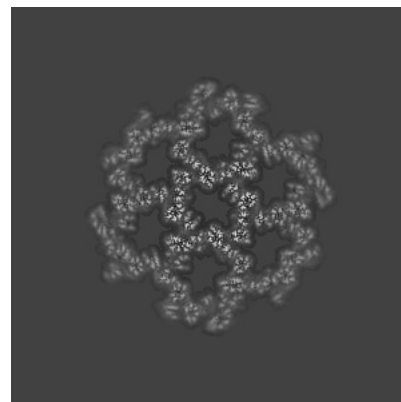
### 6.3.1 Primary map



X Index: 365

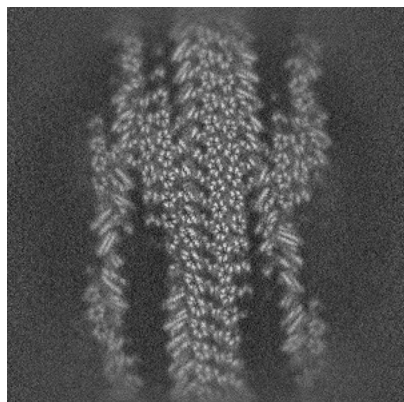


Y Index: 368

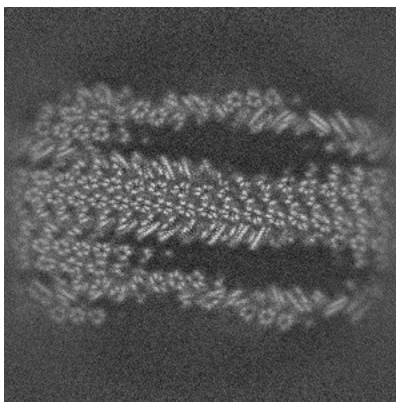


Z Index: 327

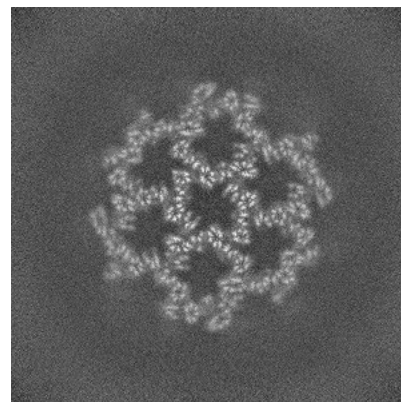
### 6.3.2 Raw map



X Index: 275



Y Index: 368

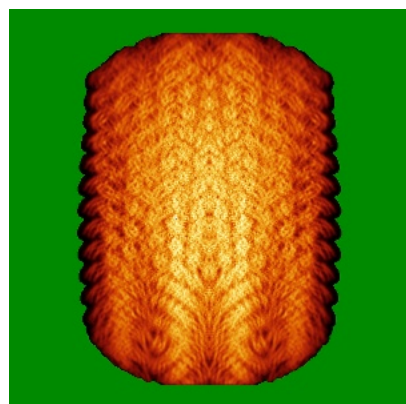


Z Index: 327

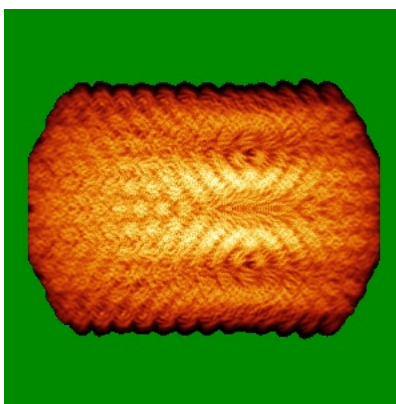
The images above show the largest variance slices of the map in three orthogonal directions.

