



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:14 AM EST

PDB ID : 1ZKU  
EMDB ID : EMD-1126  
Title : Fitting of the gp9 structure in the EM density of bacteriophage T4 extended tail  
Authors : Kostyuchenko, V.A.  
Deposited on : 2005-05-04  
Resolution : 15.00 Å(reported)  
Based on initial model : 1S2E

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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

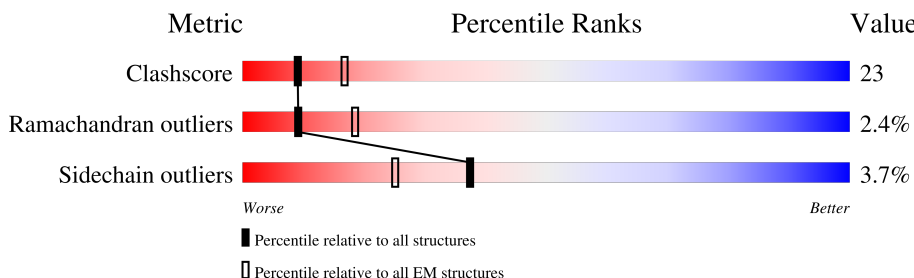
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 15.00 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            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 288    | <div> <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div> |
| 1   | B     | 288    | <div> <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div> |
| 1   | C     | 288    | <div> <div>100%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>5%</div> </div> </div> |
| 1   | D     | 288    | <div> <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div> |
| 1   | E     | 288    | <div> <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div> |
| 1   | F     | 288    | <div> <div>100%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>5%</div> </div> </div> |
| 1   | G     | 288    | <div> <div>100%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>5%</div> </div> </div> |
| 1   | H     | 288    | <div> <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | I     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | J     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | K     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | L     | 288    | <div>100%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>5%</div> </div> |
| 1   | M     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | N     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | O     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | P     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | Q     | 288    | <div>100%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> |
| 1   | R     | 288    | <div>100%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>5%</div> </div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 39420 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 Baseplate structural protein Gp9.

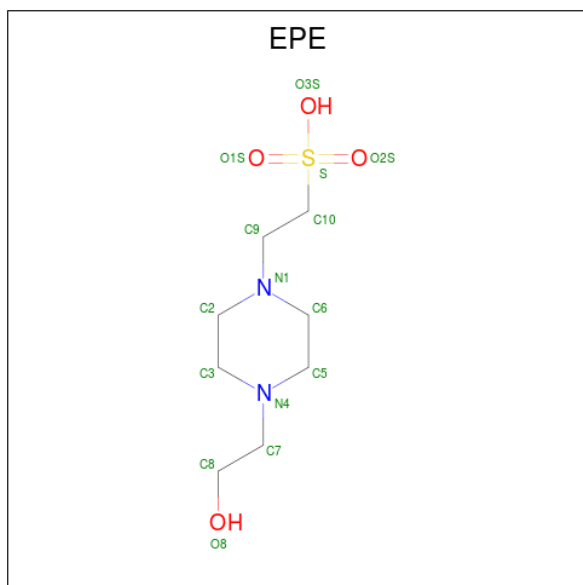
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | B     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | C     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | D     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | E     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | F     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | G     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | H     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | I     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | J     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | K     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | L     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | M     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | N     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | O     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | P     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |
| 1   | Q     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | R     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2175  | 1354 | 366 | 446 | 9 |         |       |

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 2   | A     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | B     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | C     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | D     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | E     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | F     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | G     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | H     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | I     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | J     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |

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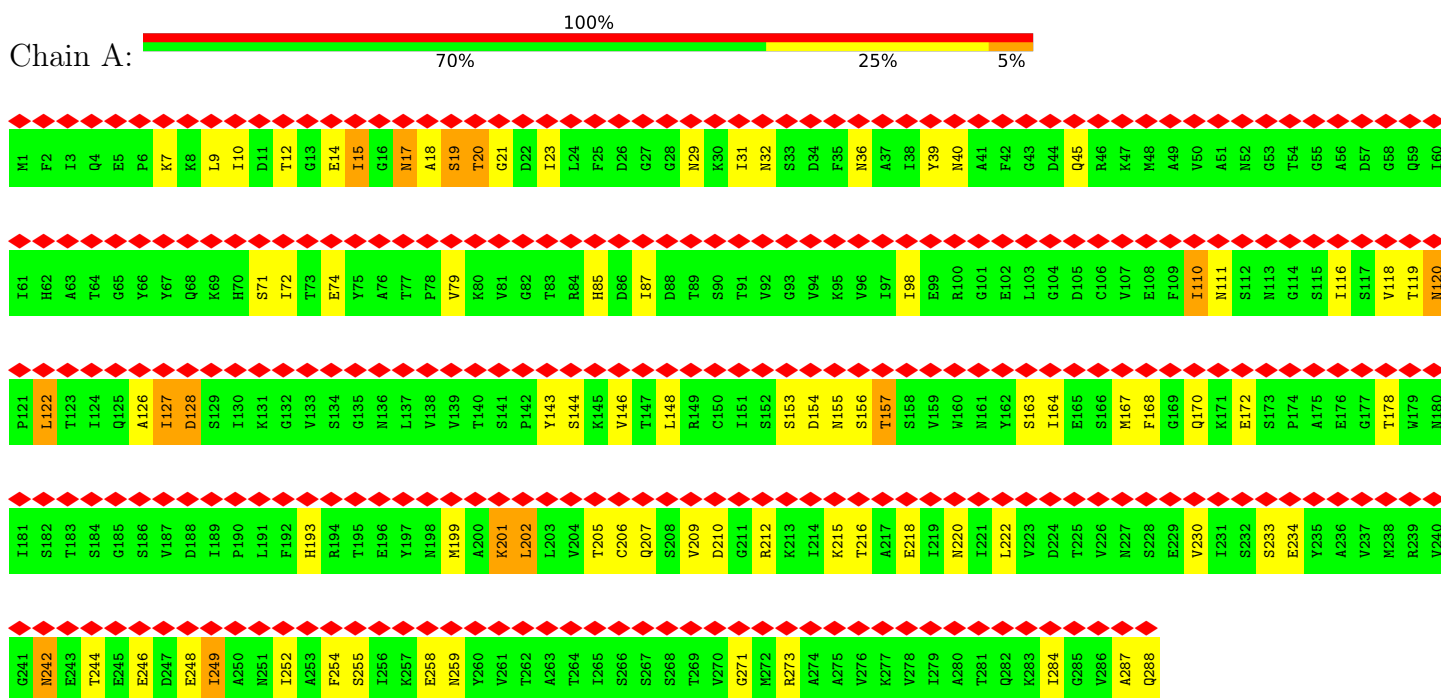
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| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 2   | K     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | L     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | M     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | N     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | O     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | P     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | Q     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |
| 2   | R     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |

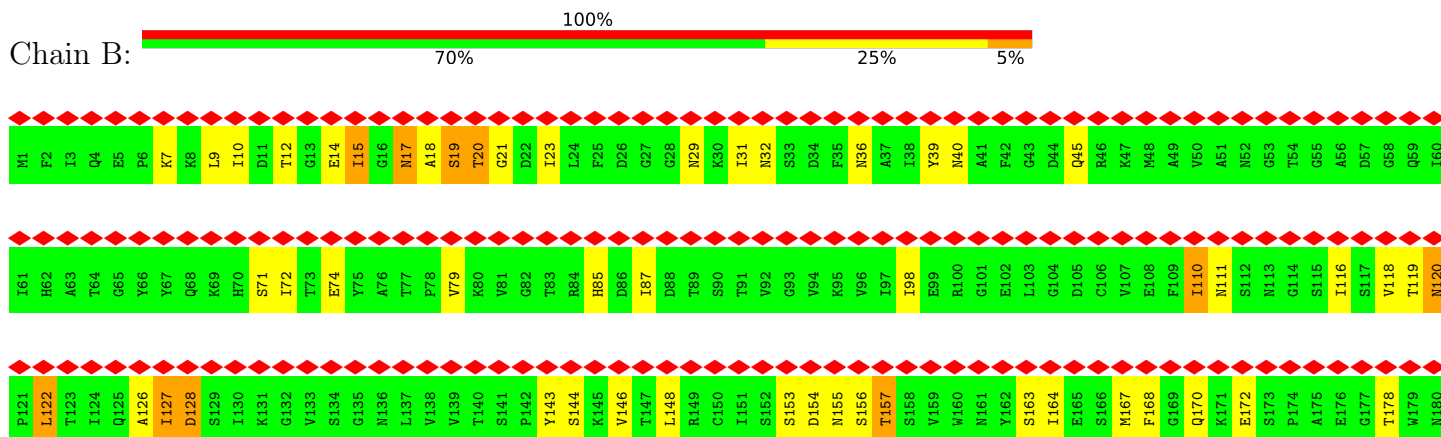
### 3 Residue-property plots

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

#### • Molecule 1: Baseplate structural protein Gp9

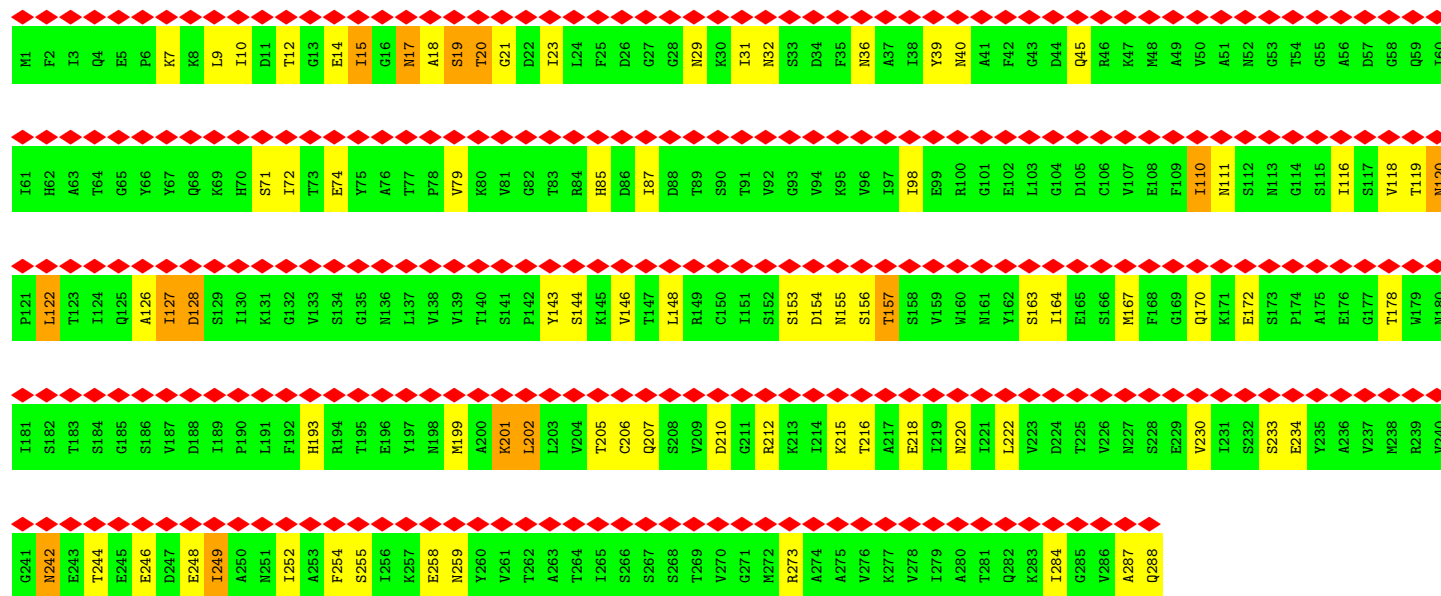


#### • Molecule 1: Baseplate structural protein Gp9

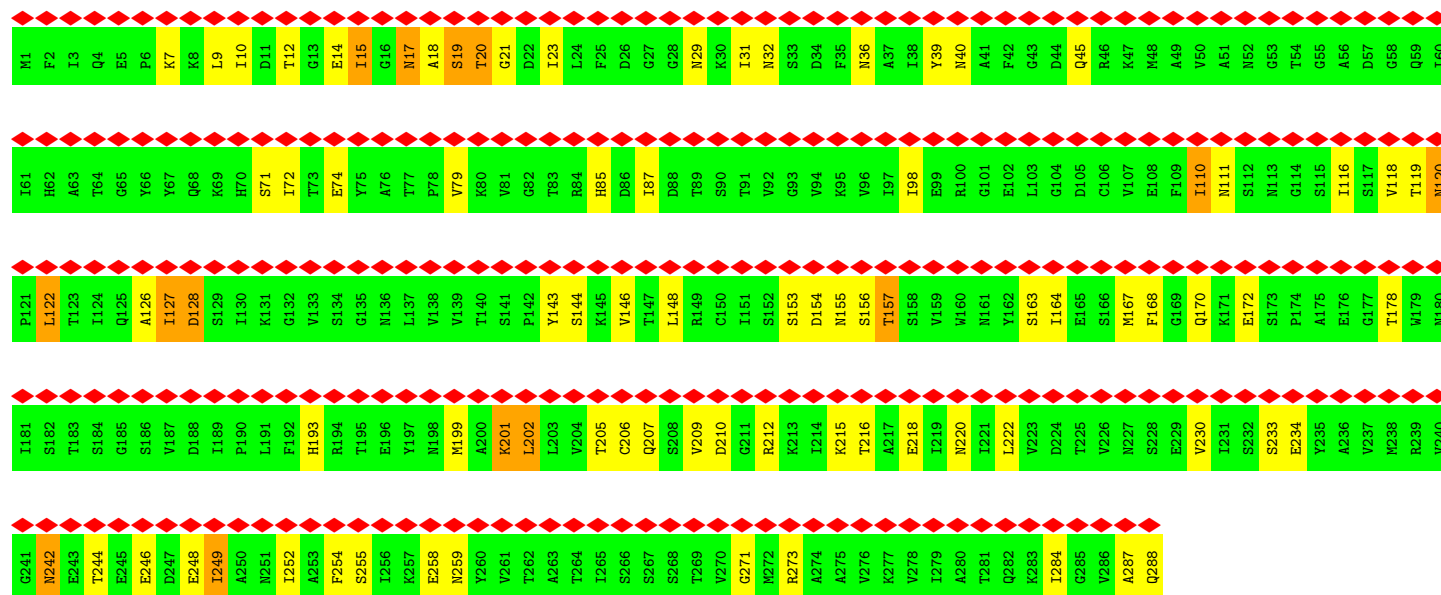




• Molecule 1: Baseplate structural protein Gp9

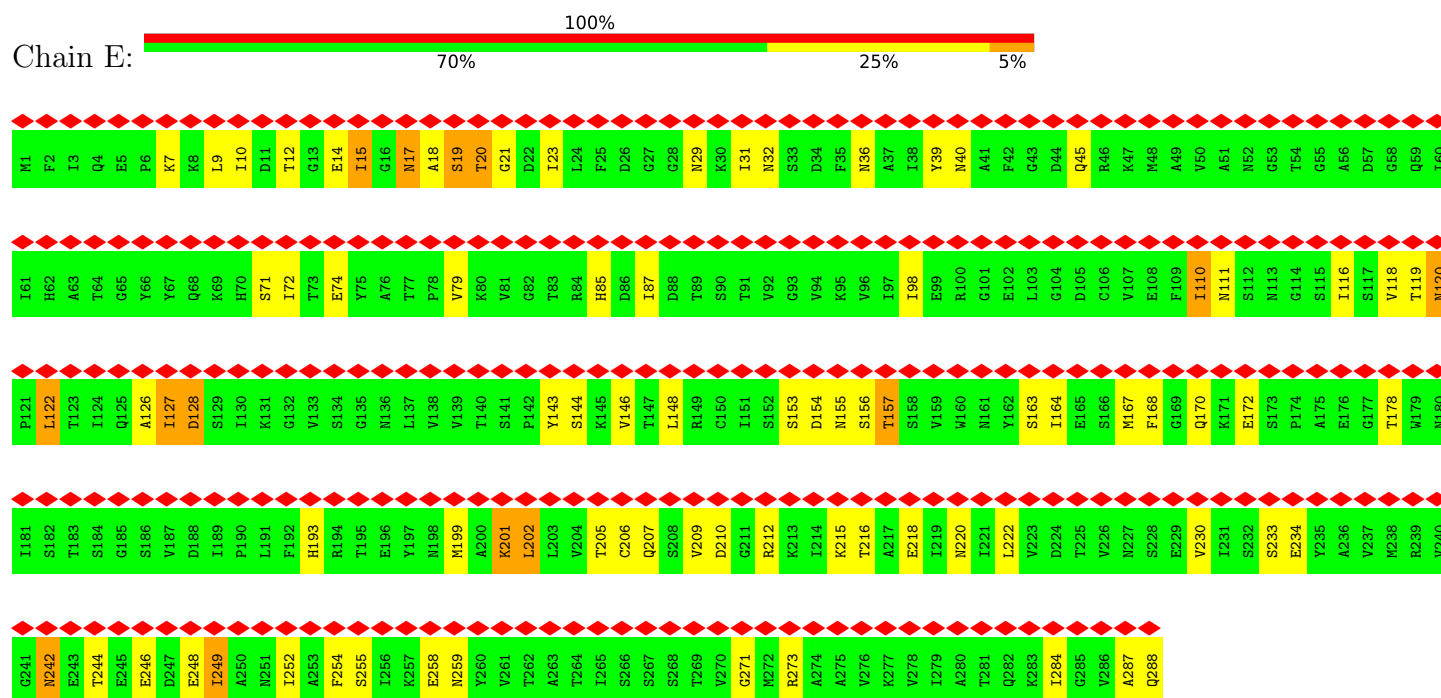


• Molecule 1: Baseplate structural protein Gp9

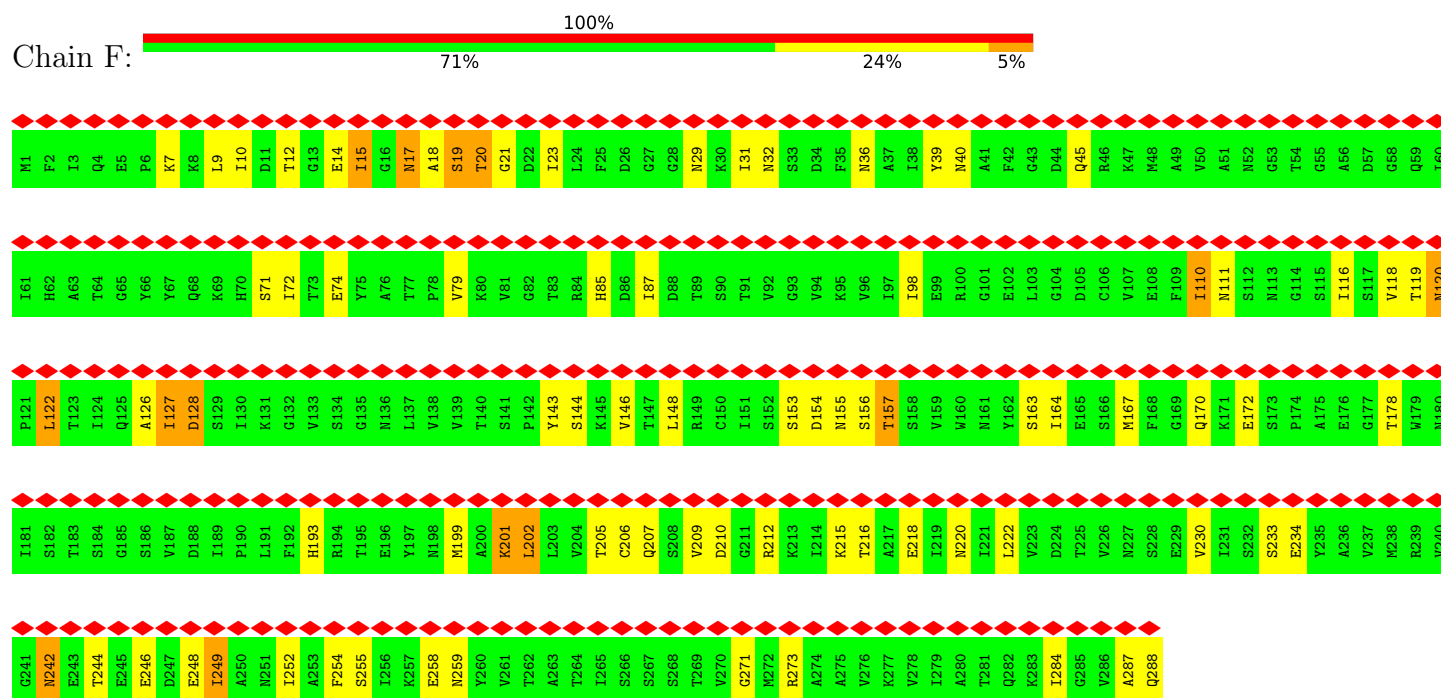




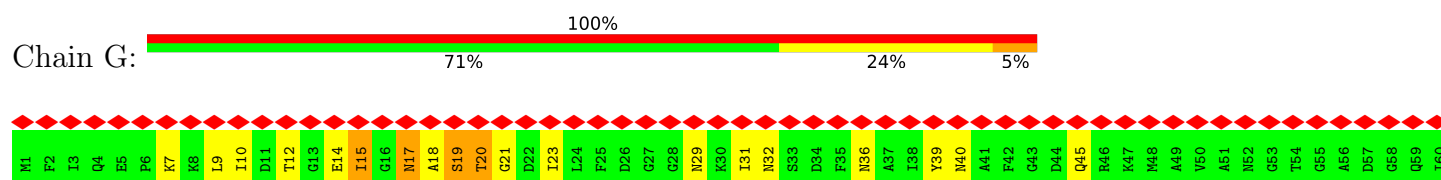
• Molecule 1: Baseplate structural protein Gp9

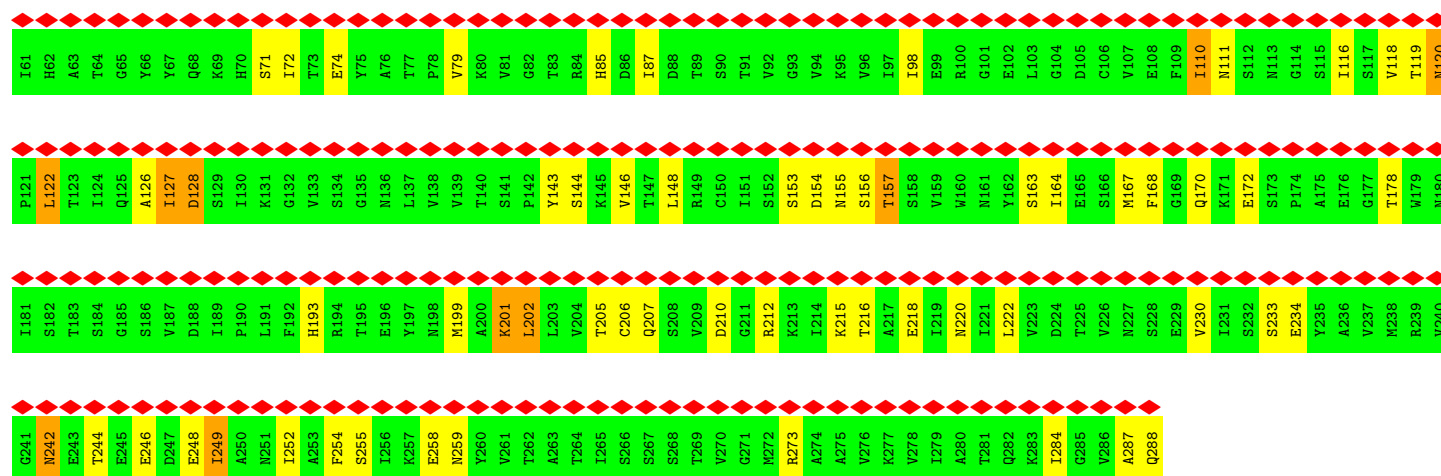


• Molecule 1: Baseplate structural protein Gp9

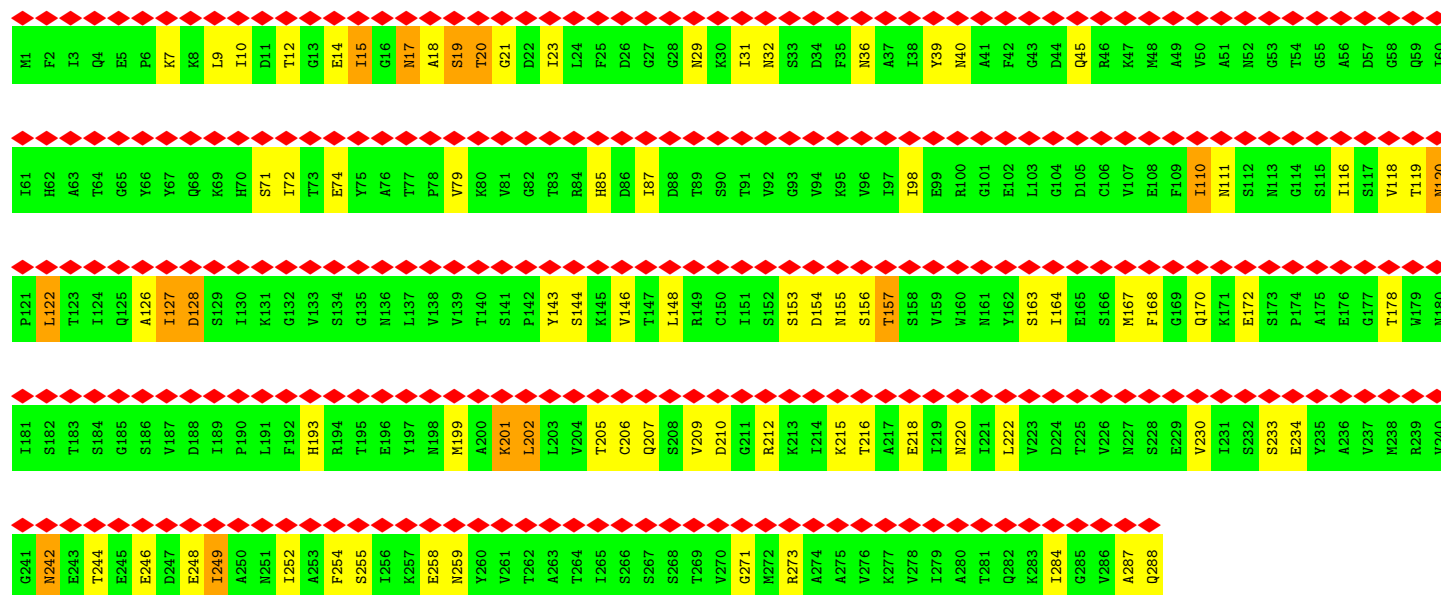


• Molecule 1: Baseplate structural protein Gp9

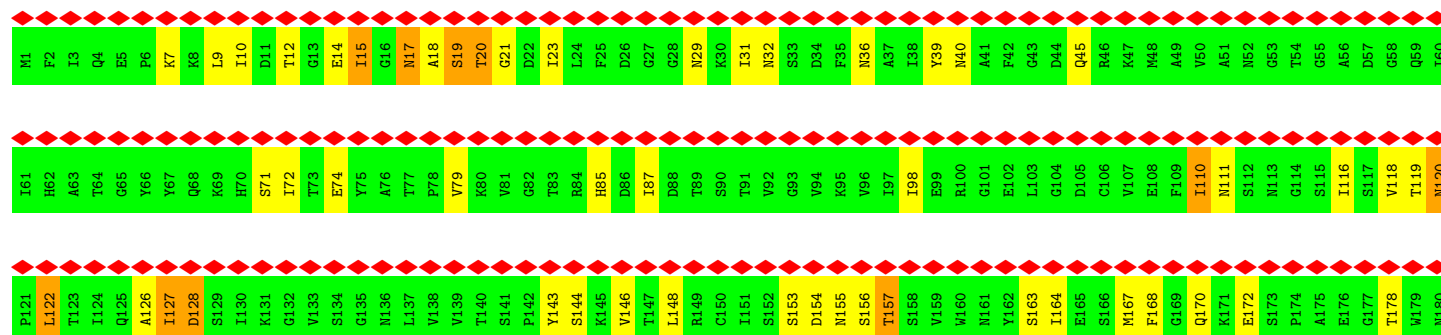


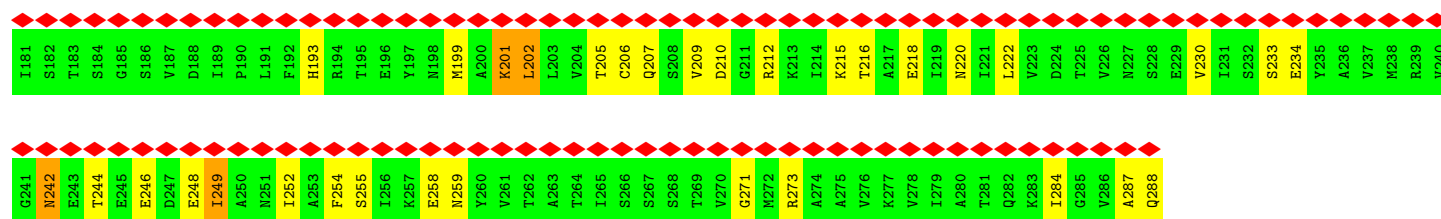


• Molecule 1: Baseplate structural protein Gp9

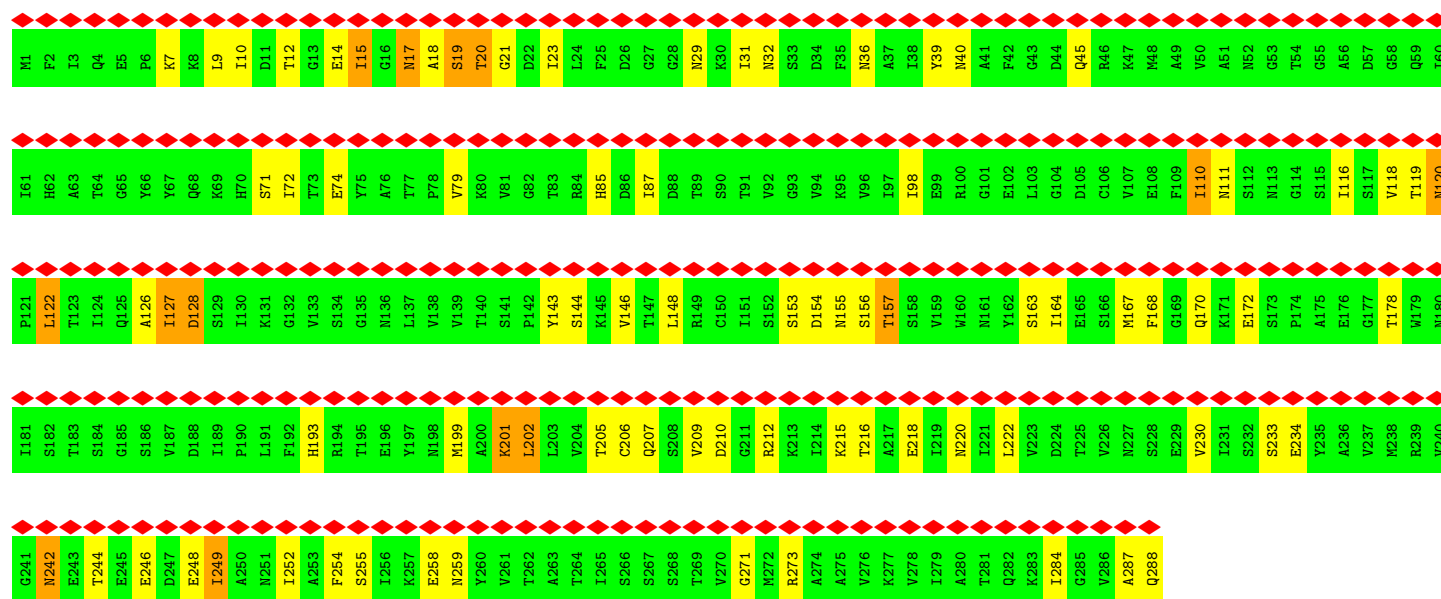


• Molecule 1: Baseplate structural protein Gp9

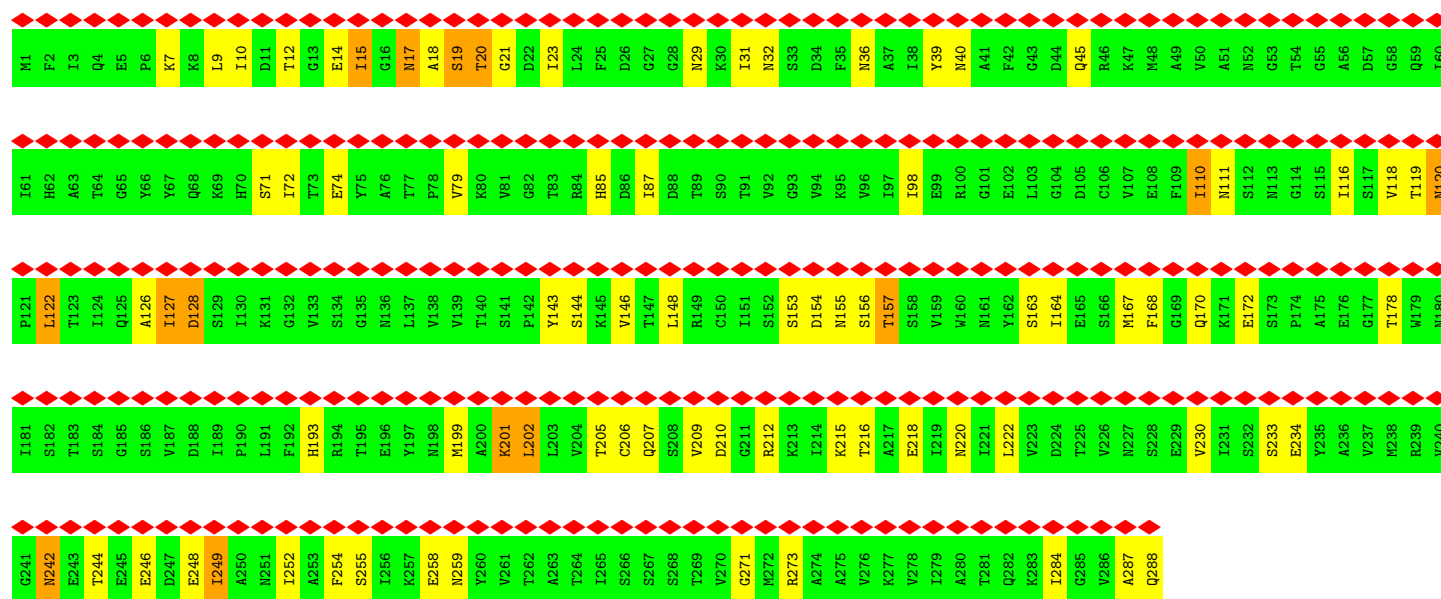




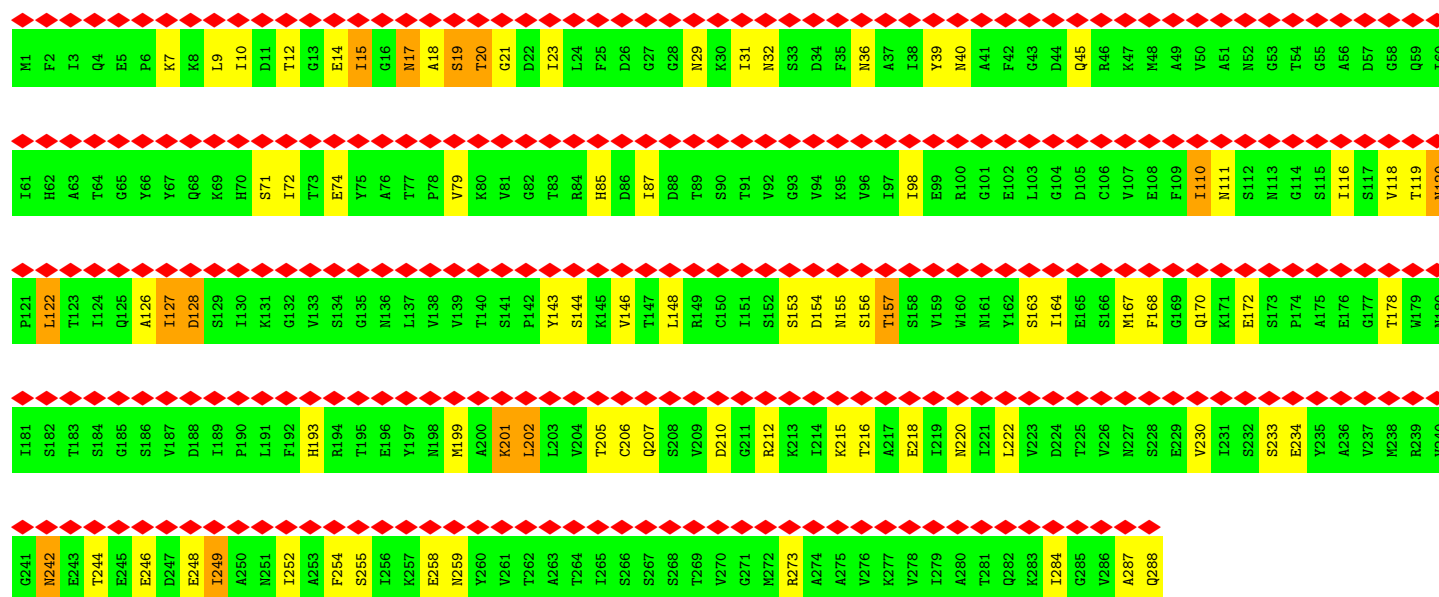
• Molecule 1: Baseplate structural protein Gp9