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

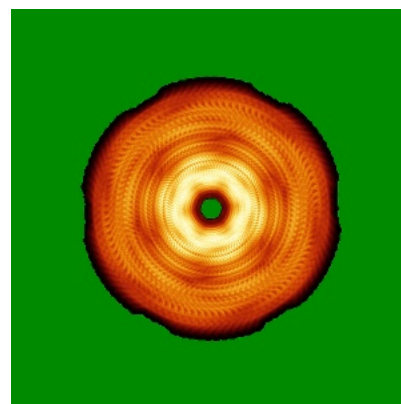
### 6.4.1 Primary map



X

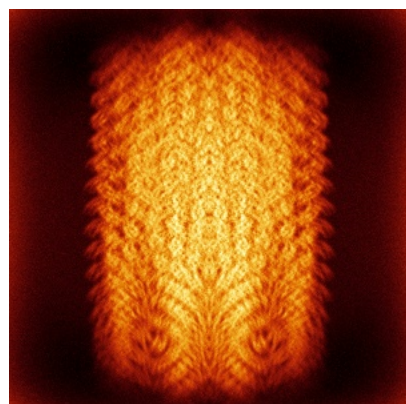


Y

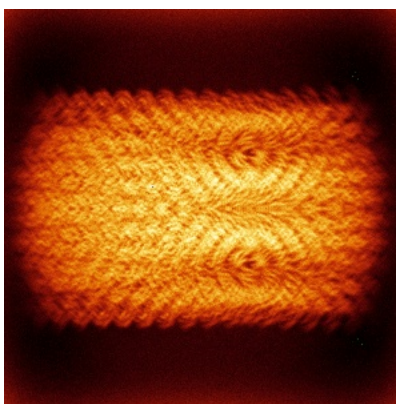


Z

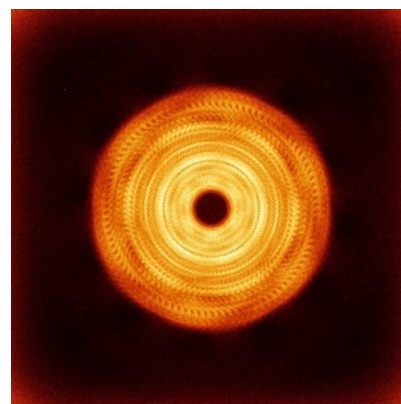
### 6.4.2 Raw map



X



Y

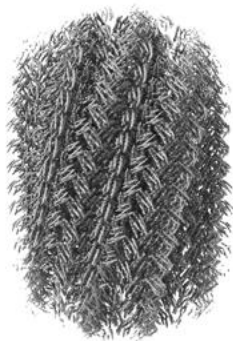


Z

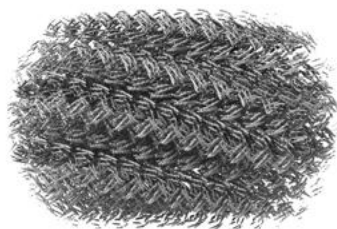
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

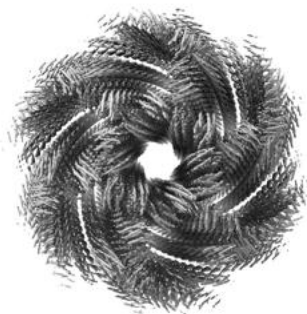
### 6.5.1 Primary map



X



Y



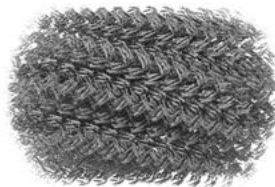
Z

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

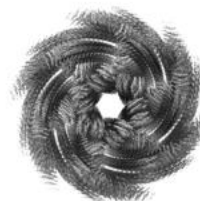
### 6.5.2 Raw map



X



Y



Z

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

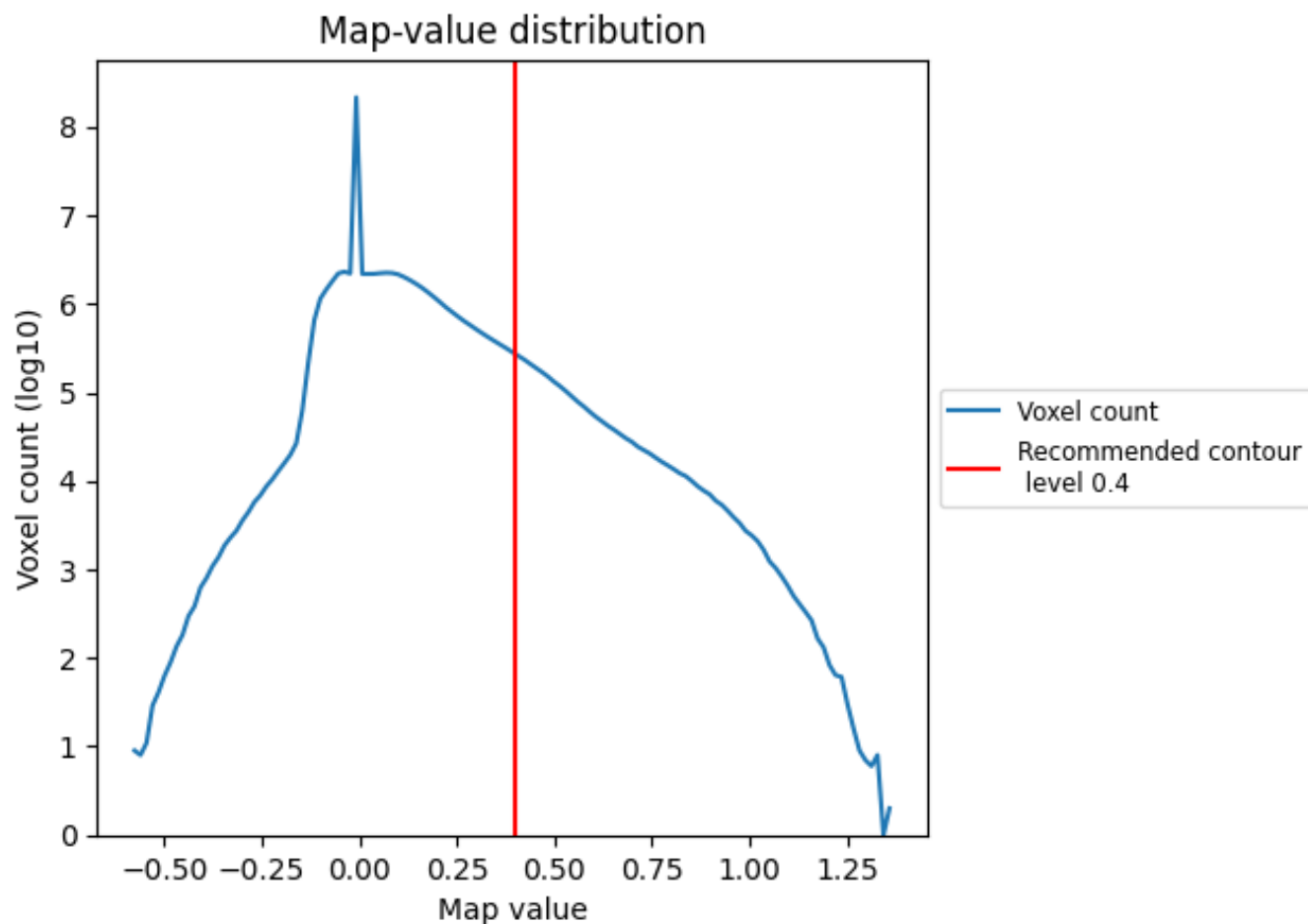
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

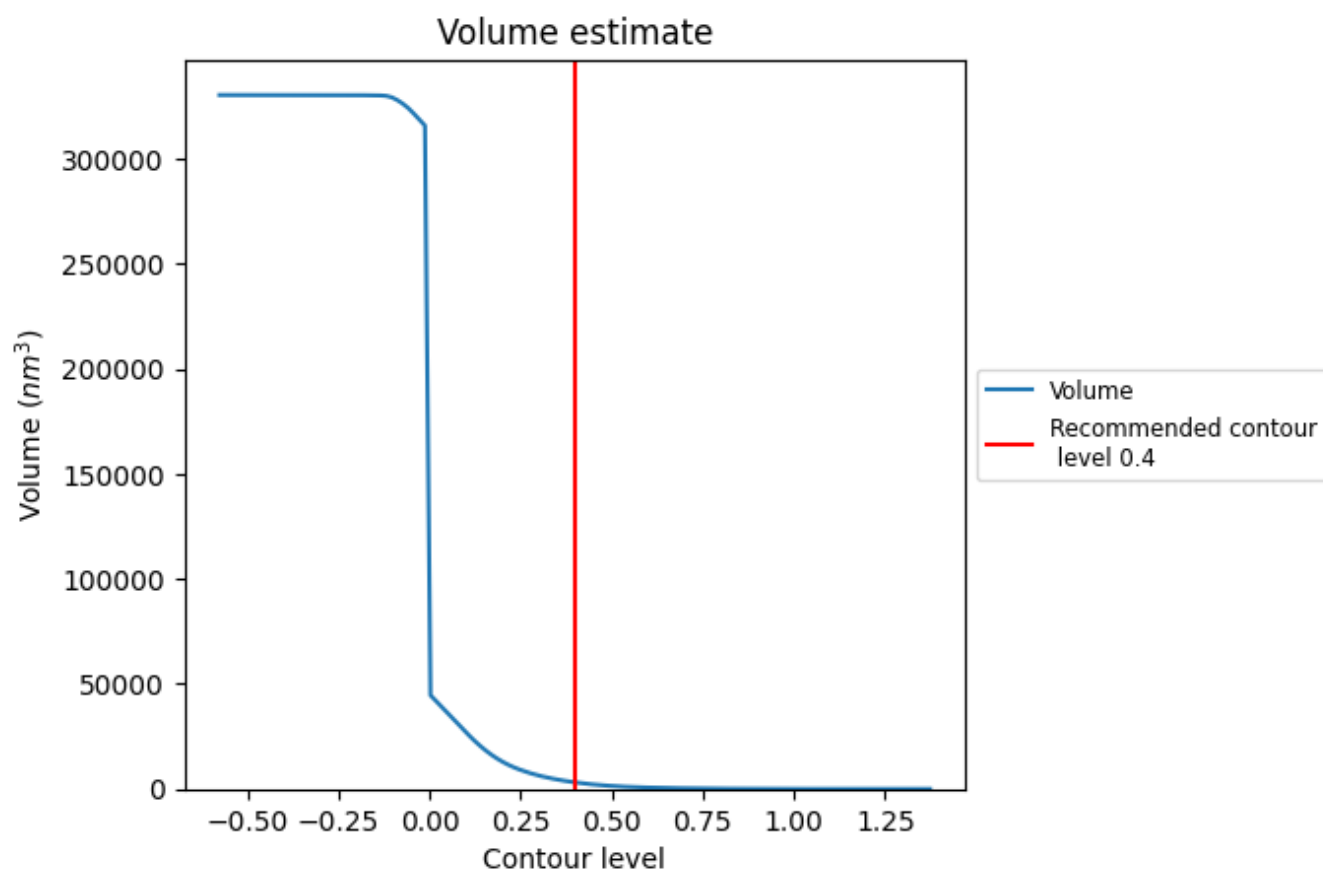
This section contains the results of statistical analysis of the map.