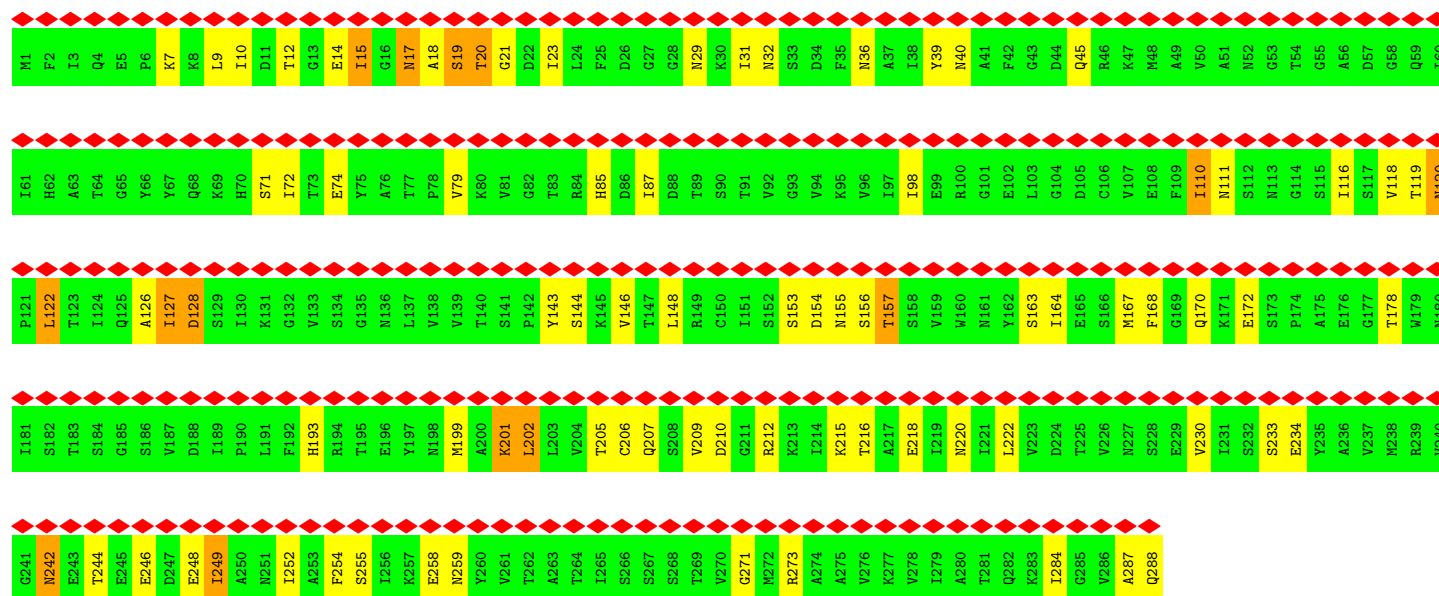
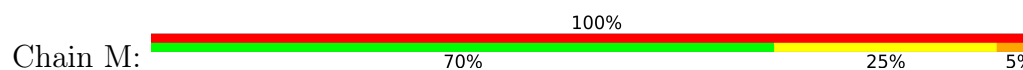
• Molecule 1: Baseplate structural protein Gp9



- Molecule 1: Baseplate structural protein Gp9

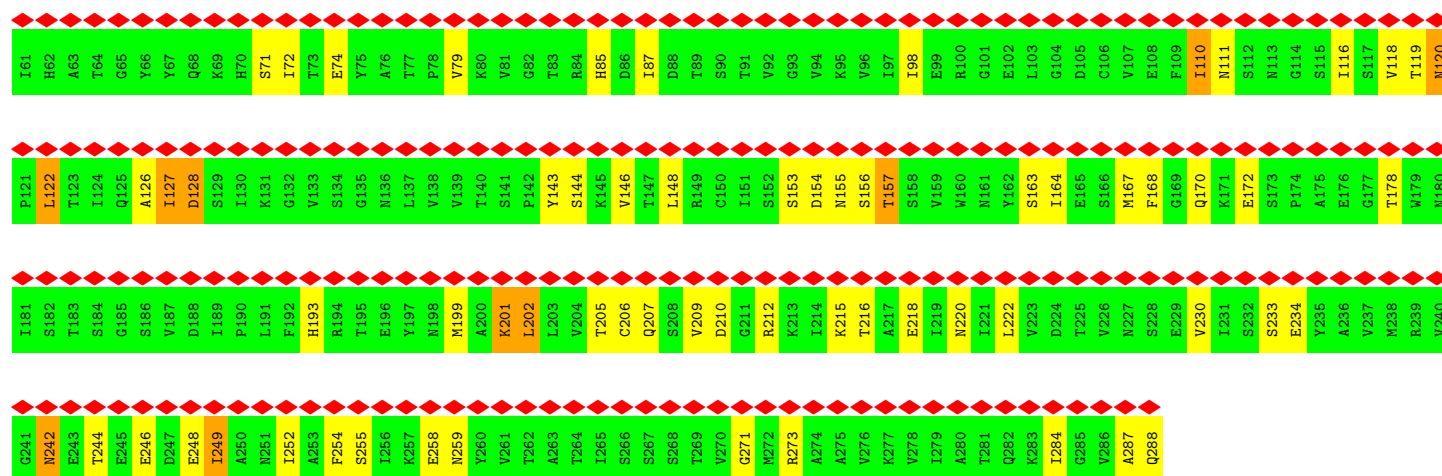


- Molecule 1: Baseplate structural protein Gp9

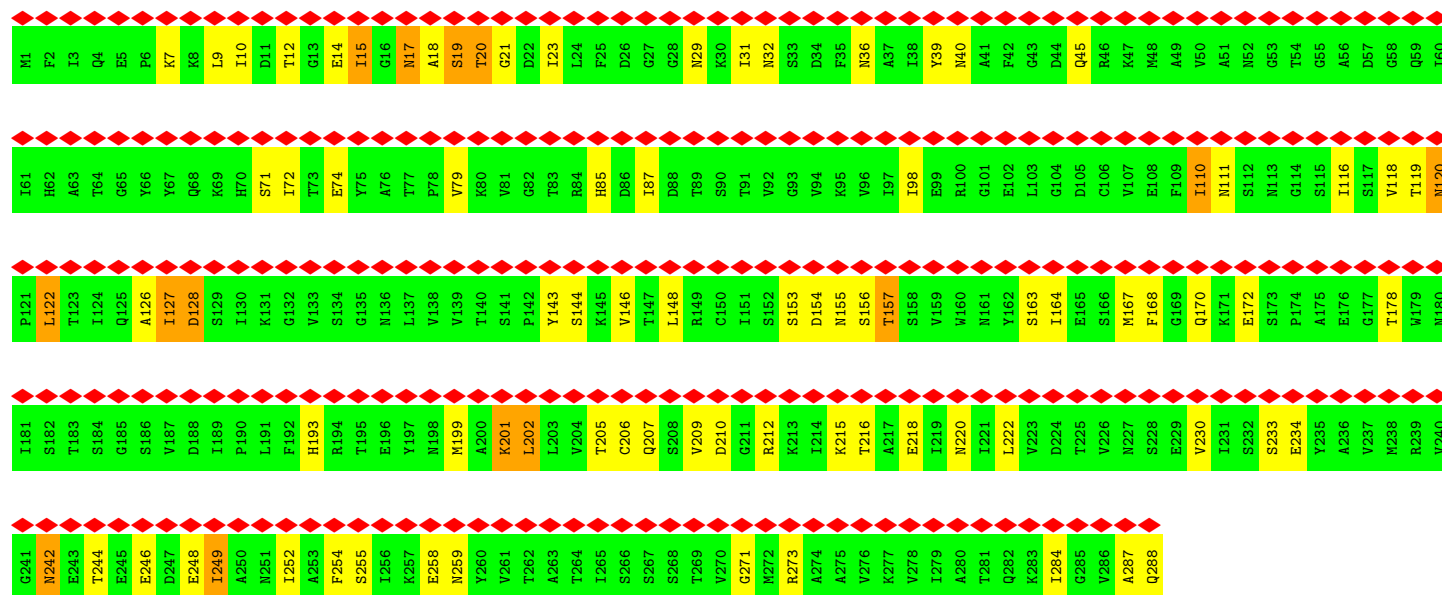


- Molecule 1: Baseplate structural protein Gp9

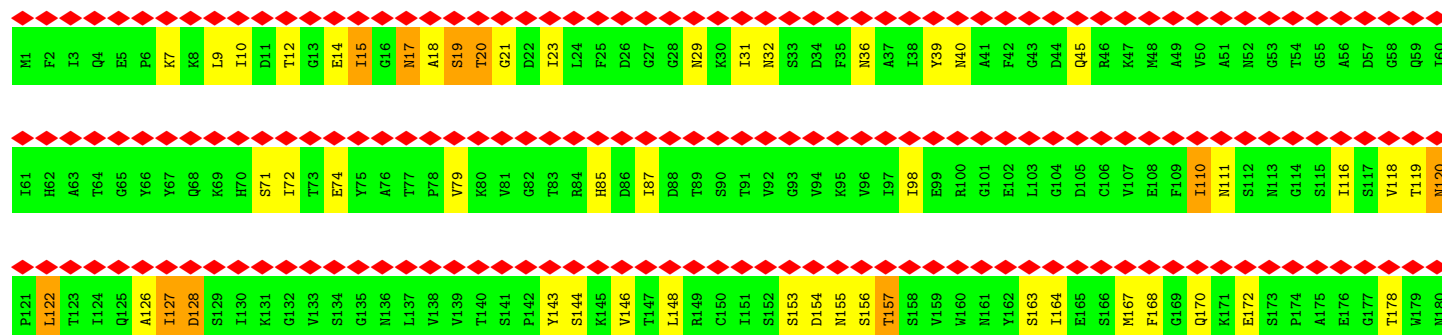


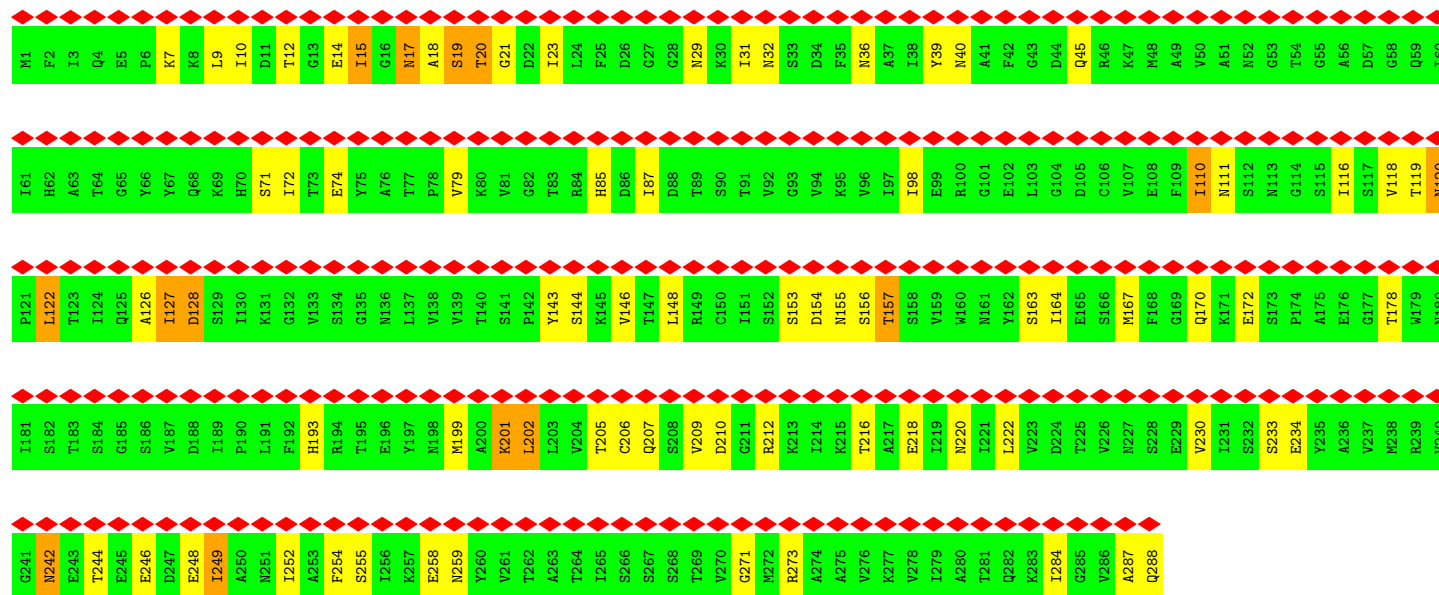


• Molecule 1: Baseplate structural protein Gp9



• Molecule 1: Baseplate structural protein Gp9





## 4 Experimental information

| Property                             | Value                  | Source    |
|--------------------------------------|------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE        | Depositor |
| Imposed symmetry                     | POINT, C6              | Depositor |
| Number of particles used             | 3029                   | Depositor |
| Resolution determination method      | Not provided           |           |
| CTF correction method                | EACH IMAGE             | Depositor |
| Microscope                           | FEI/PHILIPS CM300FEG/T | Depositor |
| Voltage (kV)                         | 300                    | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided           |           |
| Minimum defocus (nm)                 | 0.8                    | Depositor |
| Maximum defocus (nm)                 | 3.2                    | Depositor |
| Magnification                        | 47000                  | Depositor |
| Image detector                       | GENERIC FILM           | Depositor |
| Maximum map value                    | 7.953                  | Depositor |
| Minimum map value                    | -2.953                 | Depositor |
| Average map value                    | 0.059                  | Depositor |
| Map value standard deviation         | 0.533                  | Depositor |
| Recommended contour level            | 1.01                   | Depositor |
| Map size ( $\text{\AA}$ )            | 714.6, 714.6, 1508.6   | wwPDB     |
| Map dimensions                       | 180, 180, 380          | wwPDB     |
| Map angles ( $^\circ$ )              | 90, 90, 90             | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 3.97, 3.97, 3.97       | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | B     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | C     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | D     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | E     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | F     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | G     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | H     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | I     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | J     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | K     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | L     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | M     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | N     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | O     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | P     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | Q     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| 1   | R     | 0.37         | 0/2205      | 0.67        | 1/2988 (0.0%)   |
| All | All   | 0.37         | 0/39690     | 0.67        | 18/53784 (0.0%) |

There are no bond length outliers.

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 19  | SER  | CA-C-N | -7.11 | 101.56      | 117.20   |
| 1   | M     | 19  | SER  | CA-C-N | -7.11 | 101.56      | 117.20   |
| 1   | A     | 19  | SER  | CA-C-N | -7.11 | 101.57      | 117.20   |
| 1   | C     | 19  | SER  | CA-C-N | -7.11 | 101.57      | 117.20   |
| 1   | I     | 19  | SER  | CA-C-N | -7.11 | 101.57      | 117.20   |
| 1   | J     | 19  | SER  | CA-C-N | -7.11 | 101.57      | 117.20   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | L     | 19  | SER  | CA-C-N | -7.11 | 101.57      | 117.20   |
| 1   | R     | 19  | SER  | CA-C-N | -7.11 | 101.57      | 117.20   |
| 1   | F     | 19  | SER  | CA-C-N | -7.09 | 101.60      | 117.20   |
| 1   | G     | 19  | SER  | CA-C-N | -7.09 | 101.61      | 117.20   |
| 1   | O     | 19  | SER  | CA-C-N | -7.09 | 101.60      | 117.20   |
| 1   | P     | 19  | SER  | CA-C-N | -7.09 | 101.61      | 117.20   |
| 1   | B     | 19  | SER  | CA-C-N | -7.08 | 101.63      | 117.20   |
| 1   | K     | 19  | SER  | CA-C-N | -7.08 | 101.63      | 117.20   |
| 1   | H     | 19  | SER  | CA-C-N | -7.07 | 101.65      | 117.20   |
| 1   | Q     | 19  | SER  | CA-C-N | -7.07 | 101.65      | 117.20   |
| 1   | E     | 19  | SER  | CA-C-N | -7.06 | 101.66      | 117.20   |
| 1   | N     | 19  | SER  | CA-C-N | -7.06 | 101.66      | 117.20   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2175  | 0        | 2157     | 123     | 0            |
| 1   | B     | 2175  | 0        | 2157     | 121     | 0            |
| 1   | C     | 2175  | 0        | 2157     | 119     | 0            |
| 1   | D     | 2175  | 0        | 2157     | 125     | 0            |
| 1   | E     | 2175  | 0        | 2157     | 123     | 0            |
| 1   | F     | 2175  | 0        | 2157     | 122     | 0            |
| 1   | G     | 2175  | 0        | 2157     | 120     | 0            |
| 1   | H     | 2175  | 0        | 2157     | 123     | 0            |
| 1   | I     | 2175  | 0        | 2157     | 120     | 0            |
| 1   | J     | 2175  | 0        | 2157     | 121     | 0            |
| 1   | K     | 2175  | 0        | 2157     | 124     | 0            |
| 1   | L     | 2175  | 0        | 2157     | 121     | 0            |
| 1   | M     | 2175  | 0        | 2157     | 121     | 0            |
| 1   | N     | 2175  | 0        | 2157     | 124     | 0            |
| 1   | O     | 2175  | 0        | 2157     | 123     | 0            |
| 1   | P     | 2175  | 0        | 2157     | 123     | 0            |
| 1   | Q     | 2175  | 0        | 2157     | 122     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | R     | 2175  | 0        | 2157     | 121     | 0            |
| 2   | A     | 15    | 0        | 18       | 3       | 0            |
| 2   | B     | 15    | 0        | 18       | 3       | 0            |
| 2   | C     | 15    | 0        | 18       | 3       | 0            |
| 2   | D     | 15    | 0        | 18       | 4       | 0            |
| 2   | E     | 15    | 0        | 18       | 3       | 0            |
| 2   | F     | 15    | 0        | 18       | 3       | 0            |
| 2   | G     | 15    | 0        | 18       | 3       | 0            |
| 2   | H     | 15    | 0        | 18       | 3       | 0            |
| 2   | I     | 15    | 0        | 18       | 3       | 0            |
| 2   | J     | 15    | 0        | 18       | 3       | 0            |
| 2   | K     | 15    | 0        | 18       | 3       | 0            |
| 2   | L     | 15    | 0        | 18       | 3       | 0            |
| 2   | M     | 15    | 0        | 18       | 3       | 0            |
| 2   | N     | 15    | 0        | 18       | 3       | 0            |
| 2   | O     | 15    | 0        | 18       | 3       | 0            |
| 2   | P     | 15    | 0        | 18       | 3       | 0            |
| 2   | Q     | 15    | 0        | 18       | 3       | 0            |
| 2   | R     | 15    | 0        | 18       | 3       | 0            |
| All | All   | 39420 | 0        | 39150    | 1808    | 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 23.

All (1808) 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:B:18:ALA:HB3 | 1:B:23:ILE:HD11 | 1.41                     | 1.03              |
| 1:E:18:ALA:HB3 | 1:E:23:ILE:HD11 | 1.41                     | 1.02              |
| 1:Q:18:ALA:HB3 | 1:Q:23:ILE:HD11 | 1.41                     | 1.02              |
| 1:F:18:ALA:HB3 | 1:F:23:ILE:HD11 | 1.41                     | 1.02              |
| 1:I:18:ALA:HB3 | 1:I:23:ILE:HD11 | 1.41                     | 1.02              |
| 1:F:14:GLU:CA  | 1:F:17:ASN:HD21 | 1.73                     | 1.02              |
| 1:H:14:GLU:CA  | 1:H:17:ASN:HD21 | 1.73                     | 1.02              |
| 1:E:14:GLU:CA  | 1:E:17:ASN:HD21 | 1.73                     | 1.01              |
| 1:I:14:GLU:CA  | 1:I:17:ASN:HD21 | 1.73                     | 1.01              |
| 1:J:14:GLU:CA  | 1:J:17:ASN:HD21 | 1.73                     | 1.01              |
| 1:M:18:ALA:HB3 | 1:M:23:ILE:HD11 | 1.41                     | 1.01              |
| 1:C:14:GLU:CA  | 1:C:17:ASN:HD21 | 1.73                     | 1.01              |
| 1:H:18:ALA:HB3 | 1:H:23:ILE:HD11 | 1.41                     | 1.01              |
| 1:R:14:GLU:CA  | 1:R:17:ASN:HD21 | 1.73                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:14:GLU:CA    | 1:G:17:ASN:HD21  | 1.73                     | 1.01              |
| 1:K:18:ALA:HB3   | 1:K:23:ILE:HD11  | 1.41                     | 1.01              |
| 1:M:14:GLU:CA    | 1:M:17:ASN:HD21  | 1.73                     | 1.01              |
| 1:C:242:ASN:HD22 | 1:C:242:ASN:H    | 1.01                     | 1.01              |
| 1:K:14:GLU:C     | 1:K:17:ASN:HD21  | 1.64                     | 1.01              |
| 1:L:14:GLU:CA    | 1:L:17:ASN:HD21  | 1.73                     | 1.01              |
| 1:A:14:GLU:C     | 1:A:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:C:14:GLU:C     | 1:C:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:O:14:GLU:CA    | 1:O:17:ASN:HD21  | 1.73                     | 1.00              |
| 1:P:14:GLU:CA    | 1:P:17:ASN:HD21  | 1.73                     | 1.00              |
| 1:D:14:GLU:CA    | 1:D:17:ASN:HD21  | 1.73                     | 1.00              |
| 1:N:14:GLU:C     | 1:N:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:O:18:ALA:HB3   | 1:O:23:ILE:HD11  | 1.41                     | 1.00              |
| 1:Q:14:GLU:C     | 1:Q:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:R:18:ALA:HB3   | 1:R:23:ILE:HD11  | 1.41                     | 1.00              |
| 1:A:14:GLU:CA    | 1:A:17:ASN:HD21  | 1.73                     | 1.00              |
| 1:D:14:GLU:C     | 1:D:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:H:14:GLU:C     | 1:H:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:K:14:GLU:CA    | 1:K:17:ASN:HD21  | 1.73                     | 1.00              |
| 1:P:14:GLU:C     | 1:P:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:P:18:ALA:HB3   | 1:P:23:ILE:HD11  | 1.41                     | 1.00              |
| 1:B:14:GLU:C     | 1:B:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:N:18:ALA:HB3   | 1:N:23:ILE:HD11  | 1.41                     | 1.00              |
| 1:B:14:GLU:CA    | 1:B:17:ASN:HD21  | 1.73                     | 1.00              |
| 1:G:18:ALA:HB3   | 1:G:23:ILE:HD11  | 1.41                     | 1.00              |
| 1:R:14:GLU:C     | 1:R:17:ASN:HD21  | 1.64                     | 1.00              |
| 1:O:14:GLU:C     | 1:O:17:ASN:HD21  | 1.64                     | 0.99              |
| 1:J:242:ASN:H    | 1:J:242:ASN:HD22 | 1.01                     | 0.99              |
| 1:L:18:ALA:HB3   | 1:L:23:ILE:HD11  | 1.41                     | 0.99              |
| 1:C:18:ALA:HB3   | 1:C:23:ILE:HD11  | 1.41                     | 0.99              |
| 1:N:14:GLU:CA    | 1:N:17:ASN:HD21  | 1.73                     | 0.99              |
| 1:E:14:GLU:C     | 1:E:17:ASN:HD21  | 1.64                     | 0.99              |
| 1:M:14:GLU:C     | 1:M:17:ASN:HD21  | 1.64                     | 0.99              |
| 1:D:18:ALA:HB3   | 1:D:23:ILE:HD11  | 1.41                     | 0.99              |
| 1:G:14:GLU:C     | 1:G:17:ASN:HD21  | 1.64                     | 0.99              |
| 1:A:18:ALA:HB3   | 1:A:23:ILE:HD11  | 1.41                     | 0.99              |
| 1:M:242:ASN:H    | 1:M:242:ASN:HD22 | 1.01                     | 0.99              |
| 1:Q:14:GLU:CA    | 1:Q:17:ASN:HD21  | 1.73                     | 0.99              |
| 1:I:14:GLU:C     | 1:I:17:ASN:HD21  | 1.64                     | 0.98              |
| 1:J:18:ALA:HB3   | 1:J:23:ILE:HD11  | 1.41                     | 0.98              |
| 1:L:14:GLU:C     | 1:L:17:ASN:HD21  | 1.64                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:14:GLU:C     | 1:J:17:ASN:HD21  | 1.64                     | 0.98              |
| 1:R:242:ASN:H    | 1:R:242:ASN:HD22 | 1.01                     | 0.98              |
| 1:F:14:GLU:C     | 1:F:17:ASN:HD21  | 1.64                     | 0.98              |
| 1:F:242:ASN:HD22 | 1:F:242:ASN:H    | 1.01                     | 0.97              |
| 1:P:242:ASN:H    | 1:P:242:ASN:HD22 | 1.01                     | 0.96              |
| 1:G:242:ASN:H    | 1:G:242:ASN:HD22 | 1.01                     | 0.96              |
| 1:O:242:ASN:HD22 | 1:O:242:ASN:H    | 1.01                     | 0.95              |
| 1:A:242:ASN:HD22 | 1:A:242:ASN:H    | 1.01                     | 0.94              |
| 1:I:242:ASN:HD22 | 1:I:242:ASN:H    | 1.01                     | 0.94              |
| 1:L:242:ASN:HD22 | 1:L:242:ASN:H    | 1.01                     | 0.93              |
| 1:D:242:ASN:HD22 | 1:D:242:ASN:H    | 1.01                     | 0.93              |
| 1:H:242:ASN:H    | 1:H:242:ASN:HD22 | 1.01                     | 0.93              |
| 1:K:242:ASN:H    | 1:K:242:ASN:HD22 | 1.01                     | 0.92              |
| 1:Q:242:ASN:HD22 | 1:Q:242:ASN:H    | 1.01                     | 0.92              |
| 1:E:242:ASN:H    | 1:E:242:ASN:HD22 | 1.01                     | 0.91              |
| 1:N:242:ASN:ND2  | 1:N:242:ASN:H    | 1.69                     | 0.90              |
| 1:D:242:ASN:H    | 1:D:242:ASN:ND2  | 1.69                     | 0.90              |
| 1:B:242:ASN:ND2  | 1:B:242:ASN:H    | 1.69                     | 0.90              |
| 1:I:234:GLU:H    | 2:I:309:EPE:H82  | 1.37                     | 0.90              |
| 1:N:242:ASN:H    | 1:N:242:ASN:HD22 | 1.01                     | 0.90              |
| 1:A:242:ASN:H    | 1:A:242:ASN:ND2  | 1.69                     | 0.90              |
| 1:B:242:ASN:H    | 1:B:242:ASN:HD22 | 1.01                     | 0.90              |
| 1:O:234:GLU:H    | 2:O:315:EPE:H82  | 1.37                     | 0.90              |
| 1:J:234:GLU:H    | 2:J:310:EPE:H82  | 1.37                     | 0.90              |
| 1:M:234:GLU:H    | 2:M:313:EPE:H82  | 1.37                     | 0.90              |
| 1:F:234:GLU:H    | 2:F:306:EPE:H82  | 1.37                     | 0.90              |
| 1:G:242:ASN:H    | 1:G:242:ASN:ND2  | 1.69                     | 0.90              |
| 1:L:234:GLU:H    | 2:L:312:EPE:H82  | 1.37                     | 0.90              |
| 1:P:234:GLU:H    | 2:P:316:EPE:H82  | 1.37                     | 0.90              |
| 1:A:234:GLU:H    | 2:A:301:EPE:H82  | 1.37                     | 0.89              |
| 1:G:234:GLU:H    | 2:G:307:EPE:H82  | 1.37                     | 0.89              |
| 1:Q:234:GLU:H    | 2:Q:317:EPE:H82  | 1.37                     | 0.89              |
| 1:O:242:ASN:H    | 1:O:242:ASN:ND2  | 1.69                     | 0.89              |
| 1:I:242:ASN:H    | 1:I:242:ASN:ND2  | 1.69                     | 0.89              |
| 1:H:242:ASN:H    | 1:H:242:ASN:ND2  | 1.69                     | 0.89              |
| 1:F:242:ASN:H    | 1:F:242:ASN:ND2  | 1.69                     | 0.89              |
| 1:R:234:GLU:H    | 2:R:318:EPE:H82  | 1.37                     | 0.89              |
| 1:D:234:GLU:H    | 2:D:304:EPE:H82  | 1.37                     | 0.88              |
| 1:L:242:ASN:H    | 1:L:242:ASN:ND2  | 1.69                     | 0.88              |
| 1:R:242:ASN:H    | 1:R:242:ASN:ND2  | 1.69                     | 0.88              |
| 1:B:234:GLU:H    | 2:B:302:EPE:H82  | 1.37                     | 0.88              |