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



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

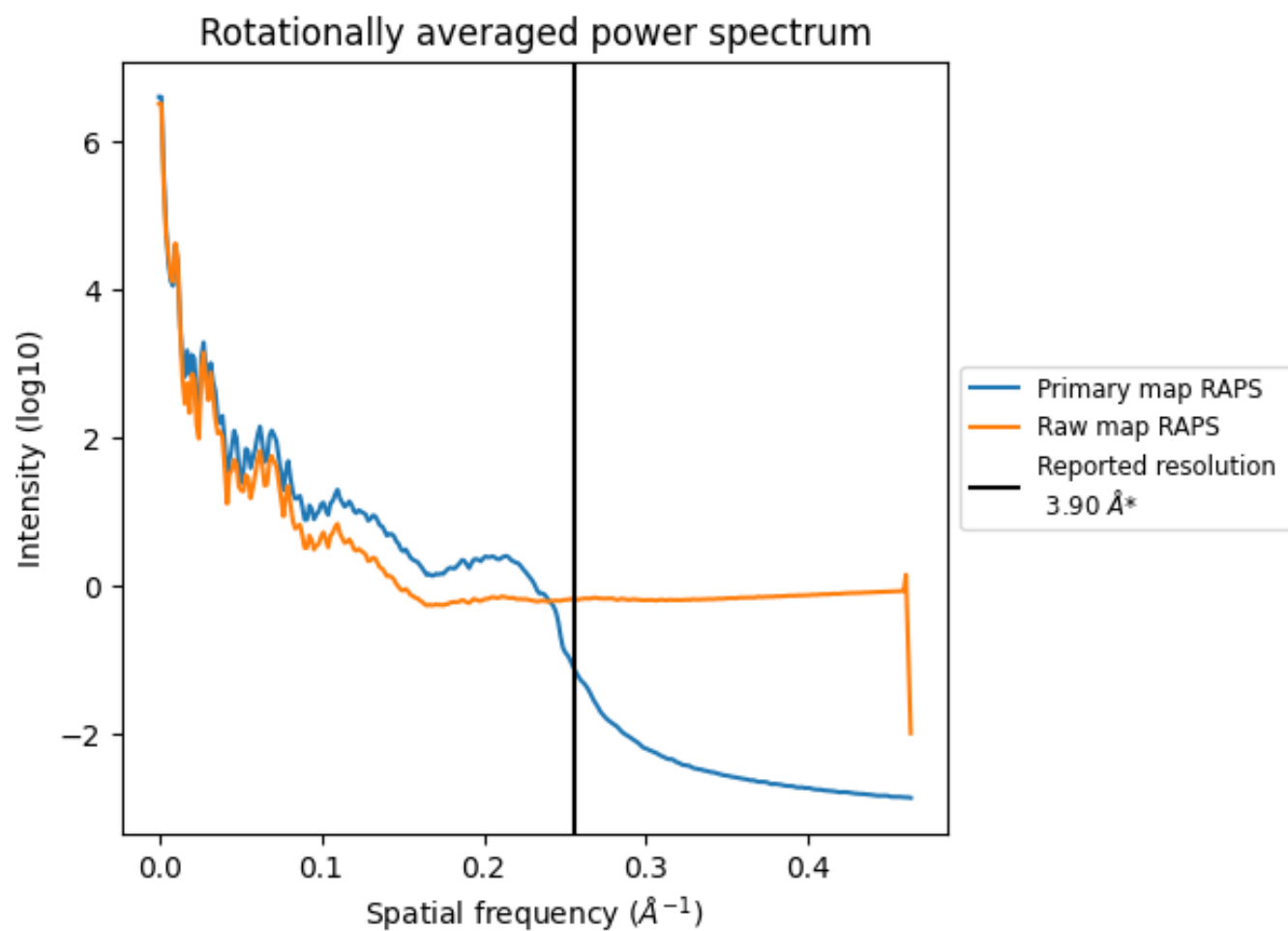
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3123  $\text{nm}^3$ ; this corresponds to an approximate mass of 2821 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