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| Atom-1        | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------|--------------------------|-------------------|
| 1:P:242:ASN:H | 1:P:242:ASN:ND2  | 1.69                     | 0.88              |
| 1:C:242:ASN:H | 1:C:242:ASN:ND2  | 1.69                     | 0.88              |
| 1:J:242:ASN:H | 1:J:242:ASN:ND2  | 1.69                     | 0.88              |
| 1:K:242:ASN:H | 1:K:242:ASN:ND2  | 1.69                     | 0.88              |
| 1:M:242:ASN:H | 1:M:242:ASN:ND2  | 1.69                     | 0.87              |
| 1:Q:242:ASN:H | 1:Q:242:ASN:ND2  | 1.69                     | 0.87              |
| 1:C:234:GLU:H | 2:C:303:EPE:H82  | 1.37                     | 0.87              |
| 1:N:234:GLU:H | 2:N:314:EPE:H82  | 1.37                     | 0.86              |
| 1:E:234:GLU:H | 2:E:305:EPE:H82  | 1.37                     | 0.86              |
| 1:K:234:GLU:H | 2:K:311:EPE:H82  | 1.37                     | 0.86              |
| 1:H:234:GLU:H | 2:H:308:EPE:H82  | 1.37                     | 0.86              |
| 1:E:242:ASN:H | 1:E:242:ASN:ND2  | 1.69                     | 0.85              |
| 1:E:119:THR:C | 1:E:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:Q:119:THR:C | 1:Q:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:F:119:THR:C | 1:F:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:A:119:THR:C | 1:A:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:K:119:THR:C | 1:K:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:M:119:THR:C | 1:M:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:P:119:THR:C | 1:P:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:B:119:THR:C | 1:B:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:R:14:GLU:C  | 1:R:17:ASN:ND2   | 2.31                     | 0.84              |
| 1:R:119:THR:C | 1:R:120:ASN:HD22 | 1.81                     | 0.84              |
| 1:N:14:GLU:C  | 1:N:17:ASN:ND2   | 2.31                     | 0.84              |
| 1:C:14:GLU:C  | 1:C:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:Q:14:GLU:C  | 1:Q:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:O:119:THR:C | 1:O:120:ASN:HD22 | 1.81                     | 0.83              |
| 1:C:119:THR:C | 1:C:120:ASN:HD22 | 1.81                     | 0.83              |
| 1:D:14:GLU:C  | 1:D:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:G:14:GLU:C  | 1:G:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:K:14:GLU:C  | 1:K:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:P:14:GLU:C  | 1:P:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:N:119:THR:C | 1:N:120:ASN:HD22 | 1.81                     | 0.83              |
| 1:E:14:GLU:C  | 1:E:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:A:14:GLU:C  | 1:A:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:G:119:THR:C | 1:G:120:ASN:HD22 | 1.81                     | 0.83              |
| 1:M:14:GLU:C  | 1:M:17:ASN:ND2   | 2.31                     | 0.83              |
| 1:O:18:ALA:O  | 1:O:23:ILE:HD13  | 1.79                     | 0.83              |
| 1:A:18:ALA:O  | 1:A:23:ILE:HD13  | 1.79                     | 0.83              |
| 1:C:18:ALA:O  | 1:C:23:ILE:HD13  | 1.79                     | 0.83              |
| 1:D:119:THR:C | 1:D:120:ASN:HD22 | 1.81                     | 0.83              |
| 1:O:14:GLU:C  | 1:O:17:ASN:ND2   | 2.31                     | 0.83              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:14:GLU:C    | 1:B:17:ASN:ND2   | 2.31                     | 0.82              |
| 1:F:14:GLU:C    | 1:F:17:ASN:ND2   | 2.31                     | 0.82              |
| 1:H:119:THR:C   | 1:H:120:ASN:HD22 | 1.81                     | 0.82              |
| 1:K:18:ALA:O    | 1:K:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:M:18:ALA:O    | 1:M:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:R:18:ALA:O    | 1:R:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:F:201:LYS:HD3 | 1:F:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:H:14:GLU:C    | 1:H:17:ASN:ND2   | 2.31                     | 0.82              |
| 1:H:18:ALA:O    | 1:H:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:I:119:THR:C   | 1:I:120:ASN:HD22 | 1.81                     | 0.82              |
| 1:I:201:LYS:HD3 | 1:I:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:J:14:GLU:C    | 1:J:17:ASN:ND2   | 2.31                     | 0.82              |
| 1:L:201:LYS:HD3 | 1:L:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:F:18:ALA:O    | 1:F:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:J:201:LYS:HD3 | 1:J:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:L:18:ALA:O    | 1:L:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:Q:18:ALA:O    | 1:Q:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:L:119:THR:C   | 1:L:120:ASN:HD22 | 1.81                     | 0.82              |
| 1:I:14:GLU:C    | 1:I:17:ASN:ND2   | 2.31                     | 0.82              |
| 1:J:119:THR:C   | 1:J:120:ASN:HD22 | 1.81                     | 0.82              |
| 1:K:201:LYS:HD3 | 1:K:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:M:201:LYS:HD3 | 1:M:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:G:18:ALA:O    | 1:G:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:A:201:LYS:HD3 | 1:A:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:B:18:ALA:O    | 1:B:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:D:201:LYS:HD3 | 1:D:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:J:18:ALA:O    | 1:J:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:O:201:LYS:HD3 | 1:O:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:P:201:LYS:HD3 | 1:P:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:G:201:LYS:HD3 | 1:G:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:L:14:GLU:C    | 1:L:17:ASN:ND2   | 2.31                     | 0.82              |
| 1:N:18:ALA:O    | 1:N:23:ILE:HD13  | 1.79                     | 0.82              |
| 1:Q:201:LYS:HD3 | 1:Q:220:ASN:OD1  | 1.80                     | 0.82              |
| 1:P:18:ALA:O    | 1:P:23:ILE:HD13  | 1.79                     | 0.81              |
| 1:C:201:LYS:HD3 | 1:C:220:ASN:OD1  | 1.80                     | 0.81              |
| 1:E:201:LYS:HD3 | 1:E:220:ASN:OD1  | 1.80                     | 0.81              |
| 1:R:201:LYS:HD3 | 1:R:220:ASN:OD1  | 1.80                     | 0.81              |
| 1:D:18:ALA:O    | 1:D:23:ILE:HD13  | 1.79                     | 0.81              |
| 1:E:18:ALA:O    | 1:E:23:ILE:HD13  | 1.79                     | 0.81              |
| 1:H:201:LYS:HD3 | 1:H:220:ASN:OD1  | 1.80                     | 0.81              |
| 1:N:201:LYS:HD3 | 1:N:220:ASN:OD1  | 1.80                     | 0.81              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:201:LYS:HD3 | 1:B:220:ASN:OD1 | 1.80                     | 0.80              |
| 1:I:18:ALA:O    | 1:I:23:ILE:HD13 | 1.79                     | 0.80              |
| 1:D:17:ASN:HD22 | 1:D:17:ASN:H    | 1.30                     | 0.80              |
| 1:B:17:ASN:HD22 | 1:B:17:ASN:H    | 1.31                     | 0.79              |
| 1:F:17:ASN:H    | 1:F:17:ASN:HD22 | 1.31                     | 0.79              |
| 1:G:17:ASN:HD22 | 1:G:17:ASN:H    | 1.31                     | 0.79              |
| 1:A:17:ASN:H    | 1:A:17:ASN:HD22 | 1.30                     | 0.79              |
| 1:Q:17:ASN:H    | 1:Q:17:ASN:HD22 | 1.31                     | 0.79              |
| 1:L:17:ASN:HD22 | 1:L:17:ASN:H    | 1.31                     | 0.79              |
| 1:I:17:ASN:H    | 1:I:17:ASN:HD22 | 1.31                     | 0.78              |
| 1:P:17:ASN:H    | 1:P:17:ASN:HD22 | 1.31                     | 0.78              |
| 1:E:17:ASN:HD22 | 1:E:17:ASN:H    | 1.31                     | 0.78              |
| 1:J:17:ASN:HD22 | 1:J:17:ASN:H    | 1.30                     | 0.78              |
| 1:C:17:ASN:H    | 1:C:17:ASN:HD22 | 1.31                     | 0.78              |
| 1:J:15:ILE:N    | 1:J:17:ASN:HD21 | 1.82                     | 0.78              |
| 1:R:15:ILE:N    | 1:R:17:ASN:HD21 | 1.82                     | 0.78              |
| 1:F:234:GLU:H   | 2:F:306:EPE:C8  | 1.97                     | 0.78              |
| 1:O:234:GLU:H   | 2:O:315:EPE:C8  | 1.97                     | 0.78              |
| 1:G:15:ILE:N    | 1:G:17:ASN:HD21 | 1.82                     | 0.78              |
| 1:L:234:GLU:H   | 2:L:312:EPE:C8  | 1.97                     | 0.78              |
| 1:M:15:ILE:N    | 1:M:17:ASN:HD21 | 1.82                     | 0.78              |
| 1:M:17:ASN:HD22 | 1:M:17:ASN:H    | 1.30                     | 0.78              |
| 1:L:15:ILE:N    | 1:L:17:ASN:HD21 | 1.82                     | 0.78              |
| 1:C:234:GLU:H   | 2:C:303:EPE:C8  | 1.97                     | 0.78              |
| 1:G:234:GLU:H   | 2:G:307:EPE:C8  | 1.97                     | 0.78              |
| 1:I:234:GLU:H   | 2:I:309:EPE:C8  | 1.97                     | 0.78              |
| 1:N:17:ASN:H    | 1:N:17:ASN:HD22 | 1.31                     | 0.77              |
| 1:D:15:ILE:N    | 1:D:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:Q:15:ILE:N    | 1:Q:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:F:15:ILE:N    | 1:F:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:O:17:ASN:HD22 | 1:O:17:ASN:H    | 1.31                     | 0.77              |
| 1:A:234:GLU:H   | 2:A:301:EPE:C8  | 1.97                     | 0.77              |
| 1:H:15:ILE:N    | 1:H:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:H:17:ASN:H    | 1:H:17:ASN:HD22 | 1.31                     | 0.77              |
| 1:M:234:GLU:H   | 2:M:313:EPE:C8  | 1.97                     | 0.77              |
| 1:N:234:GLU:H   | 2:N:314:EPE:C8  | 1.97                     | 0.77              |
| 1:B:15:ILE:N    | 1:B:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:P:234:GLU:H   | 2:P:316:EPE:C8  | 1.97                     | 0.77              |
| 1:B:234:GLU:H   | 2:B:302:EPE:C8  | 1.97                     | 0.77              |
| 1:O:15:ILE:N    | 1:O:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:R:17:ASN:HD22 | 1:R:17:ASN:H    | 1.31                     | 0.77              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:234:GLU:H   | 2:R:318:EPE:C8  | 1.97                     | 0.77              |
| 1:K:234:GLU:H   | 2:K:311:EPE:C8  | 1.97                     | 0.77              |
| 1:N:15:ILE:N    | 1:N:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:C:15:ILE:N    | 1:C:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:E:15:ILE:N    | 1:E:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:K:15:ILE:N    | 1:K:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:P:15:ILE:N    | 1:P:17:ASN:HD21 | 1.82                     | 0.77              |
| 1:E:234:GLU:H   | 2:E:305:EPE:C8  | 1.97                     | 0.77              |
| 1:K:17:ASN:H    | 1:K:17:ASN:HD22 | 1.31                     | 0.77              |
| 1:D:234:GLU:H   | 2:D:304:EPE:C8  | 1.97                     | 0.76              |
| 1:J:234:GLU:H   | 2:J:310:EPE:C8  | 1.97                     | 0.76              |
| 1:Q:234:GLU:H   | 2:Q:317:EPE:C8  | 1.97                     | 0.76              |
| 1:I:15:ILE:N    | 1:I:17:ASN:HD21 | 1.82                     | 0.76              |
| 1:A:15:ILE:N    | 1:A:17:ASN:HD21 | 1.82                     | 0.76              |
| 1:H:234:GLU:H   | 2:H:308:EPE:C8  | 1.97                     | 0.75              |
| 1:D:40:ASN:HD22 | 1:D:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:B:14:GLU:CA   | 1:B:17:ASN:ND2  | 2.50                     | 0.75              |
| 1:D:127:ILE:O   | 1:D:128:ASP:HB2 | 1.87                     | 0.75              |
| 1:J:40:ASN:HD22 | 1:J:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:K:14:GLU:CA   | 1:K:17:ASN:ND2  | 2.50                     | 0.75              |
| 1:L:40:ASN:HD22 | 1:L:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:N:40:ASN:HD22 | 1:N:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:Q:127:ILE:O   | 1:Q:128:ASP:HB2 | 1.87                     | 0.75              |
| 1:F:14:GLU:CA   | 1:F:17:ASN:ND2  | 2.50                     | 0.75              |
| 1:F:40:ASN:HD22 | 1:F:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:J:127:ILE:O   | 1:J:128:ASP:HB2 | 1.87                     | 0.75              |
| 1:L:127:ILE:O   | 1:L:128:ASP:HB2 | 1.87                     | 0.75              |
| 1:M:14:GLU:CA   | 1:M:17:ASN:ND2  | 2.50                     | 0.75              |
| 1:G:40:ASN:HD22 | 1:G:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:M:40:ASN:HD22 | 1:M:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:Q:40:ASN:HD22 | 1:Q:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:B:40:ASN:HD22 | 1:B:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:E:127:ILE:O   | 1:E:128:ASP:HB2 | 1.87                     | 0.75              |
| 1:P:40:ASN:HD22 | 1:P:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:K:40:ASN:HD22 | 1:K:45:GLN:HG2  | 1.52                     | 0.75              |
| 1:R:40:ASN:HD22 | 1:R:45:GLN:HG2  | 1.52                     | 0.74              |
| 1:Q:14:GLU:CA   | 1:Q:17:ASN:ND2  | 2.50                     | 0.74              |
| 1:R:127:ILE:O   | 1:R:128:ASP:HB2 | 1.87                     | 0.74              |
| 1:C:14:GLU:CA   | 1:C:17:ASN:ND2  | 2.50                     | 0.74              |
| 1:E:40:ASN:HD22 | 1:E:45:GLN:HG2  | 1.52                     | 0.74              |
| 1:K:127:ILE:O   | 1:K:128:ASP:HB2 | 1.87                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:40:ASN:HD22  | 1:H:45:GLN:HG2   | 1.52                     | 0.74              |
| 1:N:14:GLU:CA    | 1:N:17:ASN:ND2   | 2.50                     | 0.74              |
| 1:C:127:ILE:O    | 1:C:128:ASP:HB2  | 1.87                     | 0.74              |
| 1:M:127:ILE:O    | 1:M:128:ASP:HB2  | 1.87                     | 0.74              |
| 1:C:40:ASN:HD22  | 1:C:45:GLN:HG2   | 1.52                     | 0.74              |
| 1:O:127:ILE:O    | 1:O:128:ASP:HB2  | 1.87                     | 0.74              |
| 1:P:14:GLU:CA    | 1:P:17:ASN:ND2   | 2.50                     | 0.74              |
| 1:R:144:SER:HB2  | 1:R:164:ILE:HD11 | 1.70                     | 0.74              |
| 1:H:127:ILE:O    | 1:H:128:ASP:HB2  | 1.87                     | 0.74              |
| 1:O:40:ASN:HD22  | 1:O:45:GLN:HG2   | 1.52                     | 0.74              |
| 1:P:127:ILE:O    | 1:P:128:ASP:HB2  | 1.87                     | 0.74              |
| 1:E:14:GLU:CA    | 1:E:17:ASN:ND2   | 2.50                     | 0.73              |
| 1:L:144:SER:HB2  | 1:L:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:B:127:ILE:O    | 1:B:128:ASP:HB2  | 1.87                     | 0.73              |
| 1:C:144:SER:HB2  | 1:C:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:I:144:SER:HB2  | 1:I:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:L:14:GLU:CA    | 1:L:17:ASN:ND2   | 2.50                     | 0.73              |
| 1:A:14:GLU:CA    | 1:A:17:ASN:ND2   | 2.50                     | 0.73              |
| 1:B:144:SER:HB2  | 1:B:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:H:18:ALA:HB3   | 1:H:23:ILE:CD1   | 2.19                     | 0.73              |
| 1:I:40:ASN:HD22  | 1:I:45:GLN:HG2   | 1.52                     | 0.73              |
| 1:A:40:ASN:HD22  | 1:A:45:GLN:HG2   | 1.52                     | 0.73              |
| 1:G:127:ILE:O    | 1:G:128:ASP:HB2  | 1.87                     | 0.73              |
| 1:H:144:SER:HB2  | 1:H:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:I:127:ILE:O    | 1:I:128:ASP:HB2  | 1.87                     | 0.73              |
| 1:O:14:GLU:CA    | 1:O:17:ASN:ND2   | 2.50                     | 0.73              |
| 1:D:14:GLU:CA    | 1:D:17:ASN:ND2   | 2.50                     | 0.73              |
| 1:G:144:SER:HB2  | 1:G:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:N:127:ILE:O    | 1:N:128:ASP:HB2  | 1.87                     | 0.73              |
| 1:A:18:ALA:HB3   | 1:A:23:ILE:CD1   | 2.19                     | 0.73              |
| 1:G:120:ASN:HD22 | 1:G:120:ASN:N    | 1.87                     | 0.73              |
| 1:Q:144:SER:HB2  | 1:Q:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:G:14:GLU:CA    | 1:G:17:ASN:ND2   | 2.50                     | 0.73              |
| 1:J:15:ILE:N     | 1:J:17:ASN:ND2   | 2.37                     | 0.73              |
| 1:J:144:SER:HB2  | 1:J:164:ILE:HD11 | 1.70                     | 0.73              |
| 1:Q:15:ILE:N     | 1:Q:17:ASN:ND2   | 2.37                     | 0.73              |
| 1:P:144:SER:HB2  | 1:P:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:A:216:THR:HG21 | 1:C:199:MET:HG3  | 1.71                     | 0.72              |
| 1:B:15:ILE:N     | 1:B:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:H:199:MET:HG3  | 1:I:216:THR:HG21 | 1.72                     | 0.72              |
| 1:I:120:ASN:HD22 | 1:I:120:ASN:N    | 1.87                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:144:SER:HB2  | 1:N:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:N:199:MET:HG3  | 1:O:216:THR:HG21 | 1.72                     | 0.72              |
| 1:O:15:ILE:N     | 1:O:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:O:144:SER:HB2  | 1:O:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:P:18:ALA:HB3   | 1:P:23:ILE:CD1   | 2.19                     | 0.72              |
| 1:P:216:THR:HG21 | 1:R:199:MET:HG3  | 1.71                     | 0.72              |
| 1:R:15:ILE:N     | 1:R:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:A:144:SER:HB2  | 1:A:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:D:15:ILE:N     | 1:D:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:D:216:THR:HG21 | 1:F:199:MET:HG3  | 1.72                     | 0.72              |
| 1:F:120:ASN:HD22 | 1:F:120:ASN:N    | 1.87                     | 0.72              |
| 1:H:15:ILE:N     | 1:H:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:E:15:ILE:N     | 1:E:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:Q:199:MET:HG3  | 1:R:216:THR:HG21 | 1.72                     | 0.72              |
| 1:A:120:ASN:HD22 | 1:A:120:ASN:N    | 1.87                     | 0.72              |
| 1:B:18:ALA:HB3   | 1:B:23:ILE:CD1   | 2.19                     | 0.72              |
| 1:C:15:ILE:N     | 1:C:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:C:120:ASN:HD22 | 1:C:120:ASN:N    | 1.87                     | 0.72              |
| 1:M:18:ALA:HB3   | 1:M:23:ILE:CD1   | 2.19                     | 0.72              |
| 1:N:15:ILE:N     | 1:N:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:G:216:THR:HG21 | 1:I:199:MET:HG3  | 1.71                     | 0.72              |
| 1:K:15:ILE:N     | 1:K:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:K:199:MET:HG3  | 1:L:216:THR:HG21 | 1.71                     | 0.72              |
| 1:P:199:MET:HG3  | 1:Q:216:THR:HG21 | 1.71                     | 0.72              |
| 1:R:18:ALA:HB3   | 1:R:23:ILE:CD1   | 2.19                     | 0.72              |
| 1:D:144:SER:HB2  | 1:D:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:E:144:SER:HB2  | 1:E:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:F:127:ILE:O    | 1:F:128:ASP:HB2  | 1.87                     | 0.72              |
| 1:G:15:ILE:N     | 1:G:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:I:18:ALA:HB3   | 1:I:23:ILE:CD1   | 2.19                     | 0.72              |
| 1:J:216:THR:HG21 | 1:L:199:MET:HG3  | 1.71                     | 0.72              |
| 1:K:144:SER:HB2  | 1:K:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:L:15:ILE:N     | 1:L:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:R:120:ASN:HD22 | 1:R:120:ASN:N    | 1.87                     | 0.72              |
| 1:A:15:ILE:N     | 1:A:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:B:199:MET:HG3  | 1:C:216:THR:HG21 | 1.71                     | 0.72              |
| 1:E:199:MET:HG3  | 1:F:216:THR:HG21 | 1.72                     | 0.72              |
| 1:K:18:ALA:HB3   | 1:K:23:ILE:CD1   | 2.19                     | 0.72              |
| 1:L:120:ASN:HD22 | 1:L:120:ASN:N    | 1.87                     | 0.72              |
| 1:A:127:ILE:O    | 1:A:128:ASP:HB2  | 1.87                     | 0.72              |
| 1:F:18:ALA:HB3   | 1:F:23:ILE:CD1   | 2.19                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:15:ILE:N     | 1:I:17:ASN:ND2   | 2.37                     | 0.72              |
| 1:I:110:ILE:HD12 | 1:I:167:MET:HE3  | 1.72                     | 0.72              |
| 1:M:144:SER:HB2  | 1:M:164:ILE:HD11 | 1.70                     | 0.72              |
| 1:D:120:ASN:HD22 | 1:D:120:ASN:N    | 1.87                     | 0.71              |
| 1:D:199:MET:HG3  | 1:E:216:THR:HG21 | 1.71                     | 0.71              |
| 1:M:120:ASN:HD22 | 1:M:120:ASN:N    | 1.87                     | 0.71              |
| 1:M:216:THR:HG21 | 1:O:199:MET:HG3  | 1.72                     | 0.71              |
| 1:F:144:SER:HB2  | 1:F:164:ILE:HD11 | 1.70                     | 0.71              |
| 1:G:199:MET:HG3  | 1:H:216:THR:HG21 | 1.71                     | 0.71              |
| 1:M:15:ILE:N     | 1:M:17:ASN:ND2   | 2.37                     | 0.71              |
| 1:M:199:MET:HG3  | 1:N:216:THR:HG21 | 1.71                     | 0.71              |
| 1:P:15:ILE:N     | 1:P:17:ASN:ND2   | 2.37                     | 0.71              |
| 1:F:15:ILE:N     | 1:F:17:ASN:ND2   | 2.37                     | 0.71              |
| 1:I:14:GLU:CA    | 1:I:17:ASN:ND2   | 2.50                     | 0.71              |
| 1:N:120:ASN:HD22 | 1:N:120:ASN:N    | 1.87                     | 0.71              |
| 1:O:120:ASN:HD22 | 1:O:120:ASN:N    | 1.87                     | 0.71              |
| 1:Q:120:ASN:HD22 | 1:Q:120:ASN:N    | 1.87                     | 0.71              |
| 1:B:120:ASN:HD22 | 1:B:120:ASN:N    | 1.87                     | 0.71              |
| 1:J:14:GLU:CA    | 1:J:17:ASN:ND2   | 2.50                     | 0.71              |
| 1:R:14:GLU:CA    | 1:R:17:ASN:ND2   | 2.50                     | 0.71              |
| 1:C:242:ASN:HD22 | 1:C:242:ASN:N    | 1.85                     | 0.70              |
| 1:C:18:ALA:HB3   | 1:C:23:ILE:CD1   | 2.19                     | 0.70              |
| 1:J:120:ASN:HD22 | 1:J:120:ASN:N    | 1.87                     | 0.70              |
| 1:P:120:ASN:HD22 | 1:P:120:ASN:N    | 1.87                     | 0.70              |
| 1:G:110:ILE:HD12 | 1:G:167:MET:HE3  | 1.73                     | 0.70              |
| 1:H:14:GLU:CA    | 1:H:17:ASN:ND2   | 2.50                     | 0.70              |
| 1:E:120:ASN:HD22 | 1:E:120:ASN:N    | 1.87                     | 0.70              |
| 1:N:18:ALA:HB3   | 1:N:23:ILE:CD1   | 2.19                     | 0.70              |
| 1:J:199:MET:HG3  | 1:K:216:THR:HG21 | 1.71                     | 0.70              |
| 1:K:120:ASN:HD22 | 1:K:120:ASN:N    | 1.87                     | 0.70              |
| 1:A:199:MET:HG3  | 1:B:216:THR:HG21 | 1.71                     | 0.70              |
| 1:C:110:ILE:HD12 | 1:C:167:MET:HE3  | 1.73                     | 0.70              |
| 1:H:120:ASN:HD22 | 1:H:120:ASN:N    | 1.87                     | 0.70              |
| 1:E:18:ALA:HB3   | 1:E:23:ILE:CD1   | 2.19                     | 0.69              |
| 1:R:110:ILE:HD12 | 1:R:167:MET:HE3  | 1.71                     | 0.69              |
| 1:L:18:ALA:HB3   | 1:L:23:ILE:CD1   | 2.19                     | 0.69              |
| 1:R:242:ASN:HD22 | 1:R:242:ASN:N    | 1.85                     | 0.69              |
| 1:H:242:ASN:HD22 | 1:H:242:ASN:N    | 1.85                     | 0.69              |
| 1:K:242:ASN:HD22 | 1:K:242:ASN:N    | 1.85                     | 0.69              |
| 1:J:110:ILE:HD12 | 1:J:167:MET:HE3  | 1.75                     | 0.68              |
| 1:E:242:ASN:HD22 | 1:E:242:ASN:N    | 1.85                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:18:ALA:HB3   | 1:G:23:ILE:CD1   | 2.19                     | 0.68              |
| 1:K:14:GLU:HA    | 1:K:17:ASN:OD1   | 1.94                     | 0.68              |
| 1:L:14:GLU:HA    | 1:L:17:ASN:OD1   | 1.94                     | 0.68              |
| 1:D:14:GLU:HA    | 1:D:17:ASN:OD1   | 1.94                     | 0.68              |
| 1:J:14:GLU:HA    | 1:J:17:ASN:OD1   | 1.94                     | 0.68              |
| 1:J:18:ALA:HB3   | 1:J:23:ILE:CD1   | 2.19                     | 0.68              |
| 1:O:18:ALA:HB3   | 1:O:23:ILE:CD1   | 2.19                     | 0.68              |
| 1:O:242:ASN:HD22 | 1:O:242:ASN:N    | 1.85                     | 0.68              |
| 1:I:14:GLU:HA    | 1:I:17:ASN:OD1   | 1.94                     | 0.68              |
| 1:N:110:ILE:HD12 | 1:N:167:MET:HE3  | 1.75                     | 0.68              |
| 1:A:14:GLU:HA    | 1:A:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:E:14:GLU:HA    | 1:E:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:Q:18:ALA:HB3   | 1:Q:23:ILE:CD1   | 2.19                     | 0.67              |
| 1:N:14:GLU:HA    | 1:N:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:N:242:ASN:HD22 | 1:N:242:ASN:N    | 1.85                     | 0.67              |
| 1:O:14:GLU:HA    | 1:O:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:P:14:GLU:HA    | 1:P:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:C:14:GLU:HA    | 1:C:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:D:18:ALA:HB3   | 1:D:23:ILE:CD1   | 2.19                     | 0.67              |
| 1:J:164:ILE:HG23 | 1:K:170:GLN:HA   | 1.77                     | 0.67              |
| 1:B:242:ASN:HD22 | 1:B:242:ASN:N    | 1.85                     | 0.67              |
| 1:H:14:GLU:HA    | 1:H:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:M:164:ILE:HG23 | 1:N:170:GLN:HA   | 1.77                     | 0.67              |
| 1:P:164:ILE:HG23 | 1:Q:170:GLN:HA   | 1.77                     | 0.67              |
| 1:R:14:GLU:HA    | 1:R:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:D:164:ILE:HG23 | 1:E:170:GLN:HA   | 1.77                     | 0.67              |
| 1:E:164:ILE:HG23 | 1:F:170:GLN:HA   | 1.77                     | 0.67              |
| 1:F:14:GLU:HA    | 1:F:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:K:164:ILE:HG23 | 1:L:170:GLN:HA   | 1.77                     | 0.67              |
| 1:N:164:ILE:HG23 | 1:O:170:GLN:HA   | 1.77                     | 0.67              |
| 1:G:164:ILE:HG23 | 1:H:170:GLN:HA   | 1.77                     | 0.67              |
| 1:H:164:ILE:HG23 | 1:I:170:GLN:HA   | 1.77                     | 0.67              |
| 1:M:14:GLU:HA    | 1:M:17:ASN:OD1   | 1.94                     | 0.67              |
| 1:A:164:ILE:HG23 | 1:B:170:GLN:HA   | 1.77                     | 0.66              |
| 1:P:170:GLN:HA   | 1:R:164:ILE:HG23 | 1.77                     | 0.66              |
| 1:B:14:GLU:HA    | 1:B:17:ASN:OD1   | 1.94                     | 0.66              |
| 1:Q:242:ASN:HD22 | 1:Q:242:ASN:N    | 1.85                     | 0.66              |
| 1:B:164:ILE:HG23 | 1:C:170:GLN:HA   | 1.77                     | 0.66              |
| 1:M:170:GLN:HA   | 1:O:164:ILE:HG23 | 1.77                     | 0.66              |
| 1:G:14:GLU:HA    | 1:G:17:ASN:OD1   | 1.94                     | 0.66              |
| 1:I:205:THR:OG1  | 1:I:216:THR:HG23 | 1.96                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:14:GLU:HA    | 1:Q:17:ASN:OD1   | 1.94                     | 0.66              |
| 1:Q:14:GLU:CB    | 1:Q:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:B:14:GLU:CB    | 1:B:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:K:205:THR:OG1  | 1:K:216:THR:HG23 | 1.96                     | 0.66              |
| 1:M:110:ILE:HD12 | 1:M:167:MET:HE3  | 1.78                     | 0.66              |
| 1:N:205:THR:OG1  | 1:N:216:THR:HG23 | 1.96                     | 0.66              |
| 1:Q:205:THR:OG1  | 1:Q:216:THR:HG23 | 1.96                     | 0.66              |
| 1:D:205:THR:OG1  | 1:D:216:THR:HG23 | 1.96                     | 0.66              |
| 1:G:170:GLN:HA   | 1:I:164:ILE:HG23 | 1.77                     | 0.66              |
| 1:N:14:GLU:CB    | 1:N:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:C:205:THR:OG1  | 1:C:216:THR:HG23 | 1.96                     | 0.66              |
| 1:E:14:GLU:CB    | 1:E:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:G:205:THR:OG1  | 1:G:216:THR:HG23 | 1.96                     | 0.66              |
| 1:K:14:GLU:CB    | 1:K:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:L:14:GLU:CB    | 1:L:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:L:242:ASN:HD22 | 1:L:242:ASN:N    | 1.85                     | 0.66              |
| 1:Q:164:ILE:HG23 | 1:R:170:GLN:HA   | 1.77                     | 0.66              |
| 1:H:14:GLU:CB    | 1:H:17:ASN:HD21  | 2.09                     | 0.66              |
| 1:J:170:GLN:HA   | 1:L:164:ILE:HG23 | 1.77                     | 0.66              |
| 1:A:205:THR:OG1  | 1:A:216:THR:HG23 | 1.96                     | 0.65              |
| 1:B:205:THR:OG1  | 1:B:216:THR:HG23 | 1.96                     | 0.65              |
| 1:D:14:GLU:CB    | 1:D:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:I:14:GLU:CB    | 1:I:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:P:205:THR:OG1  | 1:P:216:THR:HG23 | 1.96                     | 0.65              |
| 1:D:170:GLN:HA   | 1:F:164:ILE:HG23 | 1.77                     | 0.65              |
| 1:F:205:THR:OG1  | 1:F:216:THR:HG23 | 1.96                     | 0.65              |
| 1:J:205:THR:OG1  | 1:J:216:THR:HG23 | 1.96                     | 0.65              |
| 1:L:205:THR:OG1  | 1:L:216:THR:HG23 | 1.96                     | 0.65              |
| 1:E:205:THR:OG1  | 1:E:216:THR:HG23 | 1.96                     | 0.65              |
| 1:H:205:THR:OG1  | 1:H:216:THR:HG23 | 1.96                     | 0.65              |
| 1:R:205:THR:OG1  | 1:R:216:THR:HG23 | 1.96                     | 0.65              |
| 1:A:170:GLN:HA   | 1:C:164:ILE:HG23 | 1.77                     | 0.65              |
| 1:G:14:GLU:CB    | 1:G:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:O:14:GLU:CB    | 1:O:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:C:14:GLU:CB    | 1:C:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:F:14:GLU:CB    | 1:F:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:P:14:GLU:CB    | 1:P:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:R:14:GLU:CB    | 1:R:17:ASN:HD21  | 2.09                     | 0.65              |
| 1:B:110:ILE:HD12 | 1:B:167:MET:HE3  | 1.78                     | 0.64              |
| 1:M:205:THR:OG1  | 1:M:216:THR:HG23 | 1.96                     | 0.64              |
| 1:A:14:GLU:CB    | 1:A:17:ASN:HD21  | 2.09                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:14:GLU:CB    | 1:J:17:ASN:HD21  | 2.09                     | 0.64              |
| 1:M:14:GLU:CB    | 1:M:17:ASN:HD21  | 2.09                     | 0.64              |
| 1:O:205:THR:OG1  | 1:O:216:THR:HG23 | 1.96                     | 0.64              |
| 1:H:110:ILE:HD12 | 1:H:167:MET:HE3  | 1.79                     | 0.64              |
| 1:B:164:ILE:CG2  | 1:C:170:GLN:HA   | 2.28                     | 0.63              |
| 1:E:164:ILE:CG2  | 1:F:170:GLN:HA   | 2.28                     | 0.63              |
| 1:H:164:ILE:CG2  | 1:I:170:GLN:HA   | 2.28                     | 0.63              |
| 1:K:164:ILE:CG2  | 1:L:170:GLN:HA   | 2.28                     | 0.63              |
| 1:M:164:ILE:CG2  | 1:N:170:GLN:HA   | 2.29                     | 0.63              |
| 1:P:170:GLN:HA   | 1:R:164:ILE:CG2  | 2.29                     | 0.63              |
| 1:J:164:ILE:CG2  | 1:K:170:GLN:HA   | 2.29                     | 0.63              |
| 1:M:170:GLN:HA   | 1:O:164:ILE:CG2  | 2.29                     | 0.63              |
| 1:F:230:VAL:HG12 | 1:F:255:SER:HA   | 1.81                     | 0.63              |
| 1:O:230:VAL:HG12 | 1:O:255:SER:HA   | 1.81                     | 0.63              |
| 1:A:170:GLN:HA   | 1:C:164:ILE:CG2  | 2.29                     | 0.63              |
| 1:G:164:ILE:CG2  | 1:H:170:GLN:HA   | 2.29                     | 0.63              |
| 1:H:230:VAL:HG12 | 1:H:255:SER:HA   | 1.81                     | 0.63              |
| 1:I:230:VAL:HG12 | 1:I:255:SER:HA   | 1.81                     | 0.63              |
| 1:N:164:ILE:CG2  | 1:O:170:GLN:HA   | 2.28                     | 0.63              |
| 1:D:170:GLN:HA   | 1:F:164:ILE:CG2  | 2.29                     | 0.63              |
| 1:G:170:GLN:HA   | 1:I:164:ILE:CG2  | 2.29                     | 0.63              |
| 1:Q:230:VAL:HG12 | 1:Q:255:SER:HA   | 1.81                     | 0.63              |
| 1:B:242:ASN:ND2  | 1:B:242:ASN:N    | 2.45                     | 0.63              |
| 1:I:242:ASN:HD22 | 1:I:242:ASN:N    | 1.85                     | 0.63              |
| 1:P:164:ILE:CG2  | 1:Q:170:GLN:HA   | 2.29                     | 0.63              |
| 1:L:230:VAL:HG12 | 1:L:255:SER:HA   | 1.81                     | 0.62              |
| 1:R:230:VAL:HG12 | 1:R:255:SER:HA   | 1.81                     | 0.62              |
| 1:A:164:ILE:CG2  | 1:B:170:GLN:HA   | 2.29                     | 0.62              |
| 1:Q:164:ILE:CG2  | 1:R:170:GLN:HA   | 2.29                     | 0.62              |
| 1:E:230:VAL:HG12 | 1:E:255:SER:HA   | 1.81                     | 0.62              |
| 1:K:230:VAL:HG12 | 1:K:255:SER:HA   | 1.81                     | 0.62              |
| 1:H:17:ASN:HD22  | 1:H:17:ASN:N     | 1.96                     | 0.62              |
| 1:J:170:GLN:HA   | 1:L:164:ILE:CG2  | 2.29                     | 0.62              |
| 1:M:230:VAL:HG12 | 1:M:255:SER:HA   | 1.81                     | 0.62              |
| 1:D:164:ILE:CG2  | 1:E:170:GLN:HA   | 2.29                     | 0.62              |
| 1:J:230:VAL:HG12 | 1:J:255:SER:HA   | 1.81                     | 0.62              |
| 1:N:230:VAL:HG12 | 1:N:255:SER:HA   | 1.81                     | 0.62              |
| 1:C:230:VAL:HG12 | 1:C:255:SER:HA   | 1.81                     | 0.62              |
| 1:A:230:VAL:HG12 | 1:A:255:SER:HA   | 1.81                     | 0.62              |
| 1:D:230:VAL:HG12 | 1:D:255:SER:HA   | 1.81                     | 0.62              |
| 1:G:230:VAL:HG12 | 1:G:255:SER:HA   | 1.81                     | 0.62              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:248:GLU:O    | 1:I:249:ILE:HB  | 2.00                     | 0.62              |
| 1:M:248:GLU:O    | 1:M:249:ILE:HB  | 2.00                     | 0.62              |
| 1:P:230:VAL:HG12 | 1:P:255:SER:HA  | 1.81                     | 0.62              |
| 1:B:230:VAL:HG12 | 1:B:255:SER:HA  | 1.81                     | 0.61              |
| 1:L:248:GLU:O    | 1:L:249:ILE:HB  | 2.00                     | 0.61              |
| 1:N:248:GLU:O    | 1:N:249:ILE:HB  | 2.00                     | 0.61              |
| 1:F:248:GLU:O    | 1:F:249:ILE:HB  | 2.00                     | 0.61              |
| 1:K:110:ILE:HD12 | 1:K:167:MET:HE3 | 1.82                     | 0.61              |
| 1:L:110:ILE:HD12 | 1:L:167:MET:HE3 | 1.82                     | 0.61              |
| 1:O:248:GLU:O    | 1:O:249:ILE:HB  | 2.00                     | 0.61              |
| 1:A:248:GLU:O    | 1:A:249:ILE:HB  | 2.00                     | 0.61              |
| 1:F:110:ILE:HD12 | 1:F:167:MET:HE3 | 1.82                     | 0.61              |
| 1:G:248:GLU:O    | 1:G:249:ILE:HB  | 2.00                     | 0.61              |
| 1:J:248:GLU:O    | 1:J:249:ILE:HB  | 2.00                     | 0.61              |
| 1:B:248:GLU:O    | 1:B:249:ILE:HB  | 2.00                     | 0.61              |
| 1:R:248:GLU:O    | 1:R:249:ILE:HB  | 2.00                     | 0.61              |
| 1:C:248:GLU:O    | 1:C:249:ILE:HB  | 2.00                     | 0.61              |
| 1:D:248:GLU:O    | 1:D:249:ILE:HB  | 2.00                     | 0.61              |
| 1:E:110:ILE:HD12 | 1:E:167:MET:HE3 | 1.80                     | 0.61              |
| 1:P:248:GLU:O    | 1:P:249:ILE:HB  | 2.00                     | 0.61              |
| 1:K:242:ASN:ND2  | 1:K:242:ASN:N   | 2.45                     | 0.61              |
| 1:Q:248:GLU:O    | 1:Q:249:ILE:HB  | 2.00                     | 0.61              |
| 1:P:110:ILE:HD12 | 1:P:167:MET:HE3 | 1.81                     | 0.61              |
| 1:D:10:ILE:H     | 1:E:32:ASN:HD21 | 1.49                     | 0.60              |
| 1:K:248:GLU:O    | 1:K:249:ILE:HB  | 2.00                     | 0.60              |
| 1:D:32:ASN:HD21  | 1:F:10:ILE:H    | 1.50                     | 0.60              |
| 1:E:248:GLU:O    | 1:E:249:ILE:HB  | 2.00                     | 0.60              |
| 1:G:32:ASN:HD21  | 1:I:10:ILE:H    | 1.49                     | 0.60              |
| 1:A:10:ILE:H     | 1:B:32:ASN:HD21 | 1.50                     | 0.60              |
| 1:H:248:GLU:O    | 1:H:249:ILE:HB  | 2.00                     | 0.60              |
| 1:J:17:ASN:HD22  | 1:J:17:ASN:N    | 1.96                     | 0.60              |
| 1:A:32:ASN:HD21  | 1:C:10:ILE:H    | 1.50                     | 0.60              |
| 1:G:10:ILE:H     | 1:H:32:ASN:HD21 | 1.50                     | 0.60              |
| 1:J:32:ASN:HD21  | 1:L:10:ILE:H    | 1.50                     | 0.60              |
| 1:L:17:ASN:HD22  | 1:L:17:ASN:N    | 1.96                     | 0.60              |
| 1:P:10:ILE:H     | 1:Q:32:ASN:HD21 | 1.50                     | 0.60              |
| 1:M:10:ILE:H     | 1:N:32:ASN:HD21 | 1.49                     | 0.60              |
| 1:M:32:ASN:HD21  | 1:O:10:ILE:H    | 1.50                     | 0.60              |
| 1:P:32:ASN:HD21  | 1:R:10:ILE:H    | 1.49                     | 0.60              |
| 1:J:10:ILE:H     | 1:K:32:ASN:HD21 | 1.50                     | 0.60              |
| 1:G:242:ASN:HD22 | 1:G:242:ASN:N   | 1.85                     | 0.60              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:M:242:ASN:ND2  | 1:M:242:ASN:N   | 2.45                     | 0.60              |
| 1:B:15:ILE:C     | 1:B:17:ASN:H    | 2.06                     | 0.59              |
| 1:F:242:ASN:HD22 | 1:F:242:ASN:N   | 1.85                     | 0.59              |
| 1:D:110:ILE:HD12 | 1:D:167:MET:HE3 | 1.84                     | 0.59              |
| 1:C:15:ILE:C     | 1:C:17:ASN:H    | 2.06                     | 0.59              |
| 1:D:15:ILE:C     | 1:D:17:ASN:H    | 2.06                     | 0.59              |
| 1:F:15:ILE:C     | 1:F:17:ASN:H    | 2.06                     | 0.59              |
| 1:Q:110:ILE:HD12 | 1:Q:167:MET:HE3 | 1.84                     | 0.59              |
| 1:G:15:ILE:C     | 1:G:17:ASN:H    | 2.06                     | 0.59              |
| 1:E:15:ILE:C     | 1:E:17:ASN:H    | 2.06                     | 0.58              |
| 1:I:242:ASN:ND2  | 1:I:242:ASN:N   | 2.45                     | 0.58              |
| 1:N:18:ALA:CB    | 1:N:23:ILE:HD11 | 2.27                     | 0.58              |
| 1:P:15:ILE:C     | 1:P:17:ASN:H    | 2.06                     | 0.58              |
| 1:O:110:ILE:HD12 | 1:O:167:MET:HE3 | 1.85                     | 0.58              |
| 1:D:242:ASN:HD22 | 1:D:242:ASN:N   | 1.85                     | 0.58              |
| 1:F:14:GLU:O     | 1:F:15:ILE:HB   | 2.04                     | 0.58              |
| 1:A:110:ILE:HD12 | 1:A:167:MET:HE3 | 1.84                     | 0.58              |
| 1:I:15:ILE:C     | 1:I:17:ASN:H    | 2.06                     | 0.58              |
| 1:N:10:ILE:H     | 1:O:32:ASN:HD21 | 1.50                     | 0.58              |
| 1:O:14:GLU:O     | 1:O:15:ILE:HB   | 2.04                     | 0.58              |
| 1:O:15:ILE:C     | 1:O:17:ASN:H    | 2.06                     | 0.58              |
| 1:I:17:ASN:HD22  | 1:I:17:ASN:N    | 1.96                     | 0.58              |
| 1:J:15:ILE:C     | 1:J:17:ASN:H    | 2.06                     | 0.58              |
| 1:P:14:GLU:O     | 1:P:15:ILE:HB   | 2.04                     | 0.58              |
| 1:B:14:GLU:O     | 1:B:15:ILE:HB   | 2.04                     | 0.58              |
| 1:H:242:ASN:ND2  | 1:H:242:ASN:N   | 2.45                     | 0.58              |
| 1:Q:10:ILE:H     | 1:R:32:ASN:HD21 | 1.50                     | 0.58              |
| 1:E:14:GLU:O     | 1:E:15:ILE:HB   | 2.04                     | 0.58              |
| 1:M:15:ILE:C     | 1:M:17:ASN:H    | 2.06                     | 0.58              |
| 1:A:14:GLU:O     | 1:A:15:ILE:HB   | 2.04                     | 0.58              |
| 1:C:14:GLU:O     | 1:C:15:ILE:HB   | 2.04                     | 0.58              |
| 1:N:14:GLU:O     | 1:N:15:ILE:HB   | 2.04                     | 0.58              |
| 1:R:14:GLU:O     | 1:R:15:ILE:HB   | 2.04                     | 0.58              |
| 1:K:10:ILE:H     | 1:L:32:ASN:HD21 | 1.50                     | 0.57              |
| 1:E:10:ILE:H     | 1:F:32:ASN:HD21 | 1.50                     | 0.57              |
| 1:H:10:ILE:H     | 1:I:32:ASN:HD21 | 1.50                     | 0.57              |
| 1:I:14:GLU:O     | 1:I:15:ILE:HB   | 2.04                     | 0.57              |
| 1:L:15:ILE:C     | 1:L:17:ASN:H    | 2.06                     | 0.57              |
| 1:L:242:ASN:ND2  | 1:L:242:ASN:N   | 2.45                     | 0.57              |
| 1:Q:17:ASN:HD22  | 1:Q:17:ASN:N    | 1.96                     | 0.57              |
| 1:H:15:ILE:C     | 1:H:17:ASN:H    | 2.06                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:15:ILE:C     | 1:K:17:ASN:H     | 2.06                     | 0.57              |
| 1:A:15:ILE:C     | 1:A:17:ASN:H     | 2.06                     | 0.57              |
| 1:J:14:GLU:O     | 1:J:15:ILE:HB    | 2.04                     | 0.57              |
| 1:L:14:GLU:O     | 1:L:15:ILE:HB    | 2.04                     | 0.57              |
| 1:B:10:ILE:H     | 1:C:32:ASN:HD21  | 1.50                     | 0.57              |
| 1:P:242:ASN:HD22 | 1:P:242:ASN:N    | 1.85                     | 0.57              |
| 1:A:242:ASN:HD22 | 1:A:242:ASN:N    | 1.85                     | 0.57              |
| 1:C:98:ILE:O     | 1:C:127:ILE:HG12 | 2.05                     | 0.57              |
| 1:D:14:GLU:O     | 1:D:15:ILE:HB    | 2.04                     | 0.57              |
| 1:H:14:GLU:O     | 1:H:15:ILE:HB    | 2.04                     | 0.57              |
| 1:A:98:ILE:O     | 1:A:127:ILE:HG12 | 2.05                     | 0.57              |
| 1:B:17:ASN:HD22  | 1:B:17:ASN:N     | 1.96                     | 0.57              |
| 1:B:98:ILE:O     | 1:B:127:ILE:HG12 | 2.05                     | 0.57              |
| 1:D:98:ILE:O     | 1:D:127:ILE:HG12 | 2.05                     | 0.57              |
| 1:M:14:GLU:O     | 1:M:15:ILE:HB    | 2.04                     | 0.57              |
| 1:Q:15:ILE:C     | 1:Q:17:ASN:H     | 2.06                     | 0.57              |
| 1:R:98:ILE:O     | 1:R:127:ILE:HG12 | 2.05                     | 0.57              |
| 1:J:18:ALA:CB    | 1:J:23:ILE:HD11  | 2.27                     | 0.56              |
| 1:N:98:ILE:O     | 1:N:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:P:98:ILE:O     | 1:P:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:Q:14:GLU:O     | 1:Q:15:ILE:HB    | 2.04                     | 0.56              |
| 1:Q:71:SER:OG    | 1:Q:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:E:71:SER:OG    | 1:E:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:E:98:ILE:O     | 1:E:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:H:98:ILE:O     | 1:H:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:J:71:SER:OG    | 1:J:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:J:98:ILE:O     | 1:J:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:K:14:GLU:O     | 1:K:15:ILE:HB    | 2.04                     | 0.56              |
| 1:L:98:ILE:O     | 1:L:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:N:71:SER:OG    | 1:N:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:O:98:ILE:O     | 1:O:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:R:71:SER:OG    | 1:R:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:B:71:SER:OG    | 1:B:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:C:18:ALA:CB    | 1:C:23:ILE:HD11  | 2.27                     | 0.56              |
| 1:K:98:ILE:O     | 1:K:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:O:71:SER:OG    | 1:O:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:P:71:SER:OG    | 1:P:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:A:71:SER:OG    | 1:A:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:O:110:ILE:HG23 | 1:O:167:MET:HE1  | 1.88                     | 0.56              |
| 1:D:71:SER:OG    | 1:D:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:M:98:ILE:O     | 1:M:127:ILE:HG12 | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:15:ILE:C     | 1:N:17:ASN:H     | 2.06                     | 0.56              |
| 1:G:14:GLU:O     | 1:G:15:ILE:HB    | 2.04                     | 0.56              |
| 1:I:71:SER:OG    | 1:I:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:O:18:ALA:CB    | 1:O:23:ILE:HD11  | 2.27                     | 0.56              |
| 1:A:14:GLU:HA    | 1:A:17:ASN:ND2   | 2.21                     | 0.56              |
| 1:A:79:VAL:HG11  | 1:A:85:HIS:HE2   | 1.71                     | 0.56              |
| 1:A:242:ASN:ND2  | 1:A:242:ASN:N    | 2.45                     | 0.56              |
| 1:M:71:SER:OG    | 1:M:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:R:15:ILE:C     | 1:R:17:ASN:H     | 2.06                     | 0.56              |
| 1:F:98:ILE:O     | 1:F:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:P:233:SER:HA   | 2:P:316:EPE:H81  | 1.88                     | 0.56              |
| 1:A:233:SER:HA   | 2:A:301:EPE:H81  | 1.88                     | 0.56              |
| 1:C:71:SER:OG    | 1:C:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:D:14:GLU:HA    | 1:D:17:ASN:ND2   | 2.21                     | 0.56              |
| 1:D:193:HIS:CD2  | 1:F:118:VAL:HG21 | 2.41                     | 0.56              |
| 1:F:71:SER:OG    | 1:F:74:GLU:HG3   | 2.06                     | 0.56              |
| 1:I:98:ILE:O     | 1:I:127:ILE:HG12 | 2.05                     | 0.56              |
| 1:K:14:GLU:HA    | 1:K:17:ASN:ND2   | 2.21                     | 0.56              |
| 1:N:118:VAL:HG21 | 1:O:193:HIS:CD2  | 2.41                     | 0.56              |
| 1:A:193:HIS:CD2  | 1:C:118:VAL:HG21 | 2.41                     | 0.55              |
| 1:G:193:HIS:CD2  | 1:I:118:VAL:HG21 | 2.41                     | 0.55              |
| 1:H:71:SER:OG    | 1:H:74:GLU:HG3   | 2.06                     | 0.55              |
| 1:H:233:SER:HA   | 2:H:308:EPE:H81  | 1.88                     | 0.55              |
| 1:N:17:ASN:HD22  | 1:N:17:ASN:N     | 1.96                     | 0.55              |
| 1:Q:18:ALA:CB    | 1:Q:23:ILE:HD11  | 2.27                     | 0.55              |
| 1:R:79:VAL:HG11  | 1:R:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:G:98:ILE:O     | 1:G:127:ILE:HG12 | 2.05                     | 0.55              |
| 1:I:111:ASN:HD22 | 1:I:143:TYR:H    | 1.55                     | 0.55              |
| 1:K:71:SER:OG    | 1:K:74:GLU:HG3   | 2.06                     | 0.55              |
| 1:K:118:VAL:HG21 | 1:L:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:L:111:ASN:HD22 | 1:L:143:TYR:H    | 1.55                     | 0.55              |
| 1:L:201:LYS:HE2  | 1:L:218:GLU:OE2  | 2.07                     | 0.55              |
| 1:N:14:GLU:HA    | 1:N:17:ASN:ND2   | 2.21                     | 0.55              |
| 1:P:14:GLU:HA    | 1:P:17:ASN:ND2   | 2.21                     | 0.55              |
| 1:Q:118:VAL:HG21 | 1:R:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:B:14:GLU:HA    | 1:B:17:ASN:ND2   | 2.21                     | 0.55              |
| 1:B:72:ILE:H     | 1:B:72:ILE:HD12  | 1.72                     | 0.55              |
| 1:F:111:ASN:HD22 | 1:F:143:TYR:H    | 1.55                     | 0.55              |
| 1:G:233:SER:HA   | 2:G:307:EPE:H81  | 1.88                     | 0.55              |
| 1:H:72:ILE:HD12  | 1:H:72:ILE:H     | 1.72                     | 0.55              |
| 1:I:144:SER:HB2  | 1:I:164:ILE:CD1  | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:79:VAL:HG11  | 1:P:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:D:118:VAL:HG21 | 1:E:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:E:233:SER:HA   | 2:E:305:EPE:H81  | 1.88                     | 0.55              |
| 1:F:144:SER:HB2  | 1:F:164:ILE:CD1  | 2.37                     | 0.55              |
| 1:H:111:ASN:HD22 | 1:H:143:TYR:H    | 1.55                     | 0.55              |
| 1:I:79:VAL:HG11  | 1:I:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:J:118:VAL:HG21 | 1:K:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:J:193:HIS:CD2  | 1:L:118:VAL:HG21 | 2.41                     | 0.55              |
| 1:L:71:SER:OG    | 1:L:74:GLU:HG3   | 2.06                     | 0.55              |
| 1:O:79:VAL:HG11  | 1:O:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:P:193:HIS:CD2  | 1:R:118:VAL:HG21 | 2.41                     | 0.55              |
| 1:Q:98:ILE:O     | 1:Q:127:ILE:HG12 | 2.05                     | 0.55              |
| 1:B:111:ASN:HD22 | 1:B:143:TYR:H    | 1.55                     | 0.55              |
| 1:C:79:VAL:HG11  | 1:C:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:G:111:ASN:HD22 | 1:G:143:TYR:H    | 1.55                     | 0.55              |
| 1:G:118:VAL:HG21 | 1:H:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:J:233:SER:HA   | 2:J:310:EPE:H81  | 1.88                     | 0.55              |
| 1:P:201:LYS:HE2  | 1:P:218:GLU:OE2  | 2.07                     | 0.55              |
| 1:Q:110:ILE:HG23 | 1:Q:167:MET:HE1  | 1.89                     | 0.55              |
| 1:A:118:VAL:HG21 | 1:B:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:A:201:LYS:HE2  | 1:A:218:GLU:OE2  | 2.07                     | 0.55              |
| 1:D:72:ILE:H     | 1:D:72:ILE:HD12  | 1.72                     | 0.55              |
| 1:I:18:ALA:CB    | 1:I:23:ILE:HD11  | 2.27                     | 0.55              |
| 1:J:72:ILE:H     | 1:J:72:ILE:HD12  | 1.72                     | 0.55              |
| 1:J:111:ASN:HD22 | 1:J:143:TYR:H    | 1.55                     | 0.55              |
| 1:L:79:VAL:HG11  | 1:L:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:M:193:HIS:CD2  | 1:O:118:VAL:HG21 | 2.41                     | 0.55              |
| 1:O:201:LYS:HE2  | 1:O:218:GLU:OE2  | 2.07                     | 0.55              |
| 1:Q:144:SER:HB2  | 1:Q:164:ILE:CD1  | 2.37                     | 0.55              |
| 1:R:72:ILE:H     | 1:R:72:ILE:HD12  | 1.72                     | 0.55              |
| 1:B:79:VAL:HG11  | 1:B:85:HIS:HE2   | 1.71                     | 0.55              |
| 1:E:111:ASN:HD22 | 1:E:143:TYR:H    | 1.55                     | 0.55              |
| 1:E:201:LYS:HE2  | 1:E:218:GLU:OE2  | 2.07                     | 0.55              |
| 1:G:14:GLU:HA    | 1:G:17:ASN:ND2   | 2.21                     | 0.55              |
| 1:H:14:GLU:HA    | 1:H:17:ASN:ND2   | 2.21                     | 0.55              |
| 1:P:210:ASP:OD2  | 1:P:212:ARG:HD3  | 2.07                     | 0.55              |
| 1:Q:14:GLU:HA    | 1:Q:17:ASN:ND2   | 2.21                     | 0.55              |
| 1:R:201:LYS:HE2  | 1:R:218:GLU:OE2  | 2.07                     | 0.55              |
| 1:B:118:VAL:HG21 | 1:C:193:HIS:CD2  | 2.41                     | 0.55              |
| 1:C:233:SER:HA   | 2:C:303:EPE:H81  | 1.88                     | 0.55              |
| 1:D:210:ASP:OD2  | 1:D:212:ARG:HD3  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:210:ASP:OD2  | 1:G:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:J:201:LYS:HE2  | 1:J:218:GLU:OE2 | 2.07                     | 0.55              |
| 1:J:210:ASP:OD2  | 1:J:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:K:210:ASP:OD2  | 1:K:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:Q:233:SER:HA   | 2:Q:317:EPE:H81 | 1.88                     | 0.55              |
| 1:A:210:ASP:OD2  | 1:A:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:C:201:LYS:HE2  | 1:C:218:GLU:OE2 | 2.07                     | 0.55              |
| 1:F:18:ALA:CB    | 1:F:23:ILE:HD11 | 2.27                     | 0.55              |
| 1:M:14:GLU:HA    | 1:M:17:ASN:ND2  | 2.21                     | 0.55              |
| 1:D:79:VAL:HG11  | 1:D:85:HIS:HE2  | 1.71                     | 0.55              |
| 1:D:201:LYS:HE2  | 1:D:218:GLU:OE2 | 2.07                     | 0.55              |
| 1:D:233:SER:HA   | 2:D:304:EPE:H81 | 1.88                     | 0.55              |
| 1:E:210:ASP:OD2  | 1:E:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:G:71:SER:OG    | 1:G:74:GLU:HG3  | 2.06                     | 0.55              |
| 1:G:72:ILE:H     | 1:G:72:ILE:HD12 | 1.72                     | 0.55              |
| 1:G:201:LYS:HE2  | 1:G:218:GLU:OE2 | 2.07                     | 0.55              |
| 1:L:144:SER:HB2  | 1:L:164:ILE:CD1 | 2.37                     | 0.55              |
| 1:M:210:ASP:OD2  | 1:M:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:N:201:LYS:HE2  | 1:N:218:GLU:OE2 | 2.07                     | 0.55              |
| 1:N:210:ASP:OD2  | 1:N:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:Q:201:LYS:HE2  | 1:Q:218:GLU:OE2 | 2.07                     | 0.55              |
| 1:Q:210:ASP:OD2  | 1:Q:212:ARG:HD3 | 2.07                     | 0.55              |
| 1:R:233:SER:HA   | 2:R:318:EPE:H81 | 1.88                     | 0.55              |
| 1:A:17:ASN:HD22  | 1:A:17:ASN:N    | 1.96                     | 0.54              |
| 1:C:144:SER:HB2  | 1:C:164:ILE:CD1 | 2.37                     | 0.54              |
| 1:F:20:THR:O     | 1:F:21:GLY:C    | 2.46                     | 0.54              |
| 1:F:233:SER:HA   | 2:F:306:EPE:H81 | 1.88                     | 0.54              |
| 1:H:118:VAL:HG21 | 1:I:193:HIS:CD2 | 2.41                     | 0.54              |
| 1:K:233:SER:HA   | 2:K:311:EPE:H81 | 1.88                     | 0.54              |
| 1:M:72:ILE:H     | 1:M:72:ILE:HD12 | 1.72                     | 0.54              |
| 1:M:242:ASN:HD22 | 1:M:242:ASN:N   | 1.85                     | 0.54              |
| 1:N:233:SER:HA   | 2:N:314:EPE:H81 | 1.88                     | 0.54              |
| 1:O:20:THR:O     | 1:O:21:GLY:C    | 2.46                     | 0.54              |
| 1:O:111:ASN:HD22 | 1:O:143:TYR:H   | 1.55                     | 0.54              |
| 1:P:72:ILE:HD12  | 1:P:72:ILE:H    | 1.72                     | 0.54              |
| 1:P:118:VAL:HG21 | 1:Q:193:HIS:CD2 | 2.41                     | 0.54              |
| 1:R:14:GLU:HA    | 1:R:17:ASN:ND2  | 2.21                     | 0.54              |
| 1:R:210:ASP:OD2  | 1:R:212:ARG:HD3 | 2.07                     | 0.54              |
| 1:A:144:SER:HB2  | 1:A:164:ILE:CD1 | 2.37                     | 0.54              |
| 1:B:201:LYS:HE2  | 1:B:218:GLU:OE2 | 2.07                     | 0.54              |
| 1:D:111:ASN:HD22 | 1:D:143:TYR:H   | 1.55                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:14:GLU:HA    | 1:I:17:ASN:ND2  | 2.21                     | 0.54              |
| 1:J:14:GLU:HA    | 1:J:17:ASN:ND2  | 2.21                     | 0.54              |
| 1:M:201:LYS:HE2  | 1:M:218:GLU:OE2 | 2.07                     | 0.54              |
| 1:O:233:SER:HA   | 2:O:315:EPE:H81 | 1.88                     | 0.54              |
| 1:O:242:ASN:ND2  | 1:O:242:ASN:N   | 2.45                     | 0.54              |
| 1:Q:72:ILE:H     | 1:Q:72:ILE:HD12 | 1.72                     | 0.54              |
| 1:Q:111:ASN:HD22 | 1:Q:143:TYR:H   | 1.55                     | 0.54              |
| 1:A:72:ILE:H     | 1:A:72:ILE:HD12 | 1.72                     | 0.54              |
| 1:C:72:ILE:HD12  | 1:C:72:ILE:H    | 1.72                     | 0.54              |
| 1:D:144:SER:HB2  | 1:D:164:ILE:CD1 | 2.37                     | 0.54              |
| 1:I:210:ASP:OD2  | 1:I:212:ARG:HD3 | 2.07                     | 0.54              |
| 1:K:111:ASN:HD22 | 1:K:143:TYR:H   | 1.55                     | 0.54              |
| 1:M:118:VAL:HG21 | 1:N:193:HIS:CD2 | 2.41                     | 0.54              |
| 1:P:144:SER:HB2  | 1:P:164:ILE:CD1 | 2.37                     | 0.54              |
| 1:R:111:ASN:HD22 | 1:R:143:TYR:H   | 1.55                     | 0.54              |
| 1:E:17:ASN:HD22  | 1:E:17:ASN:N    | 1.96                     | 0.54              |
| 1:E:72:ILE:H     | 1:E:72:ILE:HD12 | 1.72                     | 0.54              |
| 1:E:118:VAL:HG21 | 1:F:193:HIS:CD2 | 2.41                     | 0.54              |
| 1:F:79:VAL:HG11  | 1:F:85:HIS:HE2  | 1.71                     | 0.54              |
| 1:I:201:LYS:HE2  | 1:I:218:GLU:OE2 | 2.07                     | 0.54              |
| 1:K:20:THR:O     | 1:K:21:GLY:C    | 2.46                     | 0.54              |
| 1:L:14:GLU:HA    | 1:L:17:ASN:ND2  | 2.21                     | 0.54              |
| 1:M:111:ASN:HD22 | 1:M:143:TYR:H   | 1.55                     | 0.54              |
| 1:N:79:VAL:HG11  | 1:N:85:HIS:HE2  | 1.72                     | 0.54              |
| 1:O:72:ILE:H     | 1:O:72:ILE:HD12 | 1.72                     | 0.54              |
| 1:O:210:ASP:OD2  | 1:O:212:ARG:HD3 | 2.07                     | 0.54              |
| 1:Q:79:VAL:HG11  | 1:Q:85:HIS:HE2  | 1.71                     | 0.54              |
| 1:C:14:GLU:HA    | 1:C:17:ASN:ND2  | 2.21                     | 0.54              |
| 1:D:29:ASN:OD1   | 1:F:12:THR:HG21 | 2.08                     | 0.54              |
| 1:F:17:ASN:HD22  | 1:F:17:ASN:N    | 1.96                     | 0.54              |
| 1:F:201:LYS:HE2  | 1:F:218:GLU:OE2 | 2.07                     | 0.54              |
| 1:H:79:VAL:HG11  | 1:H:85:HIS:HE2  | 1.71                     | 0.54              |
| 1:H:210:ASP:OD2  | 1:H:212:ARG:HD3 | 2.07                     | 0.54              |
| 1:I:233:SER:HA   | 2:I:309:EPE:H81 | 1.88                     | 0.54              |
| 1:L:72:ILE:H     | 1:L:72:ILE:HD12 | 1.72                     | 0.54              |
| 1:O:14:GLU:HA    | 1:O:17:ASN:ND2  | 2.21                     | 0.54              |
| 1:P:29:ASN:OD1   | 1:R:12:THR:HG21 | 2.08                     | 0.54              |
| 1:A:29:ASN:OD1   | 1:C:12:THR:HG21 | 2.08                     | 0.54              |
| 1:B:20:THR:O     | 1:B:21:GLY:C    | 2.46                     | 0.54              |
| 1:B:144:SER:HB2  | 1:B:164:ILE:CD1 | 2.37                     | 0.54              |
| 1:C:111:ASN:HD22 | 1:C:143:TYR:H   | 1.55                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:210:ASP:OD2  | 1:C:212:ARG:HD3  | 2.07                     | 0.54              |
| 1:F:14:GLU:HA    | 1:F:17:ASN:ND2   | 2.21                     | 0.54              |
| 1:H:201:LYS:HE2  | 1:H:218:GLU:OE2  | 2.07                     | 0.54              |
| 1:J:79:VAL:HG11  | 1:J:85:HIS:HE2   | 1.71                     | 0.54              |
| 1:E:12:THR:HG21  | 1:F:29:ASN:OD1   | 2.08                     | 0.54              |
| 1:F:210:ASP:OD2  | 1:F:212:ARG:HD3  | 2.07                     | 0.54              |
| 1:G:144:SER:HB2  | 1:G:164:ILE:CD1  | 2.37                     | 0.54              |
| 1:H:12:THR:HG21  | 1:I:29:ASN:OD1   | 2.08                     | 0.54              |
| 1:K:146:VAL:HG22 | 1:K:164:ILE:HD13 | 1.90                     | 0.54              |
| 1:G:79:VAL:HG11  | 1:G:85:HIS:HE2   | 1.71                     | 0.54              |
| 1:H:20:THR:O     | 1:H:21:GLY:C     | 2.46                     | 0.54              |
| 1:J:144:SER:HB2  | 1:J:164:ILE:CD1  | 2.37                     | 0.54              |
| 1:K:201:LYS:HE2  | 1:K:218:GLU:OE2  | 2.07                     | 0.54              |
| 1:M:29:ASN:OD1   | 1:O:12:THR:HG21  | 2.08                     | 0.54              |
| 1:M:144:SER:HB2  | 1:M:164:ILE:CD1  | 2.37                     | 0.54              |
| 1:O:144:SER:HB2  | 1:O:164:ILE:CD1  | 2.37                     | 0.54              |
| 1:R:18:ALA:CB    | 1:R:23:ILE:HD11  | 2.27                     | 0.54              |
| 1:B:233:SER:HA   | 2:B:302:EPE:H81  | 1.88                     | 0.54              |
| 1:C:146:VAL:HG22 | 1:C:164:ILE:HD13 | 1.90                     | 0.54              |
| 1:D:20:THR:O     | 1:D:21:GLY:C     | 2.46                     | 0.54              |
| 1:D:110:ILE:HG23 | 1:D:167:MET:HE1  | 1.89                     | 0.54              |
| 1:G:12:THR:HG21  | 1:H:29:ASN:OD1   | 2.08                     | 0.54              |
| 1:I:72:ILE:H     | 1:I:72:ILE:HD12  | 1.72                     | 0.54              |
| 1:L:233:SER:HA   | 2:L:312:EPE:H81  | 1.88                     | 0.54              |
| 1:B:210:ASP:OD2  | 1:B:212:ARG:HD3  | 2.07                     | 0.54              |
| 1:H:146:VAL:HG22 | 1:H:164:ILE:HD13 | 1.90                     | 0.54              |
| 1:K:72:ILE:HD12  | 1:K:72:ILE:H     | 1.72                     | 0.54              |
| 1:A:110:ILE:HG23 | 1:A:167:MET:HE1  | 1.89                     | 0.53              |
| 1:B:164:ILE:HG21 | 1:C:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:E:164:ILE:HG21 | 1:F:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:G:164:ILE:HG21 | 1:H:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:G:170:GLN:HG2  | 1:I:164:ILE:HG21 | 1.90                     | 0.53              |
| 1:J:164:ILE:HG21 | 1:K:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:M:79:VAL:HG11  | 1:M:85:HIS:HE2   | 1.71                     | 0.53              |
| 1:N:72:ILE:H     | 1:N:72:ILE:HD12  | 1.72                     | 0.53              |
| 1:A:12:THR:HG21  | 1:B:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:B:12:THR:HG21  | 1:C:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:B:146:VAL:HG22 | 1:B:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:D:12:THR:HG21  | 1:E:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:E:79:VAL:HG11  | 1:E:85:HIS:HE2   | 1.72                     | 0.53              |
| 1:F:146:VAL:HG22 | 1:F:164:ILE:HD13 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:12:THR:HG21  | 1:Q:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:P:146:VAL:HG22 | 1:P:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:Q:164:ILE:HG21 | 1:R:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:R:144:SER:HB2  | 1:R:164:ILE:CD1  | 2.37                     | 0.53              |
| 1:B:18:ALA:CB    | 1:B:23:ILE:HD11  | 2.27                     | 0.53              |
| 1:K:79:VAL:HG11  | 1:K:85:HIS:HE2   | 1.71                     | 0.53              |
| 1:N:146:VAL:HG22 | 1:N:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:R:20:THR:O     | 1:R:21:GLY:C     | 2.46                     | 0.53              |
| 1:F:72:ILE:H     | 1:F:72:ILE:HD12  | 1.72                     | 0.53              |
| 1:G:146:VAL:HG22 | 1:G:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:P:111:ASN:HD22 | 1:P:143:TYR:H    | 1.55                     | 0.53              |
| 1:A:20:THR:O     | 1:A:21:GLY:C     | 2.46                     | 0.53              |
| 1:A:111:ASN:HD22 | 1:A:143:TYR:H    | 1.55                     | 0.53              |
| 1:D:170:GLN:HG2  | 1:F:164:ILE:HG21 | 1.90                     | 0.53              |
| 1:E:14:GLU:HA    | 1:E:17:ASN:ND2   | 2.21                     | 0.53              |
| 1:K:144:SER:HB2  | 1:K:164:ILE:CD1  | 2.37                     | 0.53              |
| 1:M:233:SER:HA   | 2:M:313:EPE:H81  | 1.88                     | 0.53              |
| 1:N:111:ASN:HD22 | 1:N:143:TYR:H    | 1.55                     | 0.53              |
| 1:Q:20:THR:O     | 1:Q:21:GLY:C     | 2.46                     | 0.53              |
| 1:J:12:THR:HG21  | 1:K:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:K:12:THR:HG21  | 1:L:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:K:17:ASN:HD22  | 1:K:17:ASN:N     | 1.96                     | 0.53              |
| 1:L:210:ASP:OD2  | 1:L:212:ARG:HD3  | 2.07                     | 0.53              |
| 1:N:164:ILE:HG21 | 1:O:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:A:146:VAL:HG22 | 1:A:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:D:39:TYR:CE2   | 1:F:7:LYS:HB2    | 2.44                     | 0.53              |
| 1:G:29:ASN:OD1   | 1:I:12:THR:HG21  | 2.08                     | 0.53              |
| 1:M:12:THR:HG21  | 1:N:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:M:146:VAL:HG22 | 1:M:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:M:164:ILE:HG21 | 1:N:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:N:12:THR:HG21  | 1:O:29:ASN:OD1   | 2.08                     | 0.53              |
| 1:R:146:VAL:HG22 | 1:R:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:D:164:ILE:HG21 | 1:E:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:E:14:GLU:HB3   | 1:E:17:ASN:HD21  | 1.74                     | 0.53              |
| 1:J:29:ASN:OD1   | 1:L:12:THR:HG21  | 2.08                     | 0.53              |
| 1:J:242:ASN:HD22 | 1:J:242:ASN:N    | 1.85                     | 0.53              |
| 1:O:146:VAL:HG22 | 1:O:164:ILE:HD13 | 1.90                     | 0.53              |
| 1:P:170:GLN:HG2  | 1:R:164:ILE:HG21 | 1.90                     | 0.53              |
| 1:A:170:GLN:HG2  | 1:C:164:ILE:HG21 | 1.91                     | 0.53              |
| 1:B:14:GLU:HB3   | 1:B:17:ASN:HD21  | 1.74                     | 0.53              |
| 1:C:111:ASN:HD21 | 1:C:116:ILE:H    | 1.57                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:7:LYS:HB2    | 1:H:39:TYR:CE2   | 2.44                     | 0.53              |
| 1:I:20:THR:O     | 1:I:21:GLY:C     | 2.46                     | 0.53              |
| 1:K:164:ILE:HG21 | 1:L:170:GLN:HG2  | 1.91                     | 0.53              |
| 1:L:18:ALA:CB    | 1:L:23:ILE:HD11  | 2.27                     | 0.53              |
| 1:N:14:GLU:HB3   | 1:N:17:ASN:HD21  | 1.74                     | 0.53              |
| 1:P:20:THR:O     | 1:P:21:GLY:C     | 2.46                     | 0.53              |
| 1:D:17:ASN:ND2   | 1:D:17:ASN:H     | 2.05                     | 0.53              |
| 1:H:144:SER:HB2  | 1:H:164:ILE:CD1  | 2.37                     | 0.53              |
| 1:J:7:LYS:HB2    | 1:K:39:TYR:CE2   | 2.44                     | 0.53              |
| 1:K:7:LYS:HB2    | 1:L:39:TYR:CE2   | 2.45                     | 0.53              |
| 1:M:111:ASN:HD21 | 1:M:116:ILE:H    | 1.57                     | 0.53              |
| 1:A:7:LYS:HB2    | 1:B:39:TYR:CE2   | 2.44                     | 0.52              |
| 1:J:111:ASN:HD21 | 1:J:116:ILE:H    | 1.57                     | 0.52              |
| 1:K:14:GLU:HB3   | 1:K:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:L:146:VAL:HG22 | 1:L:164:ILE:HD13 | 1.90                     | 0.52              |
| 1:P:18:ALA:CB    | 1:P:23:ILE:HD11  | 2.27                     | 0.52              |
| 1:Q:146:VAL:HG22 | 1:Q:164:ILE:HD13 | 1.90                     | 0.52              |
| 1:A:39:TYR:CE2   | 1:C:7:LYS:HB2    | 2.44                     | 0.52              |
| 1:H:111:ASN:HD21 | 1:H:116:ILE:H    | 1.57                     | 0.52              |
| 1:J:153:SER:HA   | 1:J:157:THR:O    | 2.10                     | 0.52              |
| 1:N:7:LYS:HB2    | 1:O:39:TYR:CE2   | 2.44                     | 0.52              |
| 1:N:20:THR:O     | 1:N:21:GLY:C     | 2.46                     | 0.52              |
| 1:R:17:ASN:ND2   | 1:R:17:ASN:H     | 2.05                     | 0.52              |
| 1:R:111:ASN:HD21 | 1:R:116:ILE:H    | 1.57                     | 0.52              |
| 1:R:153:SER:HA   | 1:R:157:THR:O    | 2.10                     | 0.52              |
| 1:G:39:TYR:CE2   | 1:I:7:LYS:HB2    | 2.44                     | 0.52              |
| 1:H:14:GLU:HB3   | 1:H:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:H:164:ILE:HG21 | 1:I:170:GLN:HG2  | 1.91                     | 0.52              |
| 1:N:111:ASN:HD21 | 1:N:116:ILE:H    | 1.57                     | 0.52              |
| 1:O:153:SER:HA   | 1:O:157:THR:O    | 2.10                     | 0.52              |
| 1:Q:12:THR:HG21  | 1:R:29:ASN:OD1   | 2.08                     | 0.52              |
| 1:Q:111:ASN:HD21 | 1:Q:116:ILE:H    | 1.57                     | 0.52              |
| 1:C:14:GLU:HB3   | 1:C:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:C:20:THR:O     | 1:C:21:GLY:C     | 2.46                     | 0.52              |
| 1:D:7:LYS:HB2    | 1:E:39:TYR:CE2   | 2.44                     | 0.52              |
| 1:I:146:VAL:HG22 | 1:I:164:ILE:HD13 | 1.90                     | 0.52              |
| 1:K:17:ASN:ND2   | 1:K:17:ASN:H     | 2.05                     | 0.52              |
| 1:M:14:GLU:HB3   | 1:M:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:M:20:THR:O     | 1:M:21:GLY:C     | 2.46                     | 0.52              |
| 1:N:153:SER:HA   | 1:N:157:THR:O    | 2.10                     | 0.52              |
| 1:D:146:VAL:HG22 | 1:D:164:ILE:HD13 | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:20:THR:O     | 1:E:21:GLY:C     | 2.46                     | 0.52              |
| 1:E:146:VAL:HG22 | 1:E:164:ILE:HD13 | 1.90                     | 0.52              |
| 1:K:110:ILE:HG23 | 1:K:167:MET:HE1  | 1.91                     | 0.52              |
| 1:O:244:THR:C    | 1:O:246:GLU:H    | 2.13                     | 0.52              |
| 1:R:14:GLU:HB3   | 1:R:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:E:18:ALA:CB    | 1:E:23:ILE:HD11  | 2.27                     | 0.52              |
| 1:E:144:SER:HB2  | 1:E:164:ILE:CD1  | 2.37                     | 0.52              |
| 1:G:153:SER:HA   | 1:G:157:THR:O    | 2.10                     | 0.52              |
| 1:H:7:LYS:HB2    | 1:I:39:TYR:CE2   | 2.44                     | 0.52              |
| 1:H:153:SER:HA   | 1:H:157:THR:O    | 2.10                     | 0.52              |
| 1:I:14:GLU:HB3   | 1:I:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:J:14:GLU:HB3   | 1:J:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:M:170:GLN:HG2  | 1:O:164:ILE:HG21 | 1.90                     | 0.52              |
| 1:P:164:ILE:HG21 | 1:Q:170:GLN:HG2  | 1.91                     | 0.52              |
| 1:Q:153:SER:HA   | 1:Q:157:THR:O    | 2.10                     | 0.52              |
| 1:A:111:ASN:HD21 | 1:A:116:ILE:H    | 1.57                     | 0.52              |
| 1:E:111:ASN:HD21 | 1:E:116:ILE:H    | 1.57                     | 0.52              |
| 1:G:18:ALA:CB    | 1:G:23:ILE:HD11  | 2.27                     | 0.52              |
| 1:H:17:ASN:ND2   | 1:H:17:ASN:H     | 2.05                     | 0.52              |
| 1:I:17:ASN:ND2   | 1:I:17:ASN:H     | 2.05                     | 0.52              |
| 1:G:244:THR:C    | 1:G:246:GLU:H    | 2.13                     | 0.52              |
| 1:J:20:THR:O     | 1:J:21:GLY:C     | 2.46                     | 0.52              |
| 1:M:17:ASN:HD22  | 1:M:17:ASN:N     | 1.96                     | 0.52              |
| 1:M:153:SER:HA   | 1:M:157:THR:O    | 2.10                     | 0.52              |
| 1:A:164:ILE:HG21 | 1:B:170:GLN:HG2  | 1.91                     | 0.52              |
| 1:E:153:SER:HA   | 1:E:157:THR:O    | 2.10                     | 0.52              |
| 1:J:146:VAL:HG22 | 1:J:164:ILE:HD13 | 1.90                     | 0.52              |
| 1:M:7:LYS:HB2    | 1:N:39:TYR:CE2   | 2.44                     | 0.52              |
| 1:P:14:GLU:HB3   | 1:P:17:ASN:HD21  | 1.74                     | 0.52              |
| 1:R:244:THR:C    | 1:R:246:GLU:H    | 2.13                     | 0.52              |
| 1:D:111:ASN:HD21 | 1:D:116:ILE:H    | 1.57                     | 0.52              |
| 1:D:153:SER:HA   | 1:D:157:THR:O    | 2.10                     | 0.52              |
| 1:G:17:ASN:ND2   | 1:G:17:ASN:H     | 2.05                     | 0.52              |
| 1:G:17:ASN:HD22  | 1:G:17:ASN:N     | 1.96                     | 0.52              |
| 1:L:111:ASN:HD21 | 1:L:116:ILE:H    | 1.57                     | 0.52              |
| 1:N:144:SER:HB2  | 1:N:164:ILE:CD1  | 2.37                     | 0.52              |
| 1:O:79:VAL:HG11  | 1:O:85:HIS:NE2   | 2.25                     | 0.52              |
| 1:P:39:TYR:CE2   | 1:R:7:LYS:HB2    | 2.44                     | 0.52              |
| 1:C:79:VAL:HG11  | 1:C:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:F:111:ASN:HD21 | 1:F:116:ILE:H    | 1.57                     | 0.51              |
| 1:G:79:VAL:HG11  | 1:G:85:HIS:NE2   | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:39:TYR:CE2   | 1:L:7:LYS:HB2    | 2.44                     | 0.51              |
| 1:J:170:GLN:HG2  | 1:L:164:ILE:HG21 | 1.91                     | 0.51              |
| 1:J:244:THR:C    | 1:J:246:GLU:H    | 2.13                     | 0.51              |
| 1:K:79:VAL:HG11  | 1:K:85:HIS:NE2   | 2.26                     | 0.51              |
| 1:O:111:ASN:HD21 | 1:O:116:ILE:H    | 1.57                     | 0.51              |