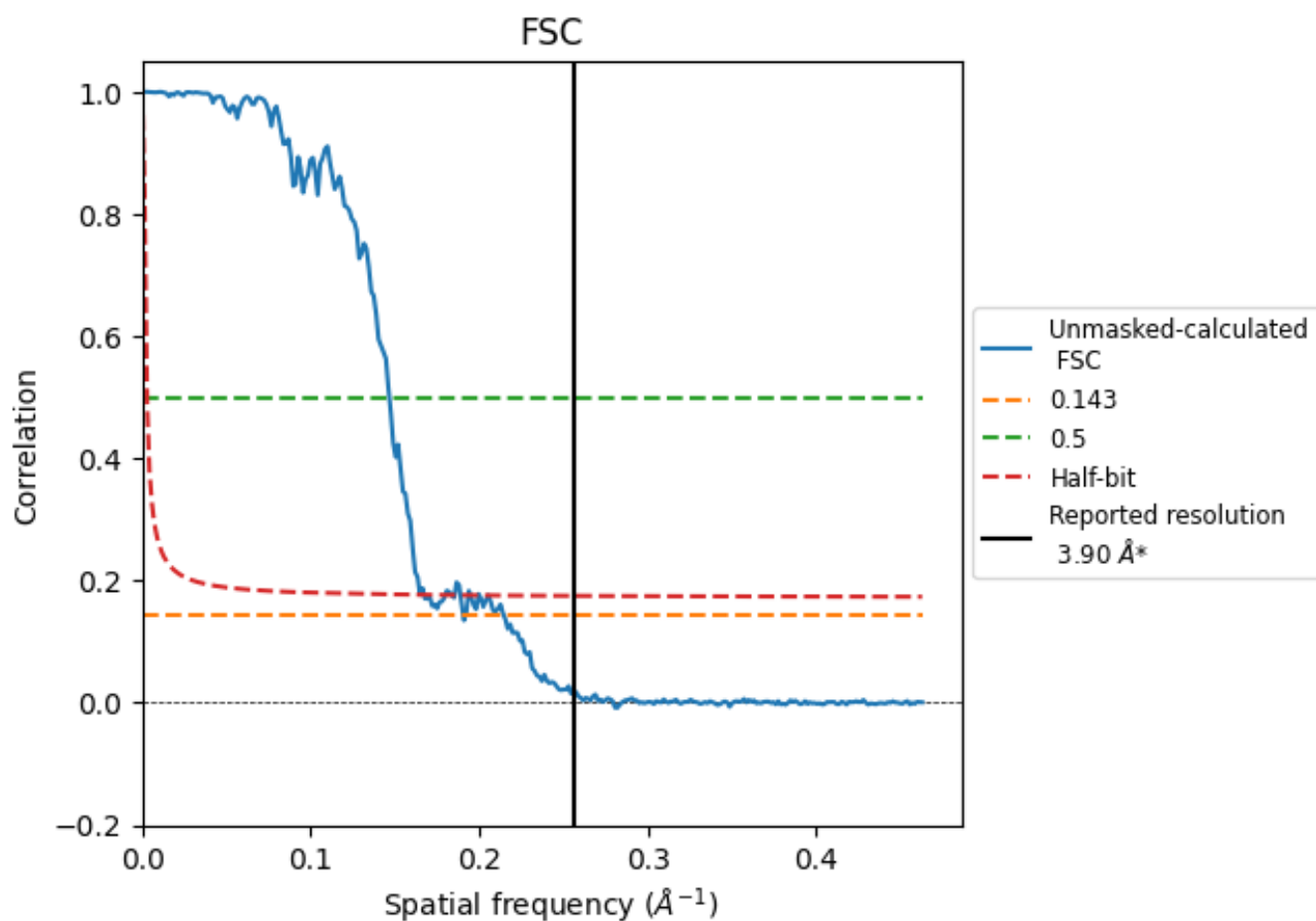


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

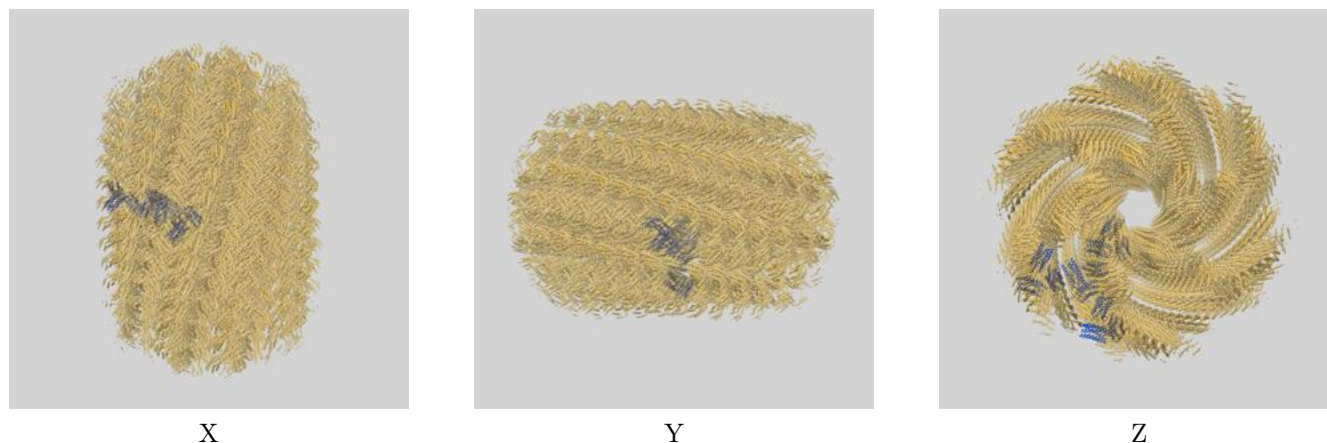
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.90                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 5.25                               | 6.82 | 6.06     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.25 differs from the reported value 3.9 by more than 10 %

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

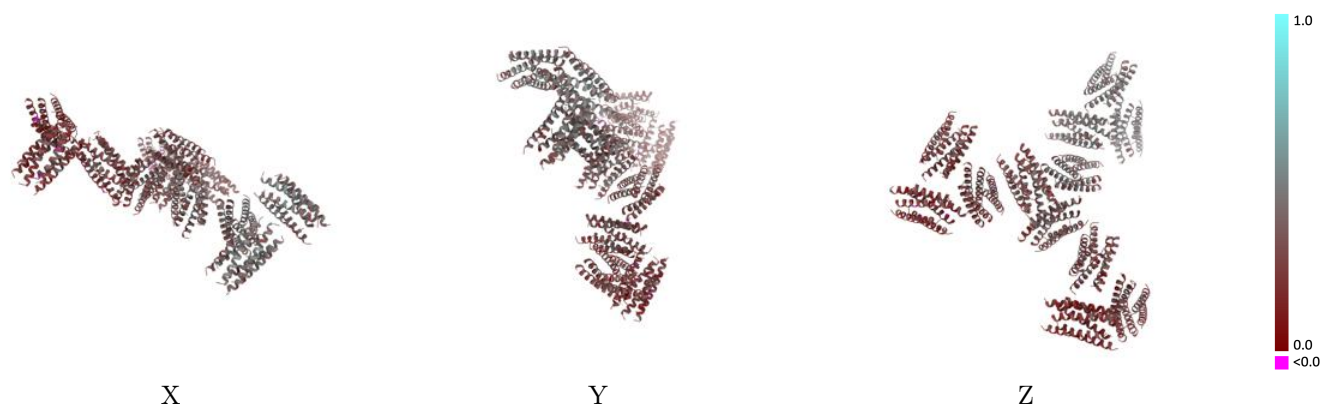
This section contains information regarding the fit between EMDB map EMD-26552 and PDB model 7UIT. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