| 1:P:7:LYS:HB2    | 1:Q:39:TYR:CE2   | 2.44                     | 0.51              |
| 1:R:79:VAL:HG11  | 1:R:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:A:14:GLU:HB3   | 1:A:17:ASN:HD21  | 1.74                     | 0.51              |
| 1:I:153:SER:HA   | 1:I:157:THR:O    | 2.10                     | 0.51              |
| 1:J:17:ASN:ND2   | 1:J:17:ASN:H     | 2.05                     | 0.51              |
| 1:L:79:VAL:HG11  | 1:L:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:L:244:THR:C    | 1:L:246:GLU:H    | 2.13                     | 0.51              |
| 1:N:79:VAL:HG11  | 1:N:85:HIS:NE2   | 2.26                     | 0.51              |
| 1:O:14:GLU:HB3   | 1:O:17:ASN:HD21  | 1.74                     | 0.51              |
| 1:P:79:VAL:HG11  | 1:P:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:G:111:ASN:HD21 | 1:G:116:ILE:H    | 1.57                     | 0.51              |
| 1:H:79:VAL:HG11  | 1:H:85:HIS:NE2   | 2.26                     | 0.51              |
| 1:I:111:ASN:HD21 | 1:I:116:ILE:H    | 1.57                     | 0.51              |
| 1:K:111:ASN:HD21 | 1:K:116:ILE:H    | 1.57                     | 0.51              |
| 1:M:39:TYR:CE2   | 1:O:7:LYS:HB2    | 2.44                     | 0.51              |
| 1:N:284:ILE:HD13 | 1:O:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:P:111:ASN:HD21 | 1:P:116:ILE:H    | 1.57                     | 0.51              |
| 1:Q:7:LYS:HB2    | 1:R:39:TYR:CE2   | 2.45                     | 0.51              |
| 1:Q:14:GLU:HB3   | 1:Q:17:ASN:HD21  | 1.74                     | 0.51              |
| 1:A:79:VAL:HG11  | 1:A:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:A:244:THR:C    | 1:A:246:GLU:H    | 2.13                     | 0.51              |
| 1:C:153:SER:HA   | 1:C:157:THR:O    | 2.10                     | 0.51              |
| 1:D:14:GLU:HB3   | 1:D:17:ASN:HD21  | 1.74                     | 0.51              |
| 1:H:284:ILE:HD13 | 1:I:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:K:153:SER:HA   | 1:K:157:THR:O    | 2.10                     | 0.51              |
| 1:M:18:ALA:CB    | 1:M:23:ILE:HD11  | 2.27                     | 0.51              |
| 1:Q:79:VAL:HG11  | 1:Q:85:HIS:NE2   | 2.26                     | 0.51              |
| 1:B:111:ASN:HD21 | 1:B:116:ILE:H    | 1.57                     | 0.51              |
| 1:E:244:THR:C    | 1:E:246:GLU:H    | 2.13                     | 0.51              |
| 1:F:244:THR:C    | 1:F:246:GLU:H    | 2.13                     | 0.51              |
| 1:G:242:ASN:ND2  | 1:G:242:ASN:N    | 2.45                     | 0.51              |
| 1:J:79:VAL:HG11  | 1:J:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:J:178:THR:O    | 1:L:287:ALA:HA   | 2.11                     | 0.51              |
| 1:L:153:SER:HA   | 1:L:157:THR:O    | 2.10                     | 0.51              |
| 1:N:244:THR:C    | 1:N:246:GLU:H    | 2.13                     | 0.51              |
| 1:A:178:THR:O    | 1:C:287:ALA:HA   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:287:ALA:HA   | 1:B:178:THR:O    | 2.11                     | 0.51              |
| 1:B:7:LYS:HB2    | 1:C:39:TYR:CE2   | 2.45                     | 0.51              |
| 1:C:17:ASN:HD22  | 1:C:17:ASN:N     | 1.96                     | 0.51              |
| 1:E:287:ALA:HA   | 1:F:178:THR:O    | 2.11                     | 0.51              |
| 1:H:244:THR:C    | 1:H:246:GLU:H    | 2.13                     | 0.51              |
| 1:L:17:ASN:ND2   | 1:L:17:ASN:H     | 2.05                     | 0.51              |
| 1:P:178:THR:O    | 1:R:287:ALA:HA   | 2.11                     | 0.51              |
| 1:P:244:THR:C    | 1:P:246:GLU:H    | 2.13                     | 0.51              |
| 1:F:110:ILE:HG23 | 1:F:167:MET:HE1  | 1.92                     | 0.51              |
| 1:F:153:SER:HA   | 1:F:157:THR:O    | 2.10                     | 0.51              |
| 1:G:14:GLU:HB3   | 1:G:17:ASN:HD21  | 1.74                     | 0.51              |
| 1:M:207:GLN:HB3  | 1:O:284:ILE:HD13 | 1.93                     | 0.51              |
| 1:P:153:SER:HA   | 1:P:157:THR:O    | 2.10                     | 0.51              |
| 1:Q:284:ILE:HD13 | 1:R:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:B:153:SER:HA   | 1:B:157:THR:O    | 2.10                     | 0.51              |
| 1:D:178:THR:O    | 1:F:287:ALA:HA   | 2.11                     | 0.51              |
| 1:E:7:LYS:HB2    | 1:F:39:TYR:CE2   | 2.44                     | 0.51              |
| 1:E:230:VAL:HG11 | 1:E:254:PHE:HB3  | 1.93                     | 0.51              |
| 1:H:18:ALA:CB    | 1:H:23:ILE:HD11  | 2.27                     | 0.51              |
| 1:H:287:ALA:HA   | 1:I:178:THR:O    | 2.11                     | 0.51              |
| 1:K:244:THR:C    | 1:K:246:GLU:H    | 2.13                     | 0.51              |
| 1:K:284:ILE:HD13 | 1:L:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:L:14:GLU:HB3   | 1:L:17:ASN:HD21  | 1.74                     | 0.51              |
| 1:O:230:VAL:HG11 | 1:O:254:PHE:HB3  | 1.93                     | 0.51              |
| 1:A:284:ILE:HD13 | 1:B:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:B:244:THR:C    | 1:B:246:GLU:H    | 2.13                     | 0.51              |
| 1:B:284:ILE:HD13 | 1:C:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:B:287:ALA:HA   | 1:C:178:THR:O    | 2.11                     | 0.51              |
| 1:C:17:ASN:ND2   | 1:C:17:ASN:H     | 2.05                     | 0.51              |
| 1:D:79:VAL:HG11  | 1:D:85:HIS:NE2   | 2.25                     | 0.51              |
| 1:E:284:ILE:HD13 | 1:F:207:GLN:HB3  | 1.93                     | 0.51              |
| 1:M:17:ASN:ND2   | 1:M:17:ASN:H     | 2.05                     | 0.51              |
| 1:N:17:ASN:ND2   | 1:N:17:ASN:H     | 2.05                     | 0.51              |
| 1:O:17:ASN:HD22  | 1:O:17:ASN:N     | 1.96                     | 0.51              |
| 1:O:72:ILE:HD12  | 1:O:72:ILE:N     | 2.26                     | 0.51              |
| 1:D:244:THR:C    | 1:D:246:GLU:H    | 2.13                     | 0.51              |
| 1:G:20:THR:O     | 1:G:21:GLY:C     | 2.46                     | 0.51              |
| 1:K:18:ALA:CB    | 1:K:23:ILE:HD11  | 2.27                     | 0.51              |
| 1:M:287:ALA:HA   | 1:N:178:THR:O    | 2.11                     | 0.51              |
| 1:A:18:ALA:CB    | 1:A:23:ILE:HD11  | 2.27                     | 0.50              |
| 1:E:79:VAL:HG11  | 1:E:85:HIS:NE2   | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:14:GLU:HB3   | 1:F:17:ASN:HD21  | 1.74                     | 0.50              |
| 1:F:157:THR:O    | 1:F:157:THR:OG1  | 2.29                     | 0.50              |
| 1:K:287:ALA:HA   | 1:L:178:THR:O    | 2.11                     | 0.50              |
| 1:L:72:ILE:HD12  | 1:L:72:ILE:N     | 2.26                     | 0.50              |
| 1:M:79:VAL:HG11  | 1:M:85:HIS:NE2   | 2.25                     | 0.50              |
| 1:P:287:ALA:HA   | 1:Q:178:THR:O    | 2.11                     | 0.50              |
| 1:R:120:ASN:N    | 1:R:120:ASN:ND2  | 2.59                     | 0.50              |
| 1:B:230:VAL:HG11 | 1:B:254:PHE:HB3  | 1.93                     | 0.50              |
| 1:J:207:GLN:HB3  | 1:L:284:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:153:SER:HA   | 1:A:157:THR:O    | 2.10                     | 0.50              |
| 1:A:153:SER:O    | 1:A:155:ASN:N    | 2.45                     | 0.50              |
| 1:B:72:ILE:HD12  | 1:B:72:ILE:N     | 2.26                     | 0.50              |
| 1:D:153:SER:O    | 1:D:155:ASN:N    | 2.45                     | 0.50              |
| 1:D:287:ALA:HA   | 1:E:178:THR:O    | 2.11                     | 0.50              |
| 1:F:79:VAL:HG11  | 1:F:85:HIS:NE2   | 2.25                     | 0.50              |
| 1:K:153:SER:O    | 1:K:155:ASN:N    | 2.45                     | 0.50              |
| 1:L:20:THR:O     | 1:L:21:GLY:C     | 2.46                     | 0.50              |
| 1:L:110:ILE:HG23 | 1:L:167:MET:HE1  | 1.92                     | 0.50              |
| 1:M:244:THR:C    | 1:M:246:GLU:H    | 2.13                     | 0.50              |
| 1:P:120:ASN:N    | 1:P:120:ASN:ND2  | 2.59                     | 0.50              |
| 1:E:17:ASN:ND2   | 1:E:17:ASN:H     | 2.05                     | 0.50              |
| 1:G:178:THR:O    | 1:I:287:ALA:HA   | 2.11                     | 0.50              |
| 1:I:79:VAL:HG11  | 1:I:85:HIS:NE2   | 2.25                     | 0.50              |
| 1:J:153:SER:O    | 1:J:155:ASN:N    | 2.45                     | 0.50              |
| 1:K:157:THR:O    | 1:K:157:THR:OG1  | 2.29                     | 0.50              |
| 1:N:153:SER:O    | 1:N:155:ASN:N    | 2.45                     | 0.50              |
| 1:N:230:VAL:HG11 | 1:N:254:PHE:HB3  | 1.93                     | 0.50              |
| 1:P:207:GLN:HB3  | 1:R:284:ILE:HD13 | 1.93                     | 0.50              |
| 1:P:242:ASN:ND2  | 1:P:242:ASN:N    | 2.45                     | 0.50              |
| 1:P:284:ILE:HD13 | 1:Q:207:GLN:HB3  | 1.93                     | 0.50              |
| 1:R:17:ASN:HD22  | 1:R:17:ASN:N     | 1.96                     | 0.50              |
| 1:B:79:VAL:HG11  | 1:B:85:HIS:NE2   | 2.26                     | 0.50              |
| 1:D:242:ASN:ND2  | 1:D:242:ASN:N    | 2.45                     | 0.50              |
| 1:E:72:ILE:HD12  | 1:E:72:ILE:N     | 2.26                     | 0.50              |
| 1:E:120:ASN:N    | 1:E:120:ASN:ND2  | 2.59                     | 0.50              |
| 1:G:284:ILE:HD13 | 1:H:207:GLN:HB3  | 1.93                     | 0.50              |
| 1:J:72:ILE:HD12  | 1:J:72:ILE:N     | 2.26                     | 0.50              |
| 1:P:230:VAL:HG11 | 1:P:254:PHE:HB3  | 1.93                     | 0.50              |
| 1:Q:244:THR:C    | 1:Q:246:GLU:H    | 2.13                     | 0.50              |
| 1:R:242:ASN:ND2  | 1:R:242:ASN:N    | 2.45                     | 0.50              |
| 1:G:153:SER:O    | 1:G:155:ASN:N    | 2.45                     | 0.50              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:230:VAL:HG11 | 1:G:254:PHE:HB3 | 1.93                     | 0.50              |
| 1:J:242:ASN:ND2  | 1:J:242:ASN:N   | 2.45                     | 0.50              |
| 1:J:287:ALA:HA   | 1:K:178:THR:O   | 2.11                     | 0.50              |
| 1:L:153:SER:O    | 1:L:155:ASN:N   | 2.45                     | 0.50              |
| 1:Q:287:ALA:HA   | 1:R:178:THR:O   | 2.11                     | 0.50              |
| 1:D:157:THR:O    | 1:D:157:THR:OG1 | 2.29                     | 0.50              |
| 1:G:287:ALA:HA   | 1:H:178:THR:O   | 2.11                     | 0.50              |
| 1:J:17:ASN:ND2   | 1:J:17:ASN:N    | 2.60                     | 0.50              |
| 1:K:72:ILE:HD12  | 1:K:72:ILE:N    | 2.26                     | 0.50              |
| 1:M:17:ASN:ND2   | 1:M:17:ASN:N    | 2.60                     | 0.50              |
| 1:M:178:THR:O    | 1:O:287:ALA:HA  | 2.11                     | 0.50              |
| 1:P:17:ASN:ND2   | 1:P:17:ASN:N    | 2.60                     | 0.50              |
| 1:Q:17:ASN:ND2   | 1:Q:17:ASN:N    | 2.60                     | 0.50              |
| 1:C:153:SER:O    | 1:C:155:ASN:N   | 2.45                     | 0.50              |
| 1:C:230:VAL:HG11 | 1:C:254:PHE:HB3 | 1.93                     | 0.50              |
| 1:C:244:THR:C    | 1:C:246:GLU:H   | 2.13                     | 0.50              |
| 1:G:17:ASN:ND2   | 1:G:17:ASN:N    | 2.60                     | 0.50              |
| 1:I:244:THR:C    | 1:I:246:GLU:H   | 2.13                     | 0.50              |
| 1:J:157:THR:O    | 1:J:157:THR:OG1 | 2.29                     | 0.50              |
| 1:O:157:THR:O    | 1:O:157:THR:OG1 | 2.29                     | 0.50              |
| 1:Q:72:ILE:HD12  | 1:Q:72:ILE:N    | 2.26                     | 0.50              |
| 1:C:120:ASN:N    | 1:C:120:ASN:ND2 | 2.59                     | 0.50              |
| 1:H:230:VAL:HG11 | 1:H:254:PHE:HB3 | 1.93                     | 0.50              |
| 1:L:230:VAL:HG11 | 1:L:254:PHE:HB3 | 1.93                     | 0.50              |
| 1:N:287:ALA:HA   | 1:O:178:THR:O   | 2.11                     | 0.50              |
| 1:B:17:ASN:ND2   | 1:B:17:ASN:N    | 2.60                     | 0.49              |
| 1:B:153:SER:O    | 1:B:155:ASN:N   | 2.45                     | 0.49              |
| 1:D:17:ASN:HD22  | 1:D:17:ASN:N    | 1.96                     | 0.49              |
| 1:D:230:VAL:HG11 | 1:D:254:PHE:HB3 | 1.93                     | 0.49              |
| 1:G:72:ILE:HD12  | 1:G:72:ILE:N    | 2.26                     | 0.49              |
| 1:H:153:SER:O    | 1:H:155:ASN:N   | 2.45                     | 0.49              |
| 1:J:120:ASN:N    | 1:J:120:ASN:ND2 | 2.59                     | 0.49              |
| 1:J:284:ILE:HD13 | 1:K:207:GLN:HB3 | 1.93                     | 0.49              |
| 1:N:72:ILE:HD12  | 1:N:72:ILE:N    | 2.26                     | 0.49              |
| 1:Q:153:SER:O    | 1:Q:155:ASN:N   | 2.45                     | 0.49              |
| 1:R:17:ASN:ND2   | 1:R:17:ASN:N    | 2.60                     | 0.49              |
| 1:R:230:VAL:HG11 | 1:R:254:PHE:HB3 | 1.93                     | 0.49              |
| 1:C:72:ILE:HD12  | 1:C:72:ILE:N    | 2.26                     | 0.49              |
| 1:D:72:ILE:HD12  | 1:D:72:ILE:N    | 2.26                     | 0.49              |
| 1:D:284:ILE:HD13 | 1:E:207:GLN:HB3 | 1.93                     | 0.49              |
| 1:E:110:ILE:HG23 | 1:E:167:MET:HE1 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:17:ASN:ND2   | 1:O:17:ASN:N     | 2.60                     | 0.49              |
| 1:P:157:THR:O    | 1:P:157:THR:OG1  | 2.29                     | 0.49              |
| 1:R:153:SER:O    | 1:R:155:ASN:N    | 2.45                     | 0.49              |
| 1:F:230:VAL:HG11 | 1:F:254:PHE:HB3  | 1.93                     | 0.49              |
| 1:H:157:THR:O    | 1:H:157:THR:OG1  | 2.29                     | 0.49              |
| 1:I:153:SER:O    | 1:I:155:ASN:N    | 2.45                     | 0.49              |
| 1:K:230:VAL:HG11 | 1:K:254:PHE:HB3  | 1.93                     | 0.49              |
| 1:L:120:ASN:N    | 1:L:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:M:153:SER:O    | 1:M:155:ASN:N    | 2.45                     | 0.49              |
| 1:P:153:SER:O    | 1:P:155:ASN:N    | 2.45                     | 0.49              |
| 1:Q:120:ASN:N    | 1:Q:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:Q:230:VAL:HG11 | 1:Q:254:PHE:HB3  | 1.93                     | 0.49              |
| 1:A:72:ILE:HD12  | 1:A:72:ILE:N     | 2.26                     | 0.49              |
| 1:A:120:ASN:N    | 1:A:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:A:230:VAL:HG11 | 1:A:254:PHE:HB3  | 1.93                     | 0.49              |
| 1:E:153:SER:O    | 1:E:155:ASN:N    | 2.45                     | 0.49              |
| 1:F:72:ILE:HD12  | 1:F:72:ILE:N     | 2.26                     | 0.49              |
| 1:G:207:GLN:HB3  | 1:I:284:ILE:HD13 | 1.93                     | 0.49              |
| 1:O:120:ASN:N    | 1:O:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:O:153:SER:O    | 1:O:155:ASN:N    | 2.45                     | 0.49              |
| 1:I:230:VAL:HG11 | 1:I:254:PHE:HB3  | 1.93                     | 0.49              |
| 1:M:284:ILE:HD13 | 1:N:207:GLN:HB3  | 1.93                     | 0.49              |
| 1:N:120:ASN:N    | 1:N:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:P:110:ILE:HG23 | 1:P:167:MET:HE1  | 1.93                     | 0.49              |
| 1:A:207:GLN:HB3  | 1:C:284:ILE:HD13 | 1.93                     | 0.49              |
| 1:E:7:LYS:HB2    | 1:F:39:TYR:CD2   | 2.48                     | 0.49              |
| 1:H:120:ASN:N    | 1:H:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:K:120:ASN:N    | 1:K:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:L:157:THR:O    | 1:L:157:THR:OG1  | 2.29                     | 0.49              |
| 1:P:72:ILE:HD12  | 1:P:72:ILE:N     | 2.26                     | 0.49              |
| 1:Q:17:ASN:ND2   | 1:Q:17:ASN:H     | 2.05                     | 0.49              |
| 1:A:17:ASN:ND2   | 1:A:17:ASN:N     | 2.60                     | 0.49              |
| 1:B:7:LYS:HB2    | 1:C:39:TYR:CD2   | 2.48                     | 0.49              |
| 1:B:120:ASN:N    | 1:B:120:ASN:ND2  | 2.59                     | 0.49              |
| 1:F:153:SER:O    | 1:F:155:ASN:N    | 2.45                     | 0.49              |
| 1:I:14:GLU:HA    | 1:I:17:ASN:CG    | 2.33                     | 0.49              |
| 1:M:72:ILE:HD12  | 1:M:72:ILE:N     | 2.26                     | 0.49              |
| 1:M:230:VAL:HG11 | 1:M:254:PHE:HB3  | 1.93                     | 0.49              |
| 1:C:18:ALA:CB    | 1:C:23:ILE:CD1   | 2.90                     | 0.49              |
| 1:E:17:ASN:ND2   | 1:E:17:ASN:N     | 2.60                     | 0.49              |
| 1:G:7:LYS:HB2    | 1:H:39:TYR:CD2   | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:7:LYS:HB2    | 1:I:39:TYR:CD2   | 2.48                     | 0.49              |
| 1:H:72:ILE:HD12  | 1:H:72:ILE:N     | 2.26                     | 0.49              |
| 1:B:17:ASN:ND2   | 1:B:17:ASN:H     | 2.05                     | 0.49              |
| 1:D:7:LYS:HB2    | 1:E:39:TYR:CD2   | 2.48                     | 0.49              |
| 1:I:72:ILE:HD12  | 1:I:72:ILE:N     | 2.26                     | 0.49              |
| 1:J:31:ILE:HD11  | 1:K:31:ILE:HD13  | 1.95                     | 0.49              |
| 1:L:14:GLU:HA    | 1:L:17:ASN:CG    | 2.33                     | 0.49              |
| 1:R:72:ILE:HD12  | 1:R:72:ILE:N     | 2.26                     | 0.49              |
| 1:R:157:THR:O    | 1:R:157:THR:OG1  | 2.29                     | 0.49              |
| 1:D:18:ALA:CB    | 1:D:23:ILE:HD11  | 2.27                     | 0.49              |
| 1:F:17:ASN:ND2   | 1:F:17:ASN:N     | 2.60                     | 0.49              |
| 1:M:157:THR:O    | 1:M:157:THR:OG1  | 2.29                     | 0.49              |
| 1:Q:31:ILE:HD11  | 1:R:31:ILE:HD13  | 1.95                     | 0.49              |
| 1:A:39:TYR:CD2   | 1:C:7:LYS:HB2    | 2.48                     | 0.48              |
| 1:A:157:THR:O    | 1:A:157:THR:OG1  | 2.29                     | 0.48              |
| 1:B:31:ILE:HD11  | 1:C:31:ILE:HD13  | 1.95                     | 0.48              |
| 1:D:207:GLN:HB3  | 1:F:284:ILE:HD13 | 1.93                     | 0.48              |
| 1:F:14:GLU:HA    | 1:F:17:ASN:CG    | 2.33                     | 0.48              |
| 1:K:17:ASN:ND2   | 1:K:17:ASN:N     | 2.60                     | 0.48              |
| 1:Q:7:LYS:HB2    | 1:R:39:TYR:CD2   | 2.48                     | 0.48              |
| 1:F:18:ALA:CB    | 1:F:23:ILE:CD1   | 2.90                     | 0.48              |
| 1:F:120:ASN:N    | 1:F:120:ASN:ND2  | 2.59                     | 0.48              |
| 1:G:14:GLU:HA    | 1:G:17:ASN:CG    | 2.33                     | 0.48              |
| 1:J:230:VAL:HG11 | 1:J:254:PHE:HB3  | 1.93                     | 0.48              |
| 1:K:31:ILE:HD11  | 1:L:31:ILE:HD13  | 1.95                     | 0.48              |
| 1:P:7:LYS:HB2    | 1:Q:39:TYR:CD2   | 2.48                     | 0.48              |
| 1:A:14:GLU:HA    | 1:A:17:ASN:CG    | 2.33                     | 0.48              |
| 1:G:31:ILE:HD13  | 1:I:31:ILE:HD11  | 1.95                     | 0.48              |
| 1:H:18:ALA:CB    | 1:H:23:ILE:CD1   | 2.90                     | 0.48              |
| 1:H:110:ILE:HG23 | 1:H:167:MET:HE1  | 1.96                     | 0.48              |
| 1:N:31:ILE:HD11  | 1:O:31:ILE:HD13  | 1.95                     | 0.48              |
| 1:P:14:GLU:HA    | 1:P:17:ASN:CG    | 2.33                     | 0.48              |
| 1:A:7:LYS:HB2    | 1:B:39:TYR:CD2   | 2.48                     | 0.48              |
| 1:A:18:ALA:CB    | 1:A:23:ILE:CD1   | 2.90                     | 0.48              |
| 1:D:39:TYR:CD2   | 1:F:7:LYS:HB2    | 2.48                     | 0.48              |
| 1:H:17:ASN:ND2   | 1:H:17:ASN:N     | 2.60                     | 0.48              |
| 1:K:7:LYS:HB2    | 1:L:39:TYR:CD2   | 2.48                     | 0.48              |
| 1:M:39:TYR:CD2   | 1:O:7:LYS:HB2    | 2.48                     | 0.48              |
| 1:O:14:GLU:HA    | 1:O:17:ASN:CG    | 2.33                     | 0.48              |
| 1:E:14:GLU:HA    | 1:E:17:ASN:CG    | 2.33                     | 0.48              |
| 1:H:14:GLU:HA    | 1:H:17:ASN:CG    | 2.33                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:J:31:ILE:HD13  | 1:L:31:ILE:HD11 | 1.95                     | 0.48              |
| 1:M:7:LYS:HB2    | 1:N:39:TYR:CD2  | 2.48                     | 0.48              |
| 1:M:31:ILE:HD11  | 1:N:31:ILE:HD13 | 1.95                     | 0.48              |
| 1:M:170:GLN:HG2  | 1:O:164:ILE:CG2 | 2.44                     | 0.48              |
| 1:P:31:ILE:HD11  | 1:Q:31:ILE:HD13 | 1.95                     | 0.48              |
| 1:C:14:GLU:HA    | 1:C:17:ASN:CG   | 2.33                     | 0.48              |
| 1:H:31:ILE:HD11  | 1:I:31:ILE:HD13 | 1.95                     | 0.48              |
| 1:J:39:TYR:CD2   | 1:L:7:LYS:HB2   | 2.48                     | 0.48              |
| 1:M:18:ALA:CB    | 1:M:23:ILE:CD1  | 2.90                     | 0.48              |
| 1:M:31:ILE:HD13  | 1:O:31:ILE:HD11 | 1.95                     | 0.48              |
| 1:P:17:ASN:ND2   | 1:P:17:ASN:H    | 2.05                     | 0.48              |
| 1:P:18:ALA:CB    | 1:P:23:ILE:CD1  | 2.90                     | 0.48              |
| 1:P:39:TYR:CD2   | 1:R:7:LYS:HB2   | 2.48                     | 0.48              |
| 1:R:14:GLU:HA    | 1:R:17:ASN:CG   | 2.33                     | 0.48              |
| 1:G:39:TYR:CD2   | 1:I:7:LYS:HB2   | 2.48                     | 0.48              |
| 1:J:14:GLU:HA    | 1:J:17:ASN:CG   | 2.33                     | 0.48              |
| 1:K:14:GLU:HA    | 1:K:17:ASN:CG   | 2.33                     | 0.48              |
| 1:M:164:ILE:CG2  | 1:N:170:GLN:HG2 | 2.44                     | 0.48              |
| 1:P:170:GLN:HG2  | 1:R:164:ILE:CG2 | 2.44                     | 0.48              |
| 1:A:31:ILE:HD13  | 1:C:31:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:14:GLU:HA    | 1:B:17:ASN:CG   | 2.33                     | 0.48              |
| 1:E:31:ILE:HD11  | 1:F:31:ILE:HD13 | 1.95                     | 0.48              |
| 1:I:17:ASN:ND2   | 1:I:17:ASN:N    | 2.60                     | 0.48              |
| 1:A:31:ILE:HD11  | 1:B:31:ILE:HD13 | 1.95                     | 0.48              |
| 1:D:14:GLU:HA    | 1:D:17:ASN:CG   | 2.33                     | 0.48              |
| 1:D:31:ILE:HD11  | 1:E:31:ILE:HD13 | 1.95                     | 0.48              |
| 1:D:164:ILE:CG2  | 1:E:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:H:164:ILE:CG2  | 1:I:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:I:120:ASN:N    | 1:I:120:ASN:ND2 | 2.59                     | 0.47              |
| 1:J:7:LYS:HB2    | 1:K:39:TYR:CD2  | 2.48                     | 0.47              |
| 1:Q:164:ILE:CG2  | 1:R:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:Q:242:ASN:ND2  | 1:Q:242:ASN:N   | 2.45                     | 0.47              |
| 1:J:164:ILE:CG2  | 1:K:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:K:110:ILE:HD13 | 1:K:110:ILE:HA  | 1.79                     | 0.47              |
| 1:K:164:ILE:CG2  | 1:L:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:N:14:GLU:HA    | 1:N:17:ASN:CG   | 2.33                     | 0.47              |
| 1:R:18:ALA:CB    | 1:R:23:ILE:CD1  | 2.90                     | 0.47              |
| 1:B:18:ALA:CB    | 1:B:23:ILE:CD1  | 2.90                     | 0.47              |
| 1:N:164:ILE:CG2  | 1:O:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:P:164:ILE:CG2  | 1:Q:170:GLN:HG2 | 2.44                     | 0.47              |
| 1:G:31:ILE:HD11  | 1:H:31:ILE:HD13 | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:170:GLN:HG2  | 1:L:164:ILE:CG2  | 2.44                     | 0.47              |
| 1:M:14:GLU:HA    | 1:M:17:ASN:CG    | 2.33                     | 0.47              |
| 1:N:7:LYS:HB2    | 1:O:39:TYR:CD2   | 2.48                     | 0.47              |
| 1:P:17:ASN:HD22  | 1:P:17:ASN:N     | 1.96                     | 0.47              |
| 1:Q:110:ILE:HD13 | 1:Q:110:ILE:HA   | 1.79                     | 0.47              |
| 1:A:164:ILE:CG2  | 1:B:170:GLN:HG2  | 2.44                     | 0.47              |
| 1:A:170:GLN:HG2  | 1:C:164:ILE:CG2  | 2.44                     | 0.47              |
| 1:I:18:ALA:CB    | 1:I:23:ILE:CD1   | 2.90                     | 0.47              |
| 1:B:157:THR:O    | 1:B:157:THR:OG1  | 2.29                     | 0.47              |
| 1:D:17:ASN:ND2   | 1:D:17:ASN:N     | 2.60                     | 0.47              |
| 1:D:31:ILE:HD13  | 1:F:31:ILE:HD11  | 1.95                     | 0.47              |
| 1:B:164:ILE:CG2  | 1:C:170:GLN:HG2  | 2.44                     | 0.47              |
| 1:E:164:ILE:CG2  | 1:F:170:GLN:HG2  | 2.44                     | 0.47              |
| 1:G:110:ILE:HD13 | 1:G:110:ILE:HA   | 1.79                     | 0.47              |
| 1:I:157:THR:O    | 1:I:157:THR:OG1  | 2.29                     | 0.47              |
| 1:N:17:ASN:ND2   | 1:N:17:ASN:N     | 2.60                     | 0.47              |
| 1:Q:14:GLU:HA    | 1:Q:17:ASN:CG    | 2.33                     | 0.47              |
| 1:G:164:ILE:CG2  | 1:H:170:GLN:HG2  | 2.44                     | 0.47              |
| 1:G:170:GLN:HG2  | 1:I:164:ILE:CG2  | 2.44                     | 0.47              |
| 1:M:287:ALA:O    | 1:M:288:GLN:HB2  | 2.15                     | 0.47              |
| 1:H:287:ALA:O    | 1:H:288:GLN:HB2  | 2.15                     | 0.47              |
| 1:N:18:ALA:CB    | 1:N:23:ILE:CD1   | 2.90                     | 0.47              |
| 1:D:120:ASN:N    | 1:D:120:ASN:ND2  | 2.59                     | 0.47              |
| 1:E:287:ALA:O    | 1:E:288:GLN:HB2  | 2.15                     | 0.47              |
| 1:F:287:ALA:O    | 1:F:288:GLN:HB2  | 2.15                     | 0.47              |
| 1:I:287:ALA:O    | 1:I:288:GLN:HB2  | 2.15                     | 0.47              |
| 1:K:287:ALA:O    | 1:K:288:GLN:HB2  | 2.15                     | 0.47              |
| 1:C:242:ASN:ND2  | 1:C:242:ASN:N    | 2.45                     | 0.46              |
| 1:K:18:ALA:CB    | 1:K:23:ILE:CD1   | 2.90                     | 0.46              |
| 1:P:31:ILE:HD13  | 1:R:31:ILE:HD11  | 1.95                     | 0.46              |
| 1:C:157:THR:O    | 1:C:157:THR:OG1  | 2.29                     | 0.46              |
| 1:P:287:ALA:O    | 1:P:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:D:287:ALA:O    | 1:D:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:L:287:ALA:O    | 1:L:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:Q:157:THR:O    | 1:Q:157:THR:OG1  | 2.29                     | 0.46              |
| 1:R:287:ALA:O    | 1:R:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:A:287:ALA:O    | 1:A:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:C:287:ALA:O    | 1:C:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:G:287:ALA:O    | 1:G:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:D:18:ALA:CB    | 1:D:23:ILE:CD1   | 2.90                     | 0.46              |
| 1:M:127:ILE:HA   | 1:M:127:ILE:HD13 | 1.82                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:170:GLN:HG2  | 1:F:164:ILE:CG2  | 2.44                     | 0.46              |
| 1:O:18:ALA:CB    | 1:O:23:ILE:CD1   | 2.90                     | 0.46              |
| 1:O:287:ALA:O    | 1:O:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:N:287:ALA:O    | 1:N:288:GLN:HB2  | 2.15                     | 0.46              |
| 1:O:17:ASN:ND2   | 1:O:17:ASN:H     | 2.05                     | 0.46              |
| 1:B:110:ILE:HG23 | 1:B:167:MET:HE1  | 1.98                     | 0.45              |
| 1:J:287:ALA:O    | 1:J:288:GLN:HB2  | 2.15                     | 0.45              |
| 1:L:18:ALA:CB    | 1:L:23:ILE:CD1   | 2.90                     | 0.45              |
| 1:E:157:THR:O    | 1:E:157:THR:OG1  | 2.29                     | 0.45              |
| 1:J:18:ALA:CB    | 1:J:23:ILE:CD1   | 2.90                     | 0.45              |
| 1:B:287:ALA:O    | 1:B:288:GLN:HB2  | 2.15                     | 0.45              |
| 1:F:17:ASN:ND2   | 1:F:17:ASN:H     | 2.05                     | 0.45              |
| 1:F:242:ASN:ND2  | 1:F:242:ASN:N    | 2.45                     | 0.45              |
| 1:Q:287:ALA:O    | 1:Q:288:GLN:HB2  | 2.15                     | 0.45              |
| 1:N:242:ASN:ND2  | 1:N:242:ASN:N    | 2.45                     | 0.45              |
| 1:P:110:ILE:HD13 | 1:P:110:ILE:HA   | 1.79                     | 0.45              |
| 1:A:202:LEU:N    | 1:A:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:C:230:VAL:HG13 | 1:C:230:VAL:O    | 2.17                     | 0.45              |
| 1:F:110:ILE:HD13 | 1:F:110:ILE:HA   | 1.79                     | 0.45              |
| 1:F:230:VAL:O    | 1:F:230:VAL:HG13 | 2.17                     | 0.45              |
| 1:K:230:VAL:HG13 | 1:K:230:VAL:O    | 2.17                     | 0.45              |
| 1:M:110:ILE:HD13 | 1:M:110:ILE:HA   | 1.79                     | 0.45              |
| 1:N:230:VAL:O    | 1:N:230:VAL:HG13 | 2.17                     | 0.45              |
| 1:R:230:VAL:HG13 | 1:R:230:VAL:O    | 2.17                     | 0.45              |
| 1:J:230:VAL:HG13 | 1:J:230:VAL:O    | 2.17                     | 0.45              |
| 1:P:202:LEU:N    | 1:P:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:B:202:LEU:N    | 1:B:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:C:17:ASN:ND2   | 1:C:17:ASN:N     | 2.60                     | 0.45              |
| 1:D:202:LEU:N    | 1:D:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:H:110:ILE:HD12 | 1:H:167:MET:CE   | 2.47                     | 0.45              |
| 1:J:222:LEU:HD13 | 1:K:216:THR:OG1  | 2.17                     | 0.45              |
| 1:K:202:LEU:N    | 1:K:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:N:202:LEU:N    | 1:N:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:Q:230:VAL:O    | 1:Q:230:VAL:HG13 | 2.17                     | 0.45              |
| 1:C:126:ALA:O    | 1:C:127:ILE:C    | 2.56                     | 0.45              |
| 1:L:202:LEU:N    | 1:L:202:LEU:HD23 | 2.32                     | 0.45              |
| 1:L:230:VAL:O    | 1:L:230:VAL:HG13 | 2.17                     | 0.45              |
| 1:M:222:LEU:HD13 | 1:N:216:THR:OG1  | 2.17                     | 0.45              |
| 1:P:110:ILE:HD12 | 1:P:167:MET:CE   | 2.47                     | 0.45              |
| 1:P:230:VAL:HG13 | 1:P:230:VAL:O    | 2.17                     | 0.45              |
| 1:Q:202:LEU:N    | 1:Q:202:LEU:HD23 | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:230:VAL:O    | 1:A:230:VAL:HG13 | 2.17                     | 0.44              |
| 1:B:222:LEU:HD13 | 1:C:216:THR:OG1  | 2.17                     | 0.44              |
| 1:F:126:ALA:O    | 1:F:127:ILE:C    | 2.56                     | 0.44              |
| 1:G:230:VAL:O    | 1:G:230:VAL:HG13 | 2.17                     | 0.44              |
| 1:G:284:ILE:HD11 | 1:H:205:THR:HG22 | 2.00                     | 0.44              |
| 1:H:230:VAL:HG13 | 1:H:230:VAL:O    | 2.17                     | 0.44              |
| 1:I:202:LEU:N    | 1:I:202:LEU:HD23 | 2.32                     | 0.44              |
| 1:O:230:VAL:O    | 1:O:230:VAL:HG13 | 2.17                     | 0.44              |
| 1:A:110:ILE:HD12 | 1:A:167:MET:CE   | 2.47                     | 0.44              |
| 1:B:284:ILE:HD11 | 1:C:205:THR:HG22 | 2.00                     | 0.44              |
| 1:E:126:ALA:O    | 1:E:127:ILE:C    | 2.56                     | 0.44              |
| 1:H:126:ALA:O    | 1:H:127:ILE:C    | 2.56                     | 0.44              |
| 1:M:126:ALA:O    | 1:M:127:ILE:C    | 2.56                     | 0.44              |
| 1:N:157:THR:O    | 1:N:157:THR:OG1  | 2.29                     | 0.44              |
| 1:R:126:ALA:O    | 1:R:127:ILE:C    | 2.56                     | 0.44              |
| 1:E:230:VAL:HG13 | 1:E:230:VAL:O    | 2.17                     | 0.44              |
| 1:I:126:ALA:O    | 1:I:127:ILE:C    | 2.56                     | 0.44              |
| 1:K:110:ILE:HD12 | 1:K:167:MET:CE   | 2.47                     | 0.44              |
| 1:Q:206:CYS:HA   | 1:Q:273:ARG:O    | 2.18                     | 0.44              |
| 1:Q:284:ILE:HD11 | 1:R:205:THR:HG22 | 2.00                     | 0.44              |
| 1:B:126:ALA:O    | 1:B:127:ILE:C    | 2.56                     | 0.44              |
| 1:B:206:CYS:HA   | 1:B:273:ARG:O    | 2.18                     | 0.44              |
| 1:E:110:ILE:HD12 | 1:E:167:MET:CE   | 2.47                     | 0.44              |
| 1:E:202:LEU:N    | 1:E:202:LEU:HD23 | 2.32                     | 0.44              |
| 1:I:230:VAL:O    | 1:I:230:VAL:HG13 | 2.17                     | 0.44              |
| 1:L:206:CYS:HA   | 1:L:273:ARG:O    | 2.18                     | 0.44              |
| 1:O:206:CYS:HA   | 1:O:273:ARG:O    | 2.18                     | 0.44              |
| 1:P:205:THR:HG22 | 1:R:284:ILE:HD11 | 2.00                     | 0.44              |
| 1:Q:222:LEU:HD13 | 1:R:216:THR:OG1  | 2.17                     | 0.44              |
| 1:R:127:ILE:HD13 | 1:R:127:ILE:HA   | 1.82                     | 0.44              |
| 1:A:205:THR:HG22 | 1:C:284:ILE:HD11 | 2.00                     | 0.44              |
| 1:A:216:THR:OG1  | 1:C:222:LEU:HD13 | 2.17                     | 0.44              |
| 1:B:230:VAL:HG13 | 1:B:230:VAL:O    | 2.17                     | 0.44              |
| 1:D:205:THR:HG22 | 1:F:284:ILE:HD11 | 2.00                     | 0.44              |
| 1:E:222:LEU:HD13 | 1:F:216:THR:OG1  | 2.17                     | 0.44              |
| 1:G:205:THR:HG22 | 1:I:284:ILE:HD11 | 2.00                     | 0.44              |
| 1:G:222:LEU:HD13 | 1:H:216:THR:OG1  | 2.17                     | 0.44              |
| 1:H:202:LEU:N    | 1:H:202:LEU:HD23 | 2.32                     | 0.44              |
| 1:J:205:THR:HG22 | 1:L:284:ILE:HD11 | 2.00                     | 0.44              |
| 1:L:126:ALA:O    | 1:L:127:ILE:C    | 2.56                     | 0.44              |
| 1:M:110:ILE:HG23 | 1:M:167:MET:HE1  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:202:LEU:N    | 1:M:202:LEU:HD23 | 2.32                     | 0.44              |
| 1:M:205:THR:HG22 | 1:O:284:ILE:HD11 | 2.00                     | 0.44              |
| 1:P:126:ALA:O    | 1:P:127:ILE:C    | 2.56                     | 0.44              |
| 1:R:202:LEU:HD23 | 1:R:202:LEU:N    | 2.32                     | 0.44              |
| 1:A:206:CYS:HA   | 1:A:273:ARG:O    | 2.18                     | 0.44              |
| 1:C:202:LEU:N    | 1:C:202:LEU:HD23 | 2.32                     | 0.44              |
| 1:D:110:ILE:HD12 | 1:D:167:MET:CE   | 2.47                     | 0.44              |
| 1:E:18:ALA:CB    | 1:E:23:ILE:CD1   | 2.90                     | 0.44              |
| 1:E:206:CYS:HA   | 1:E:273:ARG:O    | 2.18                     | 0.44              |
| 1:J:284:ILE:HD11 | 1:K:205:THR:HG22 | 2.00                     | 0.44              |
| 1:K:126:ALA:O    | 1:K:127:ILE:C    | 2.56                     | 0.44              |
| 1:L:252:ILE:HD12 | 1:L:252:ILE:N    | 2.33                     | 0.44              |
| 1:N:222:LEU:HD13 | 1:O:216:THR:OG1  | 2.17                     | 0.44              |
| 1:Q:110:ILE:HD12 | 1:Q:167:MET:CE   | 2.47                     | 0.44              |
| 1:R:110:ILE:HD13 | 1:R:110:ILE:HA   | 1.79                     | 0.44              |
| 1:A:17:ASN:ND2   | 1:A:17:ASN:H     | 2.05                     | 0.44              |
| 1:A:126:ALA:O    | 1:A:127:ILE:C    | 2.56                     | 0.44              |
| 1:D:230:VAL:O    | 1:D:230:VAL:HG13 | 2.17                     | 0.44              |
| 1:F:202:LEU:N    | 1:F:202:LEU:HD23 | 2.32                     | 0.44              |
| 1:F:206:CYS:HA   | 1:F:273:ARG:O    | 2.18                     | 0.44              |
| 1:I:206:CYS:HA   | 1:I:273:ARG:O    | 2.18                     | 0.44              |
| 1:N:206:CYS:HA   | 1:N:273:ARG:O    | 2.18                     | 0.44              |
| 1:O:202:LEU:HD23 | 1:O:202:LEU:N    | 2.32                     | 0.44              |