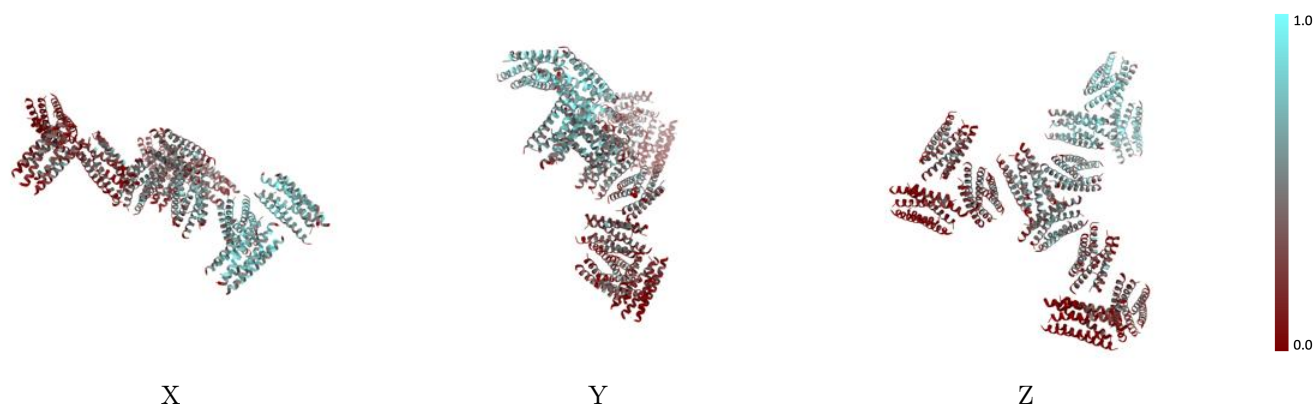
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



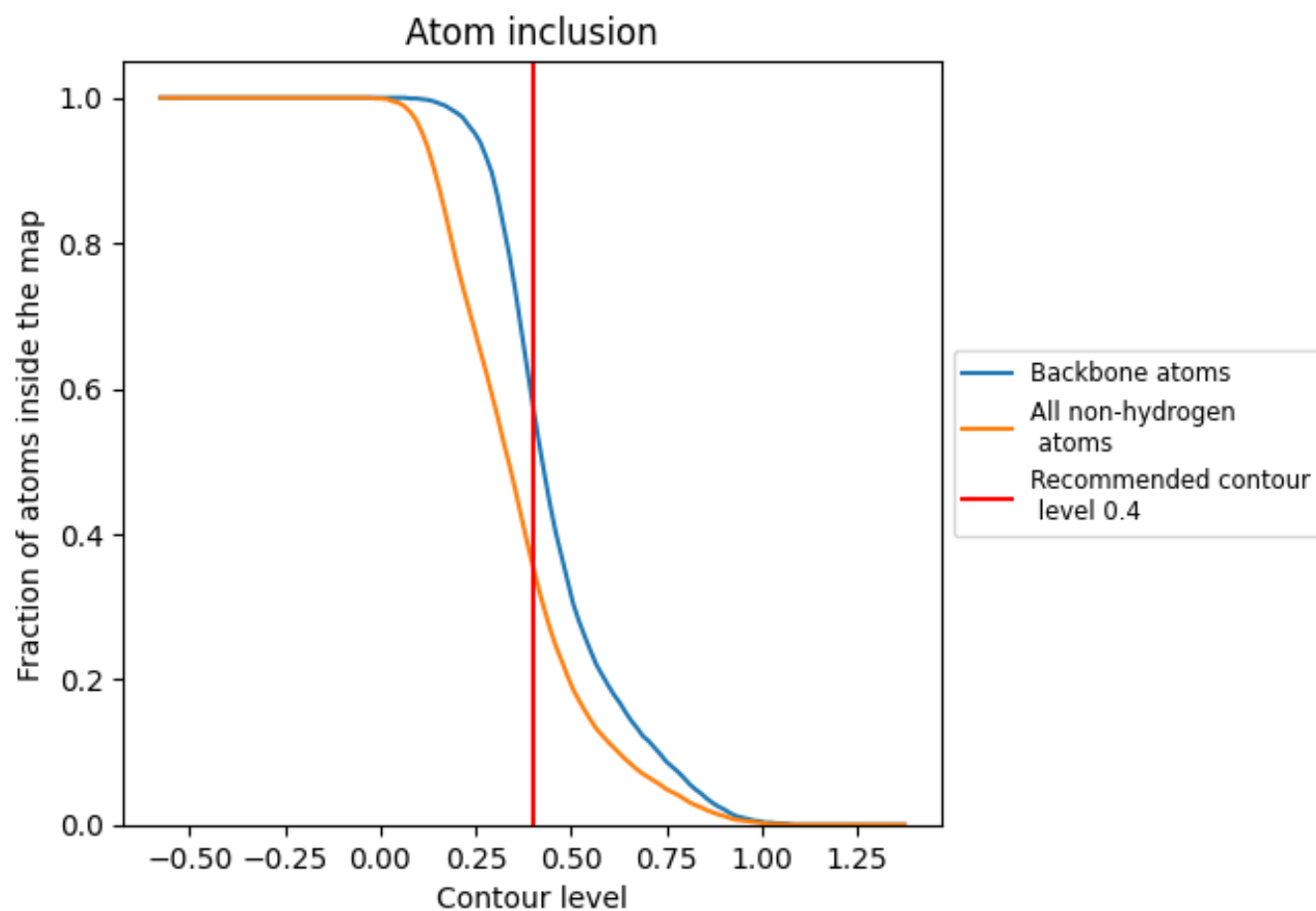
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary













































































The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.3550   |  0.3170   |
| 0     |  0.2400   |  0.3110   |
| 1     |  0.2280   |  0.2600   |
| 2     |  0.2530   |  0.2760   |
| 3     |  0.2360   |  0.2530   |
| 4     |  0.2660   |  0.2610   |
| 5     |  0.2790   |  0.3010   |
| 6     |  0.2490   |  0.2550   |
| 7     |  0.2400   |  0.2810   |
| 8     |  0.2360   |  0.2660   |
| 9     |  0.0130   |  0.2050   |
| A     |  0.0930   |  0.2200   |
| AA    |  0.0380   |  0.1880   |
| B     |  0.6410   |  0.4290   |
| BA    |  0.0590  |  0.1970  |
| C     |  0.6370 |  0.4390 |
| CA    |  0.1270 |  0.2160 |
| D     |  0.6410 |  0.4060 |
| DA    |  0.1100 |  0.2030 |
| E     |  0.6460 |  0.4180 |
| EA    |  0.0760 |  0.2180 |
| F     |  0.5780 |  0.4150 |
| FA    |  0.1010 |  0.2240 |
| G     |  0.6410 |  0.4400 |
| GA    |  0.0680 |  0.1830 |
| H     |  0.2660 |  0.2650 |
| HA    |  0.0800 |  0.1800 |
| I     |  0.3120 |  0.2740 |
| IA    |  0.1390 |  0.2110 |
| J     |  0.2660 |  0.2960 |
| JA    |  0.0250 |  0.2180 |
| K     |  0.2570 |  0.2620 |
| L     |  0.2360 |  0.2690 |
| M     |  0.2320 |  0.2900 |
| N     |  0.3420 |  0.3130 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| O     |  0.3630   |  0.3160   |
| P     |  0.3590   |  0.3150   |
| Q     |  0.3840   |  0.3240   |
| R     |  0.3670   |  0.3080   |
| S     |  0.3840   |  0.3270   |
| T     |  0.3120   |  0.2990   |
| U     |  0.2400   |  0.2870   |
| V     |  0.2490   |  0.2650   |
| W     |  0.2660   |  0.2770   |
| X     |  0.3080   |  0.2790   |
| Y     |  0.2660   |  0.2840   |
| Z     |  0.6250   |  0.4260   |
| a     |  0.6080   |  0.4110   |
| b     |  0.6370   |  0.4170   |
| c     |  0.6030   |  0.4160   |
| d     |  0.5950   |  0.4230   |
| e     |  0.6370   |  0.4400   |
| f     |  0.5650   |  0.4000   |
| g     |  0.5780   |  0.3910   |
| h     |  0.5870  |  0.3890  |
| i     |  0.5740 |  0.4000 |
| j     |  0.5610 |  0.4060 |
| k     |  0.6120 |  0.4280 |
| l     |  0.4470 |  0.3520 |
| m     |  0.4470 |  0.3810 |
| n     |  0.4600 |  0.3630 |
| o     |  0.4520 |  0.3640 |
| p     |  0.4980 |  0.3900 |
| q     |  0.4560 |  0.3830 |
| r     |  0.3970 |  0.3400 |
| s     |  0.4050 |  0.3290 |
| t     |  0.4180 |  0.3330 |
| u     |  0.4050 |  0.3290 |
| v     |  0.4350 |  0.3260 |
| w     |  0.3880 |  0.3300 |
| x     |  0.2950 |  0.3150 |
| y     |  0.2910 |  0.3040 |
| z     |  0.2190 |  0.2770 |