| 1:P:216:THR:OG1  | 1:R:222:LEU:HD13 | 2.17                     | 0.44              |
| 1:Q:18:ALA:CB    | 1:Q:23:ILE:CD1   | 2.90                     | 0.44              |
| 1:R:206:CYS:HA   | 1:R:273:ARG:O    | 2.18                     | 0.44              |
| 1:C:252:ILE:HD12 | 1:C:252:ILE:N    | 2.33                     | 0.44              |
| 1:E:252:ILE:N    | 1:E:252:ILE:HD12 | 2.33                     | 0.44              |
| 1:G:18:ALA:CB    | 1:G:23:ILE:CD1   | 2.90                     | 0.44              |
| 1:J:252:ILE:N    | 1:J:252:ILE:HD12 | 2.33                     | 0.44              |
| 1:K:206:CYS:HA   | 1:K:273:ARG:O    | 2.18                     | 0.44              |
| 1:O:110:ILE:HA   | 1:O:110:ILE:HD13 | 1.79                     | 0.44              |
| 1:O:252:ILE:HD12 | 1:O:252:ILE:N    | 2.33                     | 0.44              |
| 1:P:252:ILE:N    | 1:P:252:ILE:HD12 | 2.33                     | 0.44              |
| 1:A:252:ILE:HD12 | 1:A:252:ILE:N    | 2.33                     | 0.44              |
| 1:B:110:ILE:HD12 | 1:B:167:MET:CE   | 2.47                     | 0.44              |
| 1:D:284:ILE:HD11 | 1:E:205:THR:HG22 | 2.00                     | 0.44              |
| 1:F:110:ILE:HD12 | 1:F:167:MET:CE   | 2.47                     | 0.44              |
| 1:G:120:ASN:N    | 1:G:120:ASN:ND2  | 2.59                     | 0.44              |
| 1:G:202:LEU:HD23 | 1:G:202:LEU:N    | 2.32                     | 0.44              |
| 1:G:258:GLU:O    | 1:G:259:ASN:HB2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:87:ILE:HG21  | 1:I:122:LEU:HG   | 2.00                     | 0.44              |
| 1:I:252:ILE:HD12 | 1:I:252:ILE:N    | 2.33                     | 0.44              |
| 1:M:206:CYS:HA   | 1:M:273:ARG:O    | 2.18                     | 0.44              |
| 1:M:230:VAL:HG13 | 1:M:230:VAL:O    | 2.17                     | 0.44              |
| 1:P:222:LEU:HD13 | 1:Q:216:THR:OG1  | 2.17                     | 0.44              |
| 1:Q:126:ALA:O    | 1:Q:127:ILE:C    | 2.56                     | 0.44              |
| 1:E:284:ILE:HD11 | 1:F:205:THR:HG22 | 2.00                     | 0.43              |
| 1:G:201:LYS:HZ3  | 1:G:201:LYS:HG2  | 1.70                     | 0.43              |
| 1:H:252:ILE:N    | 1:H:252:ILE:HD12 | 2.33                     | 0.43              |
| 1:I:110:ILE:HD13 | 1:I:110:ILE:HA   | 1.79                     | 0.43              |
| 1:J:126:ALA:O    | 1:J:127:ILE:C    | 2.56                     | 0.43              |
| 1:K:222:LEU:HD13 | 1:L:216:THR:OG1  | 2.17                     | 0.43              |
| 1:N:252:ILE:HD12 | 1:N:252:ILE:N    | 2.33                     | 0.43              |
| 1:R:252:ILE:N    | 1:R:252:ILE:HD12 | 2.33                     | 0.43              |
| 1:B:252:ILE:N    | 1:B:252:ILE:HD12 | 2.33                     | 0.43              |
| 1:C:87:ILE:HG21  | 1:C:122:LEU:HG   | 2.00                     | 0.43              |
| 1:G:252:ILE:HD12 | 1:G:252:ILE:N    | 2.33                     | 0.43              |
| 1:J:206:CYS:HA   | 1:J:273:ARG:O    | 2.18                     | 0.43              |
| 1:M:216:THR:OG1  | 1:O:222:LEU:HD13 | 2.17                     | 0.43              |
| 1:P:258:GLU:O    | 1:P:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:A:258:GLU:O    | 1:A:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:D:126:ALA:O    | 1:D:127:ILE:C    | 2.56                     | 0.43              |
| 1:F:87:ILE:HG21  | 1:F:122:LEU:HG   | 2.00                     | 0.43              |
| 1:G:126:ALA:O    | 1:G:127:ILE:C    | 2.56                     | 0.43              |
| 1:M:258:GLU:O    | 1:M:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:N:126:ALA:O    | 1:N:127:ILE:C    | 2.56                     | 0.43              |
| 1:P:87:ILE:HG21  | 1:P:122:LEU:HG   | 2.00                     | 0.43              |
| 1:A:222:LEU:HD13 | 1:B:216:THR:OG1  | 2.17                     | 0.43              |
| 1:D:258:GLU:O    | 1:D:259:ASN:HB2  | 2.18                     | 0.43              |
| 1:F:258:GLU:O    | 1:F:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:G:216:THR:OG1  | 1:I:222:LEU:HD13 | 2.17                     | 0.43              |
| 1:H:222:LEU:HD13 | 1:I:216:THR:OG1  | 2.17                     | 0.43              |
| 1:J:258:GLU:O    | 1:J:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:N:40:ASN:ND2   | 1:N:45:GLN:HG2   | 2.28                     | 0.43              |
| 1:B:87:ILE:HG21  | 1:B:122:LEU:HG   | 2.00                     | 0.43              |
| 1:G:110:ILE:HD12 | 1:G:167:MET:CE   | 2.47                     | 0.43              |
| 1:M:252:ILE:N    | 1:M:252:ILE:HD12 | 2.33                     | 0.43              |
| 1:N:110:ILE:HD12 | 1:N:167:MET:CE   | 2.47                     | 0.43              |
| 1:Q:252:ILE:HD12 | 1:Q:252:ILE:N    | 2.33                     | 0.43              |
| 1:R:87:ILE:HG21  | 1:R:122:LEU:HG   | 2.00                     | 0.43              |
| 1:A:210:ASP:OD2  | 1:A:212:ARG:HB3  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:216:THR:OG1  | 1:F:222:LEU:HD13 | 2.17                     | 0.43              |
| 1:D:252:ILE:HD12 | 1:D:252:ILE:N    | 2.33                     | 0.43              |
| 1:F:252:ILE:HD12 | 1:F:252:ILE:N    | 2.33                     | 0.43              |
| 1:H:206:CYS:HA   | 1:H:273:ARG:O    | 2.18                     | 0.43              |
| 1:J:216:THR:OG1  | 1:L:222:LEU:HD13 | 2.17                     | 0.43              |
| 1:K:284:ILE:HD11 | 1:L:205:THR:HG22 | 2.00                     | 0.43              |
| 1:M:87:ILE:HG21  | 1:M:122:LEU:HG   | 2.00                     | 0.43              |
| 1:O:110:ILE:HD12 | 1:O:167:MET:CE   | 2.47                     | 0.43              |
| 1:P:127:ILE:HD13 | 1:P:127:ILE:HA   | 1.82                     | 0.43              |
| 1:A:87:ILE:HG21  | 1:A:122:LEU:HG   | 2.00                     | 0.43              |
| 1:C:206:CYS:HA   | 1:C:273:ARG:O    | 2.18                     | 0.43              |
| 1:C:258:GLU:O    | 1:C:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:H:284:ILE:HD11 | 1:I:205:THR:HG22 | 2.00                     | 0.43              |
| 1:L:210:ASP:OD2  | 1:L:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:O:210:ASP:OD2  | 1:O:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:P:284:ILE:HD11 | 1:Q:205:THR:HG22 | 2.00                     | 0.43              |
| 1:G:206:CYS:HA   | 1:G:273:ARG:O    | 2.18                     | 0.43              |
| 1:J:202:LEU:HD23 | 1:J:202:LEU:N    | 2.32                     | 0.43              |
| 1:K:258:GLU:O    | 1:K:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:L:87:ILE:HG21  | 1:L:122:LEU:HG   | 2.00                     | 0.43              |
| 1:L:110:ILE:HD12 | 1:L:167:MET:CE   | 2.47                     | 0.43              |
| 1:M:210:ASP:OD2  | 1:M:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:Q:87:ILE:HG21  | 1:Q:122:LEU:HG   | 2.00                     | 0.43              |
| 1:R:258:GLU:O    | 1:R:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:D:206:CYS:HA   | 1:D:273:ARG:O    | 2.18                     | 0.43              |
| 1:D:210:ASP:OD2  | 1:D:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:H:258:GLU:O    | 1:H:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:I:210:ASP:OD2  | 1:I:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:K:252:ILE:N    | 1:K:252:ILE:HD12 | 2.33                     | 0.43              |
| 1:P:206:CYS:HA   | 1:P:273:ARG:O    | 2.18                     | 0.43              |
| 1:A:9:LEU:HD11   | 1:B:36:ASN:HD21  | 1.84                     | 0.43              |
| 1:B:210:ASP:OD2  | 1:B:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:B:258:GLU:O    | 1:B:259:ASN:HB2  | 2.19                     | 0.43              |
| 1:D:36:ASN:HD21  | 1:F:9:LEU:HD11   | 1.84                     | 0.43              |
| 1:D:110:ILE:HG23 | 1:D:167:MET:CE   | 2.49                     | 0.43              |
| 1:D:222:LEU:HD13 | 1:E:216:THR:OG1  | 2.17                     | 0.43              |
| 1:F:210:ASP:OD2  | 1:F:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:G:157:THR:O    | 1:G:157:THR:OG1  | 2.29                     | 0.43              |
| 1:G:210:ASP:OD2  | 1:G:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:I:110:ILE:HG23 | 1:I:167:MET:CE   | 2.49                     | 0.43              |
| 1:J:164:ILE:HG13 | 1:K:172:GLU:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:210:ASP:OD2  | 1:J:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:K:87:ILE:HG21  | 1:K:122:LEU:HG   | 2.00                     | 0.43              |
| 1:M:9:LEU:HD11   | 1:N:36:ASN:HD21  | 1.84                     | 0.43              |
| 1:M:164:ILE:HG13 | 1:N:172:GLU:HB3  | 2.01                     | 0.43              |
| 1:N:110:ILE:HA   | 1:N:110:ILE:HD13 | 1.79                     | 0.43              |
| 1:N:210:ASP:OD2  | 1:N:212:ARG:HB3  | 2.19                     | 0.43              |
| 1:P:9:LEU:HD11   | 1:Q:36:ASN:HD21  | 1.84                     | 0.43              |
| 1:Q:40:ASN:ND2   | 1:Q:45:GLN:HG2   | 2.28                     | 0.43              |
| 1:B:110:ILE:HG23 | 1:B:167:MET:CE   | 2.49                     | 0.42              |
| 1:B:164:ILE:HG13 | 1:C:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:D:9:LEU:HD11   | 1:E:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:D:40:ASN:ND2   | 1:D:45:GLN:HG2   | 2.28                     | 0.42              |
| 1:E:9:LEU:HD11   | 1:F:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:K:15:ILE:C     | 1:K:17:ASN:N     | 2.73                     | 0.42              |
| 1:L:110:ILE:HG23 | 1:L:167:MET:CE   | 2.49                     | 0.42              |
| 1:L:215:LYS:HG2  | 1:L:216:THR:N    | 2.35                     | 0.42              |
| 1:N:215:LYS:HG2  | 1:N:216:THR:N    | 2.34                     | 0.42              |
| 1:O:110:ILE:HG23 | 1:O:167:MET:CE   | 2.49                     | 0.42              |
| 1:Q:110:ILE:HG23 | 1:Q:167:MET:CE   | 2.49                     | 0.42              |
| 1:Q:258:GLU:O    | 1:Q:259:ASN:HB2  | 2.19                     | 0.42              |
| 1:C:19:SER:O     | 1:C:21:GLY:N     | 2.52                     | 0.42              |
| 1:D:19:SER:O     | 1:D:21:GLY:N     | 2.52                     | 0.42              |
| 1:D:164:ILE:HG13 | 1:E:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:D:201:LYS:HZ3  | 1:D:201:LYS:HG2  | 1.72                     | 0.42              |
| 1:D:215:LYS:HG2  | 1:D:216:THR:N    | 2.34                     | 0.42              |
| 1:E:202:LEU:HD11 | 1:E:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:F:110:ILE:HG23 | 1:F:167:MET:CE   | 2.49                     | 0.42              |
| 1:F:215:LYS:HG2  | 1:F:216:THR:N    | 2.35                     | 0.42              |
| 1:G:36:ASN:HD21  | 1:I:9:LEU:HD11   | 1.84                     | 0.42              |
| 1:G:164:ILE:HG13 | 1:H:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:G:215:LYS:HG2  | 1:G:216:THR:N    | 2.34                     | 0.42              |
| 1:H:9:LEU:HD11   | 1:I:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:I:215:LYS:HG2  | 1:I:216:THR:N    | 2.35                     | 0.42              |
| 1:K:19:SER:O     | 1:K:21:GLY:N     | 2.53                     | 0.42              |
| 1:L:17:ASN:ND2   | 1:L:17:ASN:N     | 2.60                     | 0.42              |
| 1:L:127:ILE:HD13 | 1:L:127:ILE:HA   | 1.82                     | 0.42              |
| 1:N:9:LEU:HD11   | 1:O:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:N:19:SER:O     | 1:N:21:GLY:N     | 2.53                     | 0.42              |
| 1:N:202:LEU:HD11 | 1:N:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:N:284:ILE:HD11 | 1:O:205:THR:HG22 | 2.00                     | 0.42              |
| 1:O:19:SER:O     | 1:O:21:GLY:N     | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:ILE:HG23 | 1:A:167:MET:CE   | 2.49                     | 0.42              |
| 1:A:284:ILE:HD11 | 1:B:205:THR:HG22 | 2.00                     | 0.42              |
| 1:F:19:SER:O     | 1:F:21:GLY:N     | 2.52                     | 0.42              |
| 1:G:19:SER:O     | 1:G:21:GLY:N     | 2.53                     | 0.42              |
| 1:G:172:GLU:HB3  | 1:I:164:ILE:HG13 | 2.01                     | 0.42              |
| 1:H:164:ILE:HG13 | 1:I:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:J:19:SER:O     | 1:J:21:GLY:N     | 2.52                     | 0.42              |
| 1:J:215:LYS:HG2  | 1:J:216:THR:N    | 2.34                     | 0.42              |
| 1:K:202:LEU:HD11 | 1:K:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:K:210:ASP:OD2  | 1:K:212:ARG:HB3  | 2.19                     | 0.42              |
| 1:K:215:LYS:HG2  | 1:K:216:THR:N    | 2.35                     | 0.42              |
| 1:M:19:SER:O     | 1:M:21:GLY:N     | 2.52                     | 0.42              |
| 1:M:284:ILE:HD11 | 1:N:205:THR:HG22 | 2.00                     | 0.42              |
| 1:O:87:ILE:HG21  | 1:O:122:LEU:HG   | 2.00                     | 0.42              |
| 1:O:126:ALA:O    | 1:O:127:ILE:C    | 2.56                     | 0.42              |
| 1:Q:215:LYS:HG2  | 1:Q:216:THR:N    | 2.34                     | 0.42              |
| 1:C:202:LEU:HD11 | 1:C:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:110:ILE:HD13 | 1:D:110:ILE:HA   | 1.79                     | 0.42              |
| 1:D:172:GLU:HB3  | 1:F:164:ILE:HG13 | 2.01                     | 0.42              |
| 1:E:87:ILE:HG21  | 1:E:122:LEU:HG   | 2.00                     | 0.42              |
| 1:E:164:ILE:HG13 | 1:F:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:G:15:ILE:C     | 1:G:17:ASN:N     | 2.73                     | 0.42              |
| 1:G:110:ILE:HG23 | 1:G:167:MET:CE   | 2.49                     | 0.42              |
| 1:H:110:ILE:HG23 | 1:H:167:MET:CE   | 2.49                     | 0.42              |
| 1:J:15:ILE:C     | 1:J:17:ASN:N     | 2.73                     | 0.42              |
| 1:L:19:SER:O     | 1:L:21:GLY:N     | 2.52                     | 0.42              |
| 1:L:110:ILE:HD13 | 1:L:110:ILE:HA   | 1.79                     | 0.42              |
| 1:L:202:LEU:HD11 | 1:L:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:M:110:ILE:HG23 | 1:M:167:MET:CE   | 2.49                     | 0.42              |
| 1:P:202:LEU:HD11 | 1:P:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:P:210:ASP:OD2  | 1:P:212:ARG:HB3  | 2.19                     | 0.42              |
| 1:R:202:LEU:HD11 | 1:R:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:164:ILE:HG13 | 1:B:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:G:87:ILE:HG21  | 1:G:122:LEU:HG   | 2.00                     | 0.42              |
| 1:J:87:ILE:HG21  | 1:J:122:LEU:HG   | 2.00                     | 0.42              |
| 1:J:110:ILE:HG23 | 1:J:167:MET:CE   | 2.49                     | 0.42              |
| 1:Q:19:SER:O     | 1:Q:21:GLY:N     | 2.53                     | 0.42              |
| 1:R:19:SER:O     | 1:R:21:GLY:N     | 2.52                     | 0.42              |
| 1:B:9:LEU:HD11   | 1:C:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:E:210:ASP:OD2  | 1:E:212:ARG:HB3  | 2.19                     | 0.42              |
| 1:F:40:ASN:ND2   | 1:F:45:GLN:HG2   | 2.28                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:172:GLU:HB3  | 1:L:164:ILE:HG13 | 2.01                     | 0.42              |
| 1:K:110:ILE:HG23 | 1:K:167:MET:CE   | 2.49                     | 0.42              |
| 1:O:202:LEU:HD11 | 1:O:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:R:210:ASP:OD2  | 1:R:212:ARG:HB3  | 2.19                     | 0.42              |
| 1:A:36:ASN:HD21  | 1:C:9:LEU:HD11   | 1.84                     | 0.42              |
| 1:E:242:ASN:ND2  | 1:E:242:ASN:N    | 2.45                     | 0.42              |
| 1:G:9:LEU:HD11   | 1:H:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:H:87:ILE:HG21  | 1:H:122:LEU:HG   | 2.00                     | 0.42              |
| 1:M:215:LYS:HG2  | 1:M:216:THR:N    | 2.34                     | 0.42              |
| 1:N:87:ILE:HG21  | 1:N:122:LEU:HG   | 2.00                     | 0.42              |
| 1:N:110:ILE:HG23 | 1:N:167:MET:CE   | 2.49                     | 0.42              |
| 1:P:14:GLU:HB3   | 1:P:17:ASN:ND2   | 2.35                     | 0.42              |
| 1:P:19:SER:O     | 1:P:21:GLY:N     | 2.53                     | 0.42              |
| 1:P:172:GLU:OE1  | 1:R:164:ILE:HG23 | 2.20                     | 0.42              |
| 1:Q:210:ASP:OD2  | 1:Q:212:ARG:HB3  | 2.19                     | 0.42              |
| 1:A:172:GLU:OE1  | 1:C:164:ILE:HG23 | 2.20                     | 0.42              |
| 1:B:202:LEU:HD11 | 1:B:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:202:LEU:HD11 | 1:D:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:218:GLU:OE1  | 1:F:201:LYS:HE3  | 2.20                     | 0.42              |
| 1:H:202:LEU:HD11 | 1:H:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:I:202:LEU:HD11 | 1:I:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:J:9:LEU:HD11   | 1:K:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:L:14:GLU:HB3   | 1:L:17:ASN:ND2   | 2.35                     | 0.42              |
| 1:N:258:GLU:O    | 1:N:259:ASN:HB2  | 2.19                     | 0.42              |
| 1:P:164:ILE:HG13 | 1:Q:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:P:218:GLU:OE1  | 1:R:201:LYS:HE3  | 2.20                     | 0.42              |
| 1:A:19:SER:O     | 1:A:21:GLY:N     | 2.52                     | 0.42              |
| 1:C:210:ASP:OD2  | 1:C:212:ARG:HB3  | 2.19                     | 0.42              |
| 1:D:201:LYS:HE3  | 1:E:218:GLU:OE1  | 2.20                     | 0.42              |
| 1:E:201:LYS:HE3  | 1:F:218:GLU:OE1  | 2.20                     | 0.42              |
| 1:J:36:ASN:HD21  | 1:L:9:LEU:HD11   | 1.84                     | 0.42              |
| 1:J:110:ILE:HD12 | 1:J:167:MET:CE   | 2.47                     | 0.42              |
| 1:K:9:LEU:HD11   | 1:L:36:ASN:HD21  | 1.84                     | 0.42              |
| 1:K:119:THR:OG1  | 1:K:120:ASN:ND2  | 2.53                     | 0.42              |
| 1:K:201:LYS:HE3  | 1:L:218:GLU:OE1  | 2.20                     | 0.42              |
| 1:N:201:LYS:HE3  | 1:O:218:GLU:OE1  | 2.20                     | 0.42              |
| 1:Q:164:ILE:HG23 | 1:R:172:GLU:OE1  | 2.20                     | 0.42              |
| 1:Q:164:ILE:HG13 | 1:R:172:GLU:HB3  | 2.01                     | 0.42              |
| 1:R:110:ILE:HG23 | 1:R:167:MET:CE   | 2.49                     | 0.42              |
| 1:A:14:GLU:HB3   | 1:A:17:ASN:ND2   | 2.35                     | 0.42              |
| 1:A:164:ILE:HG23 | 1:B:172:GLU:OE1  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:215:LYS:HG2  | 1:C:216:THR:N    | 2.35                     | 0.42              |
| 1:H:201:LYS:HE3  | 1:I:218:GLU:OE1  | 2.20                     | 0.42              |
| 1:I:110:ILE:HD12 | 1:I:167:MET:CE   | 2.47                     | 0.42              |
| 1:L:258:GLU:O    | 1:L:259:ASN:HB2  | 2.19                     | 0.42              |
| 1:M:201:LYS:HZ3  | 1:M:201:LYS:HG2  | 1.69                     | 0.42              |
| 1:M:202:LEU:HD11 | 1:M:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:N:119:THR:OG1  | 1:N:120:ASN:ND2  | 2.53                     | 0.42              |
| 1:O:215:LYS:HG2  | 1:O:216:THR:N    | 2.35                     | 0.42              |
| 1:P:119:THR:OG1  | 1:P:120:ASN:ND2  | 2.53                     | 0.42              |
| 1:A:119:THR:OG1  | 1:A:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:A:172:GLU:HB3  | 1:C:164:ILE:HG13 | 2.01                     | 0.41              |
| 1:A:201:LYS:HE3  | 1:B:218:GLU:OE1  | 2.20                     | 0.41              |
| 1:B:19:SER:O     | 1:B:21:GLY:N     | 2.53                     | 0.41              |
| 1:B:164:ILE:HG23 | 1:C:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:C:110:ILE:HG23 | 1:C:167:MET:CE   | 2.49                     | 0.41              |
| 1:D:31:ILE:HD13  | 1:F:31:ILE:CD1   | 2.51                     | 0.41              |
| 1:D:87:ILE:HG21  | 1:D:122:LEU:HG   | 2.00                     | 0.41              |
| 1:F:202:LEU:HD11 | 1:F:254:PHE:CE2  | 2.55                     | 0.41              |
| 1:G:31:ILE:HD13  | 1:I:31:ILE:CD1   | 2.51                     | 0.41              |
| 1:H:19:SER:O     | 1:H:21:GLY:N     | 2.53                     | 0.41              |
| 1:H:210:ASP:OD2  | 1:H:212:ARG:HB3  | 2.19                     | 0.41              |
| 1:H:215:LYS:HG2  | 1:H:216:THR:N    | 2.34                     | 0.41              |
| 1:I:19:SER:O     | 1:I:21:GLY:N     | 2.52                     | 0.41              |
| 1:M:172:GLU:OE1  | 1:O:164:ILE:HG23 | 2.20                     | 0.41              |
| 1:N:164:ILE:HG13 | 1:O:172:GLU:HB3  | 2.01                     | 0.41              |
| 1:O:258:GLU:O    | 1:O:259:ASN:HB2  | 2.19                     | 0.41              |
| 1:P:110:ILE:HG23 | 1:P:167:MET:CE   | 2.49                     | 0.41              |
| 1:Q:201:LYS:HE3  | 1:R:218:GLU:OE1  | 2.20                     | 0.41              |
| 1:Q:202:LEU:HD11 | 1:Q:254:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:202:LEU:HD11 | 1:A:254:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:215:LYS:HG2  | 1:A:216:THR:N    | 2.34                     | 0.41              |
| 1:B:15:ILE:C     | 1:B:17:ASN:N     | 2.73                     | 0.41              |
| 1:B:31:ILE:CD1   | 1:C:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:D:172:GLU:OE1  | 1:F:164:ILE:HG23 | 2.20                     | 0.41              |
| 1:E:19:SER:O     | 1:E:21:GLY:N     | 2.53                     | 0.41              |
| 1:I:258:GLU:O    | 1:I:259:ASN:HB2  | 2.19                     | 0.41              |
| 1:M:119:THR:OG1  | 1:M:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:M:172:GLU:HB3  | 1:O:164:ILE:HG13 | 2.01                     | 0.41              |
| 1:N:164:ILE:HG23 | 1:O:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:Q:9:LEU:HD11   | 1:R:36:ASN:HD21  | 1.84                     | 0.41              |
| 1:A:218:GLU:OE1  | 1:C:201:LYS:HE3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:119:THR:OG1  | 1:D:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:E:110:ILE:HG23 | 1:E:167:MET:CE   | 2.49                     | 0.41              |
| 1:E:164:ILE:HG23 | 1:F:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:H:119:THR:OG1  | 1:H:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:J:31:ILE:HD13  | 1:L:31:ILE:CD1   | 2.51                     | 0.41              |
| 1:J:119:THR:OG1  | 1:J:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:M:120:ASN:N    | 1:M:120:ASN:ND2  | 2.59                     | 0.41              |
| 1:P:36:ASN:HD21  | 1:R:9:LEU:HD11   | 1.84                     | 0.41              |
| 1:P:164:ILE:HG23 | 1:Q:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:Q:31:ILE:CD1   | 1:R:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:A:31:ILE:HD13  | 1:C:31:ILE:CD1   | 2.51                     | 0.41              |
| 1:D:14:GLU:HB3   | 1:D:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:D:164:ILE:HG23 | 1:E:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:230:VAL:HG11 | 1:D:255:SER:N    | 2.36                     | 0.41              |
| 1:G:119:THR:OG1  | 1:G:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:G:230:VAL:HG11 | 1:G:255:SER:N    | 2.36                     | 0.41              |
| 1:J:218:GLU:OE1  | 1:L:201:LYS:HE3  | 2.20                     | 0.41              |
| 1:M:36:ASN:HD21  | 1:O:9:LEU:HD11   | 1.84                     | 0.41              |
| 1:P:168:PHE:HA   | 1:R:163:SER:HB3  | 2.03                     | 0.41              |
| 1:Q:119:THR:OG1  | 1:Q:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:B:215:LYS:HG2  | 1:B:216:THR:N    | 2.35                     | 0.41              |
| 1:D:163:SER:HB3  | 1:E:168:PHE:HA   | 2.03                     | 0.41              |
| 1:H:40:ASN:ND2   | 1:H:45:GLN:HG2   | 2.28                     | 0.41              |
| 1:I:119:THR:OG1  | 1:I:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:K:164:ILE:HG13 | 1:L:172:GLU:HB3  | 2.01                     | 0.41              |
| 1:R:119:THR:OG1  | 1:R:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:C:119:THR:OG1  | 1:C:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:E:15:ILE:C     | 1:E:17:ASN:N     | 2.73                     | 0.41              |
| 1:E:215:LYS:HG2  | 1:E:216:THR:N    | 2.34                     | 0.41              |
| 1:E:258:GLU:O    | 1:E:259:ASN:HB2  | 2.19                     | 0.41              |
| 1:G:14:GLU:HB3   | 1:G:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:H:230:VAL:HG11 | 1:H:255:SER:N    | 2.36                     | 0.41              |
| 1:I:230:VAL:HG11 | 1:I:255:SER:N    | 2.36                     | 0.41              |
| 1:J:168:PHE:HA   | 1:L:163:SER:HB3  | 2.03                     | 0.41              |
| 1:J:172:GLU:OE1  | 1:L:164:ILE:HG23 | 2.20                     | 0.41              |
| 1:J:202:LEU:HD11 | 1:J:254:PHE:CE2  | 2.55                     | 0.41              |
| 1:L:119:THR:OG1  | 1:L:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:M:31:ILE:HD13  | 1:O:31:ILE:CD1   | 2.51                     | 0.41              |
| 1:M:163:SER:HB3  | 1:N:168:PHE:HA   | 2.03                     | 0.41              |
| 1:M:218:GLU:OE1  | 1:O:201:LYS:HE3  | 2.20                     | 0.41              |
| 1:P:31:ILE:CD1   | 1:Q:31:ILE:HD13  | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:209:VAL:HG13 | 1:B:271:GLY:O    | 2.21                     | 0.41              |
| 1:E:31:ILE:CD1   | 1:F:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:G:168:PHE:HA   | 1:I:163:SER:HB3  | 2.03                     | 0.41              |
| 1:G:218:GLU:OE1  | 1:I:201:LYS:HE3  | 2.20                     | 0.41              |
| 1:I:14:GLU:HB3   | 1:I:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:J:163:SER:HB3  | 1:K:167:MET:O    | 2.21                     | 0.41              |
| 1:J:230:VAL:HG11 | 1:J:255:SER:N    | 2.36                     | 0.41              |
| 1:M:31:ILE:CD1   | 1:N:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:O:72:ILE:H     | 1:O:72:ILE:CD1   | 2.34                     | 0.41              |
| 1:P:201:LYS:HE3  | 1:Q:218:GLU:OE1  | 2.20                     | 0.41              |
| 1:Q:209:VAL:HG13 | 1:Q:271:GLY:O    | 2.21                     | 0.41              |
| 1:R:72:ILE:H     | 1:R:72:ILE:CD1   | 2.34                     | 0.41              |
| 1:A:163:SER:HB3  | 1:B:167:MET:O    | 2.21                     | 0.41              |
| 1:B:201:LYS:HE3  | 1:C:218:GLU:OE1  | 2.20                     | 0.41              |
| 1:C:72:ILE:H     | 1:C:72:ILE:CD1   | 2.34                     | 0.41              |
| 1:E:209:VAL:HG13 | 1:E:271:GLY:O    | 2.21                     | 0.41              |
| 1:E:230:VAL:HG11 | 1:E:255:SER:N    | 2.36                     | 0.41              |
| 1:F:72:ILE:H     | 1:F:72:ILE:CD1   | 2.34                     | 0.41              |
| 1:G:172:GLU:OE1  | 1:I:164:ILE:HG23 | 2.20                     | 0.41              |
| 1:L:230:VAL:HG11 | 1:L:255:SER:N    | 2.36                     | 0.41              |
| 1:N:163:SER:HB3  | 1:O:167:MET:O    | 2.21                     | 0.41              |
| 1:N:209:VAL:HG13 | 1:N:271:GLY:O    | 2.21                     | 0.41              |
| 1:P:31:ILE:HD13  | 1:R:31:ILE:CD1   | 2.51                     | 0.41              |
| 1:P:163:SER:HB3  | 1:Q:167:MET:O    | 2.21                     | 0.41              |
| 1:P:167:MET:O    | 1:R:163:SER:HB3  | 2.21                     | 0.41              |
| 1:A:31:ILE:CD1   | 1:B:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:A:110:ILE:HD13 | 1:A:110:ILE:HA   | 1.79                     | 0.41              |
| 1:A:167:MET:O    | 1:C:163:SER:HB3  | 2.21                     | 0.41              |
| 1:A:168:PHE:HA   | 1:C:163:SER:HB3  | 2.03                     | 0.41              |
| 1:B:119:THR:OG1  | 1:B:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:C:14:GLU:HB3   | 1:C:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:C:127:ILE:HD13 | 1:C:127:ILE:HA   | 1.82                     | 0.41              |
| 1:D:163:SER:HB3  | 1:E:167:MET:O    | 2.21                     | 0.41              |
| 1:D:209:VAL:HG13 | 1:D:271:GLY:O    | 2.21                     | 0.41              |
| 1:E:14:GLU:HB3   | 1:E:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:E:119:THR:OG1  | 1:E:120:ASN:ND2  | 2.53                     | 0.41              |
| 1:F:14:GLU:HB3   | 1:F:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:G:164:ILE:HG23 | 1:H:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:H:15:ILE:C     | 1:H:17:ASN:N     | 2.73                     | 0.41              |
| 1:H:163:SER:HB3  | 1:I:167:MET:O    | 2.21                     | 0.41              |
| 1:H:163:SER:HB3  | 1:I:168:PHE:HA   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:164:ILE:HG23 | 1:I:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:I:209:VAL:HG13 | 1:I:271:GLY:O    | 2.21                     | 0.41              |
| 1:J:31:ILE:CD1   | 1:K:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:J:164:ILE:HG23 | 1:K:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:J:209:VAL:HG13 | 1:J:271:GLY:O    | 2.21                     | 0.41              |
| 1:K:14:GLU:HB3   | 1:K:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:K:163:SER:HB3  | 1:L:167:MET:O    | 2.21                     | 0.41              |
| 1:M:164:ILE:HG23 | 1:N:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:M:168:PHE:HA   | 1:O:163:SER:HB3  | 2.03                     | 0.41              |
| 1:M:230:VAL:HG11 | 1:M:255:SER:N    | 2.36                     | 0.41              |
| 1:N:31:ILE:CD1   | 1:O:31:ILE:HD13  | 2.51                     | 0.41              |
| 1:N:110:ILE:HG23 | 1:N:167:MET:HE1  | 2.03                     | 0.41              |
| 1:N:230:VAL:HG11 | 1:N:255:SER:N    | 2.36                     | 0.41              |
| 1:O:248:GLU:O    | 1:O:249:ILE:CB   | 2.69                     | 0.41              |
| 1:P:230:VAL:HG11 | 1:P:255:SER:N    | 2.36                     | 0.41              |
| 1:Q:163:SER:HB3  | 1:R:167:MET:O    | 2.21                     | 0.41              |
| 1:R:14:GLU:HB3   | 1:R:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:A:163:SER:HB3  | 1:B:168:PHE:HA   | 2.03                     | 0.41              |
| 1:A:230:VAL:HG11 | 1:A:255:SER:N    | 2.36                     | 0.41              |
| 1:B:163:SER:HB3  | 1:C:167:MET:O    | 2.21                     | 0.41              |
| 1:E:110:ILE:HA   | 1:E:110:ILE:HD13 | 1.79                     | 0.41              |
| 1:G:163:SER:HB3  | 1:H:167:MET:O    | 2.21                     | 0.41              |
| 1:G:202:LEU:HD11 | 1:G:254:PHE:CE2  | 2.55                     | 0.41              |
| 1:H:110:ILE:HD13 | 1:H:110:ILE:HA   | 1.79                     | 0.41              |
| 1:J:201:LYS:HE3  | 1:K:218:GLU:OE1  | 2.20                     | 0.41              |
| 1:K:163:SER:HB3  | 1:L:168:PHE:HA   | 2.03                     | 0.41              |
| 1:K:164:ILE:HG23 | 1:L:172:GLU:OE1  | 2.20                     | 0.41              |
| 1:M:209:VAL:HG13 | 1:M:271:GLY:O    | 2.21                     | 0.41              |
| 1:N:14:GLU:HB3   | 1:N:17:ASN:ND2   | 2.35                     | 0.41              |
| 1:R:209:VAL:HG13 | 1:R:271:GLY:O    | 2.21                     | 0.41              |
| 1:A:14:GLU:O     | 1:A:15:ILE:CB    | 2.69                     | 0.40              |
| 1:A:209:VAL:HG13 | 1:A:271:GLY:O    | 2.21                     | 0.40              |
| 1:D:72:ILE:H     | 1:D:72:ILE:CD1   | 2.34                     | 0.40              |
| 1:E:127:ILE:HD13 | 1:E:127:ILE:HA   | 1.82                     | 0.40              |
| 1:E:163:SER:HB3  | 1:F:167:MET:O    | 2.21                     | 0.40              |
| 1:G:201:LYS:HE3  | 1:H:218:GLU:OE1  | 2.20                     | 0.40              |
| 1:H:14:GLU:O     | 1:H:15:ILE:CB    | 2.70                     | 0.40              |
| 1:K:230:VAL:HG11 | 1:K:255:SER:N    | 2.36                     | 0.40              |
| 1:O:119:THR:OG1  | 1:O:120:ASN:ND2  | 2.53                     | 0.40              |
| 1:P:209:VAL:HG13 | 1:P:271:GLY:O    | 2.21                     | 0.40              |
| 1:R:14:GLU:O     | 1:R:15:ILE:CB    | 2.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:110:ILE:HD13 | 1:C:110:ILE:HA   | 1.79                     | 0.40              |
| 1:D:234:GLU:H    | 2:D:304:EPE:H81  | 1.84                     | 0.40              |
| 1:F:119:THR:OG1  | 1:F:120:ASN:ND2  | 2.53                     | 0.40              |
| 1:F:209:VAL:HG13 | 1:F:271:GLY:O    | 2.21                     | 0.40              |
| 1:H:31:ILE:CD1   | 1:I:31:ILE:HD13  | 2.51                     | 0.40              |
| 1:J:14:GLU:HB3   | 1:J:17:ASN:ND2   | 2.35                     | 0.40              |
| 1:M:201:LYS:HE3  | 1:N:218:GLU:OE1  | 2.20                     | 0.40              |
| 1:N:230:VAL:HG12 | 1:N:255:SER:CA   | 2.51                     | 0.40              |
| 1:O:209:VAL:HG13 | 1:O:271:GLY:O    | 2.21                     | 0.40              |
| 1:F:230:VAL:HG11 | 1:F:255:SER:N    | 2.36                     | 0.40              |
| 1:G:163:SER:HB3  | 1:H:168:PHE:HA   | 2.03                     | 0.40              |
| 1:K:31:ILE:CD1   | 1:L:31:ILE:HD13  | 2.51                     | 0.40              |
| 1:N:163:SER:HB3  | 1:O:168:PHE:HA   | 2.03                     | 0.40              |
| 1:O:230:VAL:HG11 | 1:O:255:SER:N    | 2.36                     | 0.40              |
| 1:P:172:GLU:HB3  | 1:R:164:ILE:HG13 | 2.01                     | 0.40              |
| 1:R:40:ASN:ND2   | 1:R:45:GLN:HG2   | 2.28                     | 0.40              |
| 1:B:14:GLU:HB3   | 1:B:17:ASN:ND2   | 2.35                     | 0.40              |
| 1:D:168:PHE:HA   | 1:F:163:SER:HB3  | 2.03                     | 0.40              |
| 1:H:209:VAL:HG13 | 1:H:271:GLY:O    | 2.21                     | 0.40              |
| 1:K:14:GLU:CB    | 1:K:17:ASN:ND2   | 2.83                     | 0.40              |
| 1:M:167:MET:O    | 1:O:163:SER:HB3  | 2.21                     | 0.40              |
| 1:N:14:GLU:O     | 1:N:15:ILE:CB    | 2.70                     | 0.40              |
| 1:P:215:LYS:HG2  | 1:P:216:THR:N    | 2.34                     | 0.40              |
| 1:Q:230:VAL:HG11 | 1:Q:255:SER:N    | 2.36                     | 0.40              |
| 1:B:14:GLU:O     | 1:B:15:ILE:CB    | 2.70                     | 0.40              |
| 1:D:31:ILE:CD1   | 1:E:31:ILE:HD13  | 2.51                     | 0.40              |
| 1:J:14:GLU:O     | 1:J:15:ILE:CB    | 2.69                     | 0.40              |
| 1:J:163:SER:HB3  | 1:K:168:PHE:HA   | 2.03                     | 0.40              |
| 1:K:209:VAL:HG13 | 1:K:271:GLY:O    | 2.21                     | 0.40              |
| 1:P:163:SER:HB3  | 1:Q:168:PHE:HA   | 2.03                     | 0.40              |
| 1:Q:248:GLU:O    | 1:Q:249:ILE:CB   | 2.69                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | B     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | C     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | D     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | E     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | F     | 286/288 (99%)   | 264 (92%)  | 15 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | G     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | H     | 286/288 (99%)   | 264 (92%)  | 15 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | I     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | J     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | K     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | L     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | M     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | N     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | O     | 286/288 (99%)   | 264 (92%)  | 15 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | P     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | Q     | 286/288 (99%)   | 264 (92%)  | 15 (5%)  | 7 (2%)   | 6           | 33 |
| 1   | R     | 286/288 (99%)   | 265 (93%)  | 14 (5%)  | 7 (2%)   | 6           | 33 |
| All | All   | 5148/5184 (99%) | 4766 (93%) | 256 (5%) | 126 (2%) | 9           | 33 |

All (126) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | THR  |
| 1   | A     | 128 | ASP  |
| 1   | B     | 20  | THR  |
| 1   | B     | 128 | ASP  |
| 1   | C     | 20  | THR  |
| 1   | C     | 128 | ASP  |
| 1   | D     | 20  | THR  |
| 1   | D     | 128 | ASP  |
| 1   | E     | 20  | THR  |
| 1   | E     | 128 | ASP  |
| 1   | F     | 20  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 128 | ASP  |
| 1   | G     | 20  | THR  |
| 1   | G     | 128 | ASP  |
| 1   | H     | 20  | THR  |
| 1   | H     | 128 | ASP  |
| 1   | I     | 20  | THR  |
| 1   | I     | 128 | ASP  |
| 1   | J     | 20  | THR  |
| 1   | J     | 128 | ASP  |
| 1   | K     | 20  | THR  |
| 1   | K     | 128 | ASP  |
| 1   | L     | 20  | THR  |
| 1   | L     | 128 | ASP  |
| 1   | M     | 20  | THR  |
| 1   | M     | 128 | ASP  |
| 1   | N     | 20  | THR  |
| 1   | N     | 128 | ASP  |
| 1   | O     | 20  | THR  |
| 1   | O     | 128 | ASP  |
| 1   | P     | 20  | THR  |
| 1   | P     | 128 | ASP  |
| 1   | Q     | 20  | THR  |
| 1   | Q     | 128 | ASP  |
| 1   | R     | 20  | THR  |
| 1   | R     | 128 | ASP  |
| 1   | A     | 154 | ASP  |
| 1   | A     | 156 | SER  |
| 1   | B     | 154 | ASP  |
| 1   | B     | 156 | SER  |
| 1   | C     | 154 | ASP  |
| 1   | C     | 156 | SER  |
| 1   | D     | 154 | ASP  |
| 1   | D     | 156 | SER  |
| 1   | E     | 154 | ASP  |
| 1   | E     | 156 | SER  |
| 1   | F     | 154 | ASP  |
| 1   | F     | 156 | SER  |
| 1   | G     | 154 | ASP  |
| 1   | G     | 156 | SER  |
| 1   | H     | 154 | ASP  |
| 1   | H     | 156 | SER  |
| 1   | I     | 154 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 156 | SER  |
| 1   | J     | 154 | ASP  |
| 1   | J     | 156 | SER  |
| 1   | K     | 154 | ASP  |
| 1   | K     | 156 | SER  |
| 1   | L     | 154 | ASP  |
| 1   | L     | 156 | SER  |
| 1   | M     | 154 | ASP  |
| 1   | M     | 156 | SER  |
| 1   | N     | 154 | ASP  |
| 1   | N     | 156 | SER  |
| 1   | O     | 154 | ASP  |
| 1   | O     | 156 | SER  |
| 1   | P     | 154 | ASP  |
| 1   | P     | 156 | SER  |
| 1   | Q     | 154 | ASP  |
| 1   | Q     | 156 | SER  |
| 1   | R     | 154 | ASP  |
| 1   | R     | 156 | SER  |
| 1   | A     | 127 | ILE  |
| 1   | B     | 127 | ILE  |
| 1   | C     | 127 | ILE  |
| 1   | D     | 127 | ILE  |
| 1   | E     | 127 | ILE  |
| 1   | F     | 127 | ILE  |
| 1   | G     | 127 | ILE  |
| 1   | H     | 127 | ILE  |
| 1   | I     | 127 | ILE  |
| 1   | J     | 127 | ILE  |
| 1   | K     | 127 | ILE  |
| 1   | L     | 127 | ILE  |
| 1   | M     | 127 | ILE  |
| 1   | N     | 127 | ILE  |
| 1   | O     | 127 | ILE  |
| 1   | P     | 127 | ILE  |
| 1   | Q     | 127 | ILE  |
| 1   | R     | 127 | ILE  |
| 1   | B     | 15  | ILE  |
| 1   | E     | 15  | ILE  |
| 1   | H     | 15  | ILE  |
| 1   | K     | 15  | ILE  |
| 1   | N     | 15  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 15  | ILE  |
| 1   | A     | 15  | ILE  |
| 1   | C     | 15  | ILE  |
| 1   | D     | 15  | ILE  |
| 1   | F     | 15  | ILE  |
| 1   | G     | 15  | ILE  |
| 1   | I     | 15  | ILE  |
| 1   | J     | 15  | ILE  |
| 1   | L     | 15  | ILE  |
| 1   | M     | 15  | ILE  |
| 1   | O     | 15  | ILE  |
| 1   | P     | 15  | ILE  |
| 1   | R     | 15  | ILE  |
| 1   | A     | 249 | ILE  |
| 1   | B     | 249 | ILE  |
| 1   | C     | 249 | ILE  |
| 1   | D     | 249 | ILE  |
| 1   | E     | 249 | ILE  |
| 1   | F     | 249 | ILE  |
| 1   | G     | 249 | ILE  |
| 1   | H     | 249 | ILE  |
| 1   | I     | 249 | ILE  |
| 1   | J     | 249 | ILE  |
| 1   | K     | 249 | ILE  |
| 1   | L     | 249 | ILE  |
| 1   | M     | 249 | ILE  |
| 1   | N     | 249 | ILE  |
| 1   | O     | 249 | ILE  |
| 1   | P     | 249 | ILE  |
| 1   | Q     | 249 | ILE  |
| 1   | R     | 249 | ILE  |

### 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.

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | A     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | B     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | C     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | D     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | E     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | F     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | G     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | H     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | I     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | J     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | K     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | L     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | M     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | N     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | O     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | P     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | Q     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| 1   | R     | 244/244 (100%)   | 235 (96%)  | 9 (4%)   | 34          | 58 |
| All | All   | 4392/4392 (100%) | 4230 (96%) | 162 (4%) | 37          | 58 |

All (162) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | ASN  |
| 1   | A     | 110 | ILE  |
| 1   | A     | 120 | ASN  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 148 | LEU  |
| 1   | A     | 157 | THR  |
| 1   | A     | 201 | LYS  |
| 1   | A     | 202 | LEU  |
| 1   | A     | 242 | ASN  |
| 1   | B     | 17  | ASN  |
| 1   | B     | 110 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 120 | ASN  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 148 | LEU  |
| 1   | B     | 157 | THR  |
| 1   | B     | 201 | LYS  |
| 1   | B     | 202 | LEU  |
| 1   | B     | 242 | ASN  |
| 1   | C     | 17  | ASN  |
| 1   | C     | 110 | ILE  |
| 1   | C     | 120 | ASN  |
| 1   | C     | 122 | LEU  |
| 1   | C     | 148 | LEU  |
| 1   | C     | 157 | THR  |
| 1   | C     | 201 | LYS  |
| 1   | C     | 202 | LEU  |
| 1   | C     | 242 | ASN  |
| 1   | D     | 17  | ASN  |
| 1   | D     | 110 | ILE  |
| 1   | D     | 120 | ASN  |
| 1   | D     | 122 | LEU  |
| 1   | D     | 148 | LEU  |
| 1   | D     | 157 | THR  |
| 1   | D     | 201 | LYS  |
| 1   | D     | 202 | LEU  |
| 1   | D     | 242 | ASN  |
| 1   | E     | 17  | ASN  |
| 1   | E     | 110 | ILE  |
| 1   | E     | 120 | ASN  |
| 1   | E     | 122 | LEU  |
| 1   | E     | 148 | LEU  |
| 1   | E     | 157 | THR  |
| 1   | E     | 201 | LYS  |
| 1   | E     | 202 | LEU  |
| 1   | E     | 242 | ASN  |
| 1   | F     | 17  | ASN  |
| 1   | F     | 110 | ILE  |
| 1   | F     | 120 | ASN  |
| 1   | F     | 122 | LEU  |
| 1   | F     | 148 | LEU  |
| 1   | F     | 157 | THR  |
| 1   | F     | 201 | LYS  |
| 1   | F     | 202 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 242 | ASN  |
| 1   | G     | 17  | ASN  |
| 1   | G     | 110 | ILE  |
| 1   | G     | 120 | ASN  |
| 1   | G     | 122 | LEU  |
| 1   | G     | 148 | LEU  |
| 1   | G     | 157 | THR  |
| 1   | G     | 201 | LYS  |
| 1   | G     | 202 | LEU  |
| 1   | G     | 242 | ASN  |
| 1   | H     | 17  | ASN  |
| 1   | H     | 110 | ILE  |
| 1   | H     | 120 | ASN  |
| 1   | H     | 122 | LEU  |
| 1   | H     | 148 | LEU  |
| 1   | H     | 157 | THR  |
| 1   | H     | 201 | LYS  |
| 1   | H     | 202 | LEU  |
| 1   | H     | 242 | ASN  |
| 1   | I     | 17  | ASN  |
| 1   | I     | 110 | ILE  |
| 1   | I     | 120 | ASN  |
| 1   | I     | 122 | LEU  |
| 1   | I     | 148 | LEU  |
| 1   | I     | 157 | THR  |
| 1   | I     | 201 | LYS  |
| 1   | I     | 202 | LEU  |
| 1   | I     | 242 | ASN  |
| 1   | J     | 17  | ASN  |
| 1   | J     | 110 | ILE  |
| 1   | J     | 120 | ASN  |
| 1   | J     | 122 | LEU  |
| 1   | J     | 148 | LEU  |
| 1   | J     | 157 | THR  |
| 1   | J     | 201 | LYS  |
| 1   | J     | 202 | LEU  |
| 1   | J     | 242 | ASN  |
| 1   | K     | 17  | ASN  |
| 1   | K     | 110 | ILE  |
| 1   | K     | 120 | ASN  |
| 1   | K     | 122 | LEU  |
| 1   | K     | 148 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 157 | THR  |
| 1   | K     | 201 | LYS  |
| 1   | K     | 202 | LEU  |
| 1   | K     | 242 | ASN  |
| 1   | L     | 17  | ASN  |
| 1   | L     | 110 | ILE  |
| 1   | L     | 120 | ASN  |
| 1   | L     | 122 | LEU  |
| 1   | L     | 148 | LEU  |
| 1   | L     | 157 | THR  |
| 1   | L     | 201 | LYS  |
| 1   | L     | 202 | LEU  |
| 1   | L     | 242 | ASN  |
| 1   | M     | 17  | ASN  |
| 1   | M     | 110 | ILE  |
| 1   | M     | 120 | ASN  |
| 1   | M     | 122 | LEU  |
| 1   | M     | 148 | LEU  |
| 1   | M     | 157 | THR  |
| 1   | M     | 201 | LYS  |
| 1   | M     | 202 | LEU  |
| 1   | M     | 242 | ASN  |
| 1   | N     | 17  | ASN  |
| 1   | N     | 110 | ILE  |
| 1   | N     | 120 | ASN  |
| 1   | N     | 122 | LEU  |
| 1   | N     | 148 | LEU  |
| 1   | N     | 157 | THR  |
| 1   | N     | 201 | LYS  |
| 1   | N     | 202 | LEU  |
| 1   | N     | 242 | ASN  |
| 1   | O     | 17  | ASN  |
| 1   | O     | 110 | ILE  |
| 1   | O     | 120 | ASN  |
| 1   | O     | 122 | LEU  |
| 1   | O     | 148 | LEU  |
| 1   | O     | 157 | THR  |
| 1   | O     | 201 | LYS  |
| 1   | O     | 202 | LEU  |
| 1   | O     | 242 | ASN  |
| 1   | P     | 17  | ASN  |
| 1   | P     | 110 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 120 | ASN  |
| 1   | P     | 122 | LEU  |
| 1   | P     | 148 | LEU  |
| 1   | P     | 157 | THR  |
| 1   | P     | 201 | LYS  |
| 1   | P     | 202 | LEU  |
| 1   | P     | 242 | ASN  |
| 1   | Q     | 17  | ASN  |
| 1   | Q     | 110 | ILE  |
| 1   | Q     | 120 | ASN  |
| 1   | Q     | 122 | LEU  |
| 1   | Q     | 148 | LEU  |
| 1   | Q     | 157 | THR  |
| 1   | Q     | 201 | LYS  |
| 1   | Q     | 202 | LEU  |
| 1   | Q     | 242 | ASN  |
| 1   | R     | 17  | ASN  |
| 1   | R     | 110 | ILE  |
| 1   | R     | 120 | ASN  |
| 1   | R     | 122 | LEU  |
| 1   | R     | 148 | LEU  |
| 1   | R     | 157 | THR  |
| 1   | R     | 201 | LYS  |
| 1   | R     | 202 | LEU  |
| 1   | R     | 242 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | ASN  |
| 1   | A     | 32  | ASN  |
| 1   | A     | 36  | ASN  |
| 1   | A     | 40  | ASN  |
| 1   | A     | 59  | GLN  |
| 1   | A     | 111 | ASN  |
| 1   | A     | 120 | ASN  |
| 1   | A     | 125 | GLN  |
| 1   | A     | 155 | ASN  |
| 1   | A     | 227 | ASN  |
| 1   | A     | 242 | ASN  |
| 1   | B     | 17  | ASN  |
| 1   | B     | 32  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 36  | ASN  |
| 1   | B     | 40  | ASN  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 120 | ASN  |
| 1   | B     | 125 | GLN  |
| 1   | B     | 155 | ASN  |
| 1   | B     | 227 | ASN  |
| 1   | B     | 242 | ASN  |
| 1   | C     | 17  | ASN  |
| 1   | C     | 32  | ASN  |
| 1   | C     | 36  | ASN  |
| 1   | C     | 40  | ASN  |
| 1   | C     | 59  | GLN  |
| 1   | C     | 111 | ASN  |
| 1   | C     | 120 | ASN  |
| 1   | C     | 125 | GLN  |
| 1   | C     | 155 | ASN  |
| 1   | C     | 227 | ASN  |
| 1   | C     | 242 | ASN  |
| 1   | D     | 17  | ASN  |
| 1   | D     | 32  | ASN  |
| 1   | D     | 36  | ASN  |
| 1   | D     | 40  | ASN  |
| 1   | D     | 59  | GLN  |
| 1   | D     | 111 | ASN  |
| 1   | D     | 120 | ASN  |
| 1   | D     | 125 | GLN  |
| 1   | D     | 155 | ASN  |
| 1   | D     | 227 | ASN  |
| 1   | D     | 242 | ASN  |
| 1   | E     | 17  | ASN  |
| 1   | E     | 32  | ASN  |
| 1   | E     | 36  | ASN  |
| 1   | E     | 40  | ASN  |
| 1   | E     | 59  | GLN  |
| 1   | E     | 111 | ASN  |
| 1   | E     | 120 | ASN  |
| 1   | E     | 125 | GLN  |
| 1   | E     | 155 | ASN  |
| 1   | E     | 227 | ASN  |
| 1   | E     | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 17  | ASN  |
| 1   | F     | 32  | ASN  |
| 1   | F     | 36  | ASN  |
| 1   | F     | 40  | ASN  |
| 1   | F     | 59  | GLN  |
| 1   | F     | 111 | ASN  |
| 1   | F     | 120 | ASN  |
| 1   | F     | 125 | GLN  |
| 1   | F     | 155 | ASN  |
| 1   | F     | 227 | ASN  |
| 1   | F     | 242 | ASN  |
| 1   | G     | 17  | ASN  |
| 1   | G     | 32  | ASN  |
| 1   | G     | 36  | ASN  |
| 1   | G     | 40  | ASN  |
| 1   | G     | 59  | GLN  |
| 1   | G     | 111 | ASN  |
| 1   | G     | 120 | ASN  |
| 1   | G     | 125 | GLN  |
| 1   | G     | 155 | ASN  |
| 1   | G     | 227 | ASN  |
| 1   | G     | 242 | ASN  |
| 1   | H     | 17  | ASN  |
| 1   | H     | 32  | ASN  |
| 1   | H     | 36  | ASN  |
| 1   | H     | 40  | ASN  |
| 1   | H     | 59  | GLN  |
| 1   | H     | 111 | ASN  |
| 1   | H     | 120 | ASN  |
| 1   | H     | 125 | GLN  |
| 1   | H     | 155 | ASN  |
| 1   | H     | 227 | ASN  |
| 1   | H     | 242 | ASN  |
| 1   | I     | 17  | ASN  |
| 1   | I     | 32  | ASN  |
| 1   | I     | 36  | ASN  |
| 1   | I     | 40  | ASN  |
| 1   | I     | 59  | GLN  |
| 1   | I     | 111 | ASN  |
| 1   | I     | 120 | ASN  |
| 1   | I     | 125 | GLN  |
| 1   | I     | 155 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 227 | ASN  |
| 1   | I     | 242 | ASN  |
| 1   | J     | 17  | ASN  |
| 1   | J     | 32  | ASN  |
| 1   | J     | 36  | ASN  |
| 1   | J     | 40  | ASN  |
| 1   | J     | 59  | GLN  |
| 1   | J     | 111 | ASN  |
| 1   | J     | 120 | ASN  |
| 1   | J     | 125 | GLN  |
| 1   | J     | 155 | ASN  |
| 1   | J     | 227 | ASN  |
| 1   | J     | 242 | ASN  |
| 1   | K     | 17  | ASN  |
| 1   | K     | 32  | ASN  |
| 1   | K     | 36  | ASN  |
| 1   | K     | 40  | ASN  |
| 1   | K     | 59  | GLN  |
| 1   | K     | 111 | ASN  |
| 1   | K     | 120 | ASN  |
| 1   | K     | 125 | GLN  |
| 1   | K     | 155 | ASN  |
| 1   | K     | 227 | ASN  |
| 1   | K     | 242 | ASN  |
| 1   | L     | 17  | ASN  |
| 1   | L     | 32  | ASN  |
| 1   | L     | 36  | ASN  |
| 1   | L     | 40  | ASN  |
| 1   | L     | 59  | GLN  |
| 1   | L     | 111 | ASN  |
| 1   | L     | 120 | ASN  |
| 1   | L     | 125 | GLN  |
| 1   | L     | 155 | ASN  |
| 1   | L     | 227 | ASN  |
| 1   | L     | 242 | ASN  |
| 1   | M     | 17  | ASN  |
| 1   | M     | 32  | ASN  |
| 1   | M     | 36  | ASN  |
| 1   | M     | 40  | ASN  |
| 1   | M     | 59  | GLN  |
| 1   | M     | 111 | ASN  |
| 1   | M     | 120 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 125 | GLN  |
| 1   | M     | 155 | ASN  |
| 1   | M     | 227 | ASN  |
| 1   | M     | 242 | ASN  |
| 1   | N     | 17  | ASN  |
| 1   | N     | 32  | ASN  |
| 1   | N     | 36  | ASN  |
| 1   | N     | 40  | ASN  |
| 1   | N     | 59  | GLN  |
| 1   | N     | 111 | ASN  |
| 1   | N     | 120 | ASN  |
| 1   | N     | 125 | GLN  |
| 1   | N     | 155 | ASN  |
| 1   | N     | 227 | ASN  |
| 1   | N     | 242 | ASN  |
| 1   | O     | 17  | ASN  |
| 1   | O     | 32  | ASN  |
| 1   | O     | 36  | ASN  |
| 1   | O     | 40  | ASN  |
| 1   | O     | 59  | GLN  |
| 1   | O     | 111 | ASN  |
| 1   | O     | 120 | ASN  |
| 1   | O     | 125 | GLN  |
| 1   | O     | 155 | ASN  |
| 1   | O     | 227 | ASN  |
| 1   | O     | 242 | ASN  |
| 1   | P     | 17  | ASN  |
| 1   | P     | 32  | ASN  |
| 1   | P     | 36  | ASN  |
| 1   | P     | 40  | ASN  |
| 1   | P     | 59  | GLN  |
| 1   | P     | 111 | ASN  |
| 1   | P     | 120 | ASN  |
| 1   | P     | 125 | GLN  |
| 1   | P     | 155 | ASN  |
| 1   | P     | 227 | ASN  |
| 1   | P     | 242 | ASN  |
| 1   | Q     | 17  | ASN  |
| 1   | Q     | 32  | ASN  |
| 1   | Q     | 36  | ASN  |
| 1   | Q     | 40  | ASN  |
| 1   | Q     | 59  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 111 | ASN  |
| 1   | Q     | 120 | ASN  |
| 1   | Q     | 125 | GLN  |
| 1   | Q     | 155 | ASN  |
| 1   | Q     | 227 | ASN  |
| 1   | Q     | 242 | ASN  |
| 1   | R     | 17  | ASN  |
| 1   | R     | 32  | ASN  |
| 1   | R     | 36  | ASN  |
| 1   | R     | 40  | ASN  |
| 1   | R     | 59  | GLN  |
| 1   | R     | 111 | ASN  |
| 1   | R     | 120 | ASN  |
| 1   | R     | 125 | GLN  |
| 1   | R     | 155 | ASN  |
| 1   | R     | 227 | ASN  |
| 1   | R     | 242 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands 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 |
| 2   | EPE  | E     | 305 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | N     | 314 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | F     | 306 | -    | 15,15,15     | 1.77 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | D     | 304 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | H     | 308 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.61 | 12 (66%) |
| 2   | EPE  | A     | 301 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | K     | 311 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | O     | 315 | -    | 15,15,15     | 1.77 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | L     | 312 | -    | 15,15,15     | 1.78 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | B     | 302 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | P     | 316 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.59 | 12 (66%) |
| 2   | EPE  | Q     | 317 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | I     | 309 | -    | 15,15,15     | 1.78 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | J     | 310 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | M     | 313 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | G     | 307 | -    | 15,15,15     | 1.79 | 2 (13%)  | 18,20,20    | 3.59 | 12 (66%) |
| 2   | EPE  | C     | 303 | -    | 15,15,15     | 1.78 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |
| 2   | EPE  | R     | 318 | -    | 15,15,15     | 1.78 | 2 (13%)  | 18,20,20    | 3.60 | 12 (66%) |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | EPE  | E     | 305 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | N     | 314 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | F     | 306 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | D     | 304 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | H     | 308 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | A     | 301 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | K     | 311 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | O     | 315 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | L     | 312 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | B     | 302 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | P     | 316 | -    | -       | 6/9/19/19 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | EPE  | Q     | 317 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | I     | 309 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | J     | 310 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | M     | 313 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | G     | 307 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | C     | 303 | -    | -       | 6/9/19/19 | 0/1/1/1 |
| 2   | EPE  | R     | 318 | -    | -       | 6/9/19/19 | 0/1/1/1 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | B     | 302 | EPE  | O3S-S | 4.81 | 1.64        | 1.47     |
| 2   | K     | 311 | EPE  | O3S-S | 4.81 | 1.64        | 1.47     |
| 2   | H     | 308 | EPE  | O3S-S | 4.81 | 1.64        | 1.47     |
| 2   | Q     | 317 | EPE  | O3S-S | 4.81 | 1.64        | 1.47     |
| 2   | E     | 305 | EPE  | O3S-S | 4.81 | 1.64        | 1.47     |
| 2   | N     | 314 | EPE  | O3S-S | 4.81 | 1.64        | 1.47     |
| 2   | D     | 304 | EPE  | O3S-S | 4.79 | 1.64        | 1.47     |
| 2   | M     | 313 | EPE  | O3S-S | 4.79 | 1.64        | 1.47     |
| 2   | F     | 306 | EPE  | O3S-S | 4.79 | 1.64        | 1.47     |
| 2   | O     | 315 | EPE  | O3S-S | 4.79 | 1.64        | 1.47     |
| 2   | I     | 309 | EPE  | O3S-S | 4.78 | 1.64        | 1.47     |
| 2   | R     | 318 | EPE  | O3S-S | 4.78 | 1.64        | 1.47     |
| 2   | C     | 303 | EPE  | O3S-S | 4.78 | 1.64        | 1.47     |
| 2   | L     | 312 | EPE  | O3S-S | 4.78 | 1.64        | 1.47     |
| 2   | A     | 301 | EPE  | O3S-S | 4.78 | 1.64        | 1.47     |
| 2   | J     | 310 | EPE  | O3S-S | 4.78 | 1.64        | 1.47     |
| 2   | G     | 307 | EPE  | O3S-S | 4.77 | 1.64        | 1.47     |
| 2   | P     | 316 | EPE  | O3S-S | 4.77 | 1.64        | 1.47     |
| 2   | B     | 302 | EPE  | C10-S | 4.08 | 1.83        | 1.77     |
| 2   | K     | 311 | EPE  | C10-S | 4.08 | 1.83        | 1.77     |
| 2   | A     | 301 | EPE  | C10-S | 4.08 | 1.83        | 1.77     |
| 2   | J     | 310 | EPE  | C10-S | 4.08 | 1.83        | 1.77     |
| 2   | D     | 304 | EPE  | C10-S | 4.08 | 1.83        | 1.77     |
| 2   | M     | 313 | EPE  | C10-S | 4.08 | 1.83        | 1.77     |
| 2   | G     | 307 | EPE  | C10-S | 4.07 | 1.83        | 1.77     |
| 2   | P     | 316 | EPE  | C10-S | 4.07 | 1.83        | 1.77     |
| 2   | E     | 305 | EPE  | C10-S | 4.06 | 1.83        | 1.77     |
| 2   | N     | 314 | EPE  | C10-S | 4.06 | 1.83        | 1.77     |
| 2   | H     | 308 | EPE  | C10-S | 4.06 | 1.83        | 1.77     |
| 2   | Q     | 317 | EPE  | C10-S | 4.06 | 1.83        | 1.77     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | I     | 309 | EPE  | C10-S | 4.05 | 1.83        | 1.77     |
| 2   | R     | 318 | EPE  | C10-S | 4.05 | 1.83        | 1.77     |
| 2   | C     | 303 | EPE  | C10-S | 4.04 | 1.83        | 1.77     |
| 2   | L     | 312 | EPE  | C10-S | 4.04 | 1.83        | 1.77     |
| 2   | F     | 306 | EPE  | C10-S | 3.99 | 1.83        | 1.77     |
| 2   | O     | 315 | EPE  | C10-S | 3.99 | 1.83        | 1.77     |

All (216) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2   | F     | 306 | EPE  | O2S-S-C10 | 7.02 | 115.37      | 106.92   |
| 2   | O     | 315 | EPE  | O2S-S-C10 | 7.02 | 115.37      | 106.92   |
| 2   | C     | 303 | EPE  | O2S-S-C10 | 7.01 | 115.36      | 106.92   |
| 2   | L     | 312 | EPE  | O2S-S-C10 | 7.01 | 115.36      | 106.92   |
| 2   | E     | 305 | EPE  | O2S-S-C10 | 7.00 | 115.35      | 106.92   |
| 2   | N     | 314 | EPE  | O2S-S-C10 | 7.00 | 115.35      | 106.92   |
| 2   | I     | 309 | EPE  | O2S-S-C10 | 7.00 | 115.34      | 106.92   |
| 2   | R     | 318 | EPE  | O2S-S-C10 | 7.00 | 115.34      | 106.92   |
| 2   | H     | 308 | EPE  | O2S-S-C10 | 6.99 | 115.34      | 106.92   |
| 2   | Q     | 317 | EPE  | O2S-S-C10 | 6.99 | 115.34      | 106.92   |
| 2   | B     | 302 | EPE  | O2S-S-C10 | 6.99 | 115.33      | 106.92   |
| 2   | K     | 311 | EPE  | O2S-S-C10 | 6.99 | 115.33      | 106.92   |
| 2   | A     | 301 | EPE  | O2S-S-C10 | 6.98 | 115.33      | 106.92   |
| 2   | J     | 310 | EPE  | O2S-S-C10 | 6.98 | 115.33      | 106.92   |
| 2   | D     | 304 | EPE  | O2S-S-C10 | 6.98 | 115.31      | 106.92   |
| 2   | M     | 313 | EPE  | O2S-S-C10 | 6.98 | 115.31      | 106.92   |
| 2   | G     | 307 | EPE  | O2S-S-C10 | 6.97 | 115.31      | 106.92   |
| 2   | P     | 316 | EPE  | O2S-S-C10 | 6.97 | 115.31      | 106.92   |
| 2   | O     | 315 | EPE  | C7-N4-C3  | 5.62 | 125.60      | 111.23   |
| 2   | R     | 318 | EPE  | C7-N4-C3  | 5.61 | 125.59      | 111.23   |
| 2   | Q     | 317 | EPE  | C7-N4-C3  | 5.61 | 125.59      | 111.23   |
| 2   | B     | 302 | EPE  | C7-N4-C3  | 5.61 | 125.59      | 111.23   |
| 2   | K     | 311 | EPE  | C7-N4-C3  | 5.61 | 125.59      | 111.23   |
| 2   | N     | 314 | EPE  | C7-N4-C3  | 5.61 | 125.59      | 111.23   |
| 2   | H     | 308 | EPE  | C7-N4-C3  | 5.61 | 125.57      | 111.23   |
| 2   | C     | 303 | EPE  | C7-N4-C3  | 5.60 | 125.56      | 111.23   |
| 2   | L     | 312 | EPE  | C7-N4-C3  | 5.60 | 125.56      | 111.23   |
| 2   | E     | 305 | EPE  | C7-N4-C3  | 5.60 | 125.55      | 111.23   |
| 2   | F     | 306 | EPE  | C7-N4-C3  | 5.60 | 125.55      | 111.23   |
| 2   | H     | 308 | EPE  | C5-C6-N1  | 5.59 | 122.11      | 110.64   |
| 2   | Q     | 317 | EPE  | C5-C6-N1  | 5.59 | 122.11      | 110.64   |
| 2   | I     | 309 | EPE  | C7-N4-C3  | 5.59 | 125.53      | 111.23   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | G     | 307 | EPE  | C7-N4-C3  | 5.59  | 125.53      | 111.23   |
| 2   | P     | 316 | EPE  | C7-N4-C3  | 5.59  | 125.53      | 111.23   |
| 2   | A     | 301 | EPE  | C7-N4-C3  | 5.58  | 125.51      | 111.23   |
| 2   | J     | 310 | EPE  | C7-N4-C3  | 5.58  | 125.51      | 111.23   |
| 2   | E     | 305 | EPE  | C5-C6-N1  | 5.58  | 122.09      | 110.64   |
| 2   | N     | 314 | EPE  | C5-C6-N1  | 5.58  | 122.09      | 110.64   |
| 2   | G     | 307 | EPE  | C5-C6-N1  | 5.58  | 122.09      | 110.64   |
| 2   | P     | 316 | EPE  | C5-C6-N1  | 5.58  | 122.09      | 110.64   |
| 2   | D     | 304 | EPE  | C5-C6-N1  | 5.58  | 122.09      | 110.64   |
| 2   | M     | 313 | EPE  | C5-C6-N1  | 5.58  | 122.09      | 110.64   |
| 2   | D     | 304 | EPE  | C7-N4-C3  | 5.58  | 125.49      | 111.23   |
| 2   | M     | 313 | EPE  | C7-N4-C3  | 5.58  | 125.49      | 111.23   |
| 2   | B     | 302 | EPE  | C5-C6-N1  | 5.57  | 122.07      | 110.64   |
| 2   | K     | 311 | EPE  | C5-C6-N1  | 5.57  | 122.07      | 110.64   |
| 2   | A     | 301 | EPE  | C5-C6-N1  | 5.57  | 122.07      | 110.64   |
| 2   | J     | 310 | EPE  | C5-C6-N1  | 5.57  | 122.07      | 110.64   |
| 2   | C     | 303 | EPE  | C5-C6-N1  | 5.54  | 122.00      | 110.64   |
| 2   | L     | 312 | EPE  | C5-C6-N1  | 5.54  | 122.00      | 110.64   |
| 2   | I     | 309 | EPE  | C5-C6-N1  | 5.53  | 122.00      | 110.64   |
| 2   | F     | 306 | EPE  | C5-C6-N1  | 5.53  | 121.99      | 110.64   |
| 2   | O     | 315 | EPE  | C5-C6-N1  | 5.53  | 121.98      | 110.64   |
| 2   | R     | 318 | EPE  | C5-C6-N1  | 5.53  | 121.98      | 110.64   |
| 2   | H     | 308 | EPE  | O8-C8-C7  | 4.57  | 130.15      | 111.19   |
| 2   | E     | 305 | EPE  | O8-C8-C7  | 4.57  | 130.13      | 111.19   |
| 2   | B     | 302 | EPE  | O8-C8-C7  | 4.57  | 130.12      | 111.19   |
| 2   | K     | 311 | EPE  | O8-C8-C7  | 4.57  | 130.12      | 111.19   |
| 2   | Q     | 317 | EPE  | O8-C8-C7  | 4.57  | 130.12      | 111.19   |
| 2   | N     | 314 | EPE  | O8-C8-C7  | 4.56  | 130.09      | 111.19   |
| 2   | M     | 313 | EPE  | O8-C8-C7  | 4.56  | 130.09      | 111.19   |
| 2   | A     | 301 | EPE  | O8-C8-C7  | 4.55  | 130.05      | 111.19   |
| 2   | J     | 310 | EPE  | O8-C8-C7  | 4.55  | 130.05      | 111.19   |
| 2   | D     | 304 | EPE  | O8-C8-C7  | 4.55  | 130.04      | 111.19   |
| 2   | G     | 307 | EPE  | O8-C8-C7  | 4.54  | 130.03      | 111.19   |
| 2   | P     | 316 | EPE  | O8-C8-C7  | 4.54  | 130.03      | 111.19   |
| 2   | I     | 309 | EPE  | O8-C8-C7  | 4.54  | 130.00      | 111.19   |
| 2   | R     | 318 | EPE  | O8-C8-C7  | 4.54  | 130.00      | 111.19   |
| 2   | C     | 303 | EPE  | O8-C8-C7  | 4.53  | 129.97      | 111.19   |
| 2   | L     | 312 | EPE  | O8-C8-C7  | 4.53  | 129.97      | 111.19   |
| 2   | F     | 306 | EPE  | O8-C8-C7  | 4.53  | 129.97      | 111.19   |
| 2   | O     | 315 | EPE  | O8-C8-C7  | 4.53  | 129.97      | 111.19   |
| 2   | B     | 302 | EPE  | O3S-S-O1S | -4.43 | 100.45      | 111.27   |
| 2   | E     | 305 | EPE  | O3S-S-O1S | -4.43 | 100.45      | 111.27   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | K     | 311 | EPE  | O3S-S-O1S | -4.43 | 100.45      | 111.27   |
| 2   | N     | 314 | EPE  | O3S-S-O1S | -4.43 | 100.45      | 111.27   |
| 2   | H     | 308 | EPE  | O3S-S-O1S | -4.43 | 100.46      | 111.27   |
| 2   | Q     | 317 | EPE  | O3S-S-O1S | -4.43 | 100.46      | 111.27   |
| 2   | C     | 303 | EPE  | O3S-S-O1S | -4.42 | 100.47      | 111.27   |
| 2   | L     | 312 | EPE  | O3S-S-O1S | -4.42 | 100.47      | 111.27   |
| 2   | I     | 309 | EPE  | O3S-S-O1S | -4.42 | 100.48      | 111.27   |
| 2   | R     | 318 | EPE  | O3S-S-O1S | -4.42 | 100.48      | 111.27   |
| 2   | A     | 301 | EPE  | O3S-S-O1S | -4.42 | 100.48      | 111.27   |
| 2   | J     | 310 | EPE  | O3S-S-O1S | -4.42 | 100.48      | 111.27   |
| 2   | F     | 306 | EPE  | O3S-S-O1S | -4.41 | 100.49      | 111.27   |
| 2   | O     | 315 | EPE  | O3S-S-O1S | -4.41 | 100.49      | 111.27   |
| 2   | D     | 304 | EPE  | O3S-S-O1S | -4.41 | 100.49      | 111.27   |
| 2   | M     | 313 | EPE  | O3S-S-O1S | -4.41 | 100.49      | 111.27   |
| 2   | G     | 307 | EPE  | O3S-S-O1S | -4.40 | 100.52      | 111.27   |
| 2   | P     | 316 | EPE  | O3S-S-O1S | -4.40 | 100.52      | 111.27   |
| 2   | O     | 315 | EPE  | C2-C3-N4  | 3.88  | 118.60      | 110.64   |
| 2   | B     | 302 | EPE  | C2-C3-N4  | 3.88  | 118.59      | 110.64   |
| 2   | K     | 311 | EPE  | C2-C3-N4  | 3.88  | 118.59      | 110.64   |
| 2   | R     | 318 | EPE  | C2-C3-N4  | 3.88  | 118.59      | 110.64   |
| 2   | H     | 308 | EPE  | C2-C3-N4  | 3.87  | 118.59      | 110.64   |
| 2   | Q     | 317 | EPE  | C2-C3-N4  | 3.87  | 118.59      | 110.64   |
| 2   | G     | 307 | EPE  | C2-C3-N4  | 3.87  | 118.58      | 110.64   |
| 2   | P     | 316 | EPE  | C2-C3-N4  | 3.87  | 118.58      | 110.64   |
| 2   | E     | 305 | EPE  | C2-C3-N4  | 3.87  | 118.58      | 110.64   |
| 2   | N     | 314 | EPE  | C2-C3-N4  | 3.87  | 118.58      | 110.64   |
| 2   | D     | 304 | EPE  | C2-C3-N4  | 3.87  | 118.58      | 110.64   |
| 2   | M     | 313 | EPE  | C2-C3-N4  | 3.87  | 118.58      | 110.64   |
| 2   | C     | 303 | EPE  | C2-C3-N4  | 3.87  | 118.57      | 110.64   |
| 2   | L     | 312 | EPE  | C2-C3-N4  | 3.87  | 118.57      | 110.64   |
| 2   | I     | 309 | EPE  | C2-C3-N4  | 3.86  | 118.57      | 110.64   |
| 2   | A     | 301 | EPE  | C2-C3-N4  | 3.86  | 118.57      | 110.64   |
| 2   | J     | 310 | EPE  | C2-C3-N4  | 3.86  | 118.57      | 110.64   |
| 2   | F     | 306 | EPE  | C2-C3-N4  | 3.86  | 118.56      | 110.64   |
| 2   | E     | 305 | EPE  | C7-N4-C5  | 3.79  | 120.92      | 111.23   |
| 2   | D     | 304 | EPE  | C7-N4-C5  | 3.78  | 120.91      | 111.23   |
| 2   | M     | 313 | EPE  | C7-N4-C5  | 3.78  | 120.91      | 111.23   |
| 2   | H     | 308 | EPE  | C7-N4-C5  | 3.78  | 120.91      | 111.23   |
| 2   | I     | 309 | EPE  | C7-N4-C5  | 3.78  | 120.89      | 111.23   |
| 2   | N     | 314 | EPE  | C7-N4-C5  | 3.77  | 120.89      | 111.23   |
| 2   | Q     | 317 | EPE  | C7-N4-C5  | 3.77  | 120.89      | 111.23   |
| 2   | A     | 301 | EPE  | C7-N4-C5  | 3.77  | 120.88      | 111.23   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | J     | 310 | EPE  | C7-N4-C5 | 3.77 | 120.88      | 111.23   |
| 2   | G     | 307 | EPE  | C7-N4-C5 | 3.77 | 120.88      | 111.23   |
| 2   | P     | 316 | EPE  | C7-N4-C5 | 3.77 | 120.88      | 111.23   |
| 2   | F     | 306 | EPE  | C7-N4-C5 | 3.77 | 120.87      | 111.23   |
| 2   | B     | 302 | EPE  | C7-N4-C5 | 3.77 | 120.87      | 111.23   |
| 2   | K     | 311 | EPE  | C7-N4-C5 | 3.77 | 120.87      | 111.23   |
| 2   | C     | 303 | EPE  | C7-N4-C5 | 3.76 | 120.86      | 111.23   |
| 2   | L     | 312 | EPE  | C7-N4-C5 | 3.76 | 120.86      | 111.23   |
| 2   | O     | 315 | EPE  | C7-N4-C5 | 3.76 | 120.86      | 111.23   |
| 2   | R     | 318 | EPE  | C7-N4-C5 | 3.75 | 120.84      | 111.23   |
| 2   | E     | 305 | EPE  | C6-C5-N4 | 3.65 | 118.12      | 110.64   |
| 2   | N     | 314 | EPE  | C6-C5-N4 | 3.65 | 118.12      | 110.64   |
| 2   | O     | 315 | EPE  | C6-C5-N4 | 3.64 | 118.11      | 110.64   |
| 2   | B     | 302 | EPE  | C6-C5-N4 | 3.64 | 118.11      | 110.64   |
| 2   | K     | 311 | EPE  | C6-C5-N4 | 3.64 | 118.11      | 110.64   |
| 2   | C     | 303 | EPE  | C6-C5-N4 | 3.64 | 118.10      | 110.64   |
| 2   | L     | 312 | EPE  | C6-C5-N4 | 3.64 | 118.10      | 110.64   |
| 2   | I     | 309 | EPE  | C6-C5-N4 | 3.64 | 118.10      | 110.64   |
| 2   | H     | 308 | EPE  | C6-C5-N4 | 3.63 | 118.10      | 110.64   |
| 2   | Q     | 317 | EPE  | C6-C5-N4 | 3.63 | 118.10      | 110.64   |
| 2   | F     | 306 | EPE  | C6-C5-N4 | 3.63 | 118.09      | 110.64   |
| 2   | R     | 318 | EPE  | C6-C5-N4 | 3.63 | 118.08      | 110.64   |
| 2   | A     | 301 | EPE  | C6-C5-N4 | 3.61 | 118.05      | 110.64   |
| 2   | D     | 304 | EPE  | C6-C5-N4 | 3.61 | 118.05      | 110.64   |
| 2   | J     | 310 | EPE  | C6-C5-N4 | 3.61 | 118.05      | 110.64   |
| 2   | M     | 313 | EPE  | C6-C5-N4 | 3.61 | 118.05      | 110.64   |
| 2   | G     | 307 | EPE  | C6-C5-N4 | 3.60 | 118.04      | 110.64   |
| 2   | P     | 316 | EPE  | C6-C5-N4 | 3.60 | 118.04      | 110.64   |
| 2   | H     | 308 | EPE  | C9-N1-C6 | 3.37 | 119.86      | 111.23   |
| 2   | Q     | 317 | EPE  | C9-N1-C6 | 3.37 | 119.86      | 111.23   |
| 2   | E     | 305 | EPE  | C9-N1-C6 | 3.37 | 119.85      | 111.23   |
| 2   | N     | 314 | EPE  | C9-N1-C6 | 3.37 | 119.85      | 111.23   |
| 2   | D     | 304 | EPE  | C9-N1-C6 | 3.37 | 119.84      | 111.23   |
| 2   | M     | 313 | EPE  | C9-N1-C6 | 3.37 | 119.84      | 111.23   |
| 2   | G     | 307 | EPE  | C9-N1-C6 | 3.36 | 119.84      | 111.23   |
| 2   | P     | 316 | EPE  | C9-N1-C6 | 3.36 | 119.84      | 111.23   |
| 2   | A     | 301 | EPE  | C9-N1-C6 | 3.36 | 119.83      | 111.23   |
| 2   | J     | 310 | EPE  | C9-N1-C6 | 3.36 | 119.83      | 111.23   |
| 2   | B     | 302 | EPE  | C9-N1-C6 | 3.36 | 119.83      | 111.23   |
| 2   | K     | 311 | EPE  | C9-N1-C6 | 3.36 | 119.83      | 111.23   |
| 2   | I     | 309 | EPE  | C9-N1-C6 | 3.35 | 119.81      | 111.23   |
| 2   | C     | 303 | EPE  | C9-N1-C6 | 3.34 | 119.79      | 111.23   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | L     | 312 | EPE  | C9-N1-C6 | 3.34 | 119.79      | 111.23   |
| 2   | F     | 306 | EPE  | C9-N1-C6 | 3.33 | 119.75      | 111.23   |
| 2   | O     | 315 | EPE  | C9-N1-C6 | 3.33 | 119.75      | 111.23   |
| 2   | R     | 318 | EPE  | C9-N1-C6 | 3.33 | 119.74      | 111.23   |
| 2   | R     | 318 | EPE  | C9-N1-C2 | 3.08 | 119.10      | 111.23   |
| 2   | E     | 305 | EPE  | C9-N1-C2 | 3.07 | 119.09      | 111.23   |
| 2   | N     | 314 | EPE  | C9-N1-C2 | 3.07 | 119.09      | 111.23   |
| 2   | B     | 302 | EPE  | C9-N1-C2 | 3.07 | 119.09      | 111.23   |
| 2   | K     | 311 | EPE  | C9-N1-C2 | 3.07 | 119.09      | 111.23   |
| 2   | C     | 303 | EPE  | C9-N1-C2 | 3.07 | 119.08      | 111.23   |
| 2   | L     | 312 | EPE  | C9-N1-C2 | 3.07 | 119.08      | 111.23   |
| 2   | H     | 308 | EPE  | C9-N1-C2 | 3.06 | 119.07      | 111.23   |
| 2   | Q     | 317 | EPE  | C9-N1-C2 | 3.06 | 119.07      | 111.23   |
| 2   | I     | 309 | EPE  | C9-N1-C2 | 3.06 | 119.07      | 111.23   |
| 2   | F     | 306 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | O     | 315 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | A     | 301 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | D     | 304 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | J     | 310 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | M     | 313 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | G     | 307 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | P     | 316 | EPE  | C9-N1-C2 | 3.06 | 119.06      | 111.23   |
| 2   | F     | 306 | EPE  | C6-N1-C2 | 2.89 | 115.34      | 108.83   |
| 2   | O     | 315 | EPE  | C6-N1-C2 | 2.89 | 115.34      | 108.83   |
| 2   | R     | 318 | EPE  | C6-N1-C2 | 2.88 | 115.31      | 108.83   |
| 2   | I     | 309 | EPE  | C6-N1-C2 | 2.88 | 115.31      | 108.83   |
| 2   | C     | 303 | EPE  | C6-N1-C2 | 2.87 | 115.30      | 108.83   |
| 2   | L     | 312 | EPE  | C6-N1-C2 | 2.87 | 115.30      | 108.83   |
| 2   | A     | 301 | EPE  | C6-N1-C2 | 2.86 | 115.26      | 108.83   |
| 2   | J     | 310 | EPE  | C6-N1-C2 | 2.86 | 115.26      | 108.83   |
| 2   | G     | 307 | EPE  | C6-N1-C2 | 2.85 | 115.25      | 108.83   |
| 2   | P     | 316 | EPE  | C6-N1-C2 | 2.85 | 115.25      | 108.83   |
| 2   | D     | 304 | EPE  | C6-N1-C2 | 2.85 | 115.25      | 108.83   |
| 2   | M     | 313 | EPE  | C6-N1-C2 | 2.85 | 115.25      | 108.83   |
| 2   | B     | 302 | EPE  | C6-N1-C2 | 2.84 | 115.22      | 108.83   |
| 2   | K     | 311 | EPE  | C6-N1-C2 | 2.84 | 115.22      | 108.83   |
| 2   | H     | 308 | EPE  | C6-N1-C2 | 2.83 | 115.20      | 108.83   |
| 2   | Q     | 317 | EPE  | C6-N1-C2 | 2.83 | 115.20      | 108.83   |
| 2   | E     | 305 | EPE  | C6-N1-C2 | 2.83 | 115.19      | 108.83   |
| 2   | N     | 314 | EPE  | C6-N1-C2 | 2.83 | 115.19      | 108.83   |
| 2   | A     | 301 | EPE  | C5-N4-C3 | 2.12 | 113.59      | 108.83   |
| 2   | J     | 310 | EPE  | C5-N4-C3 | 2.12 | 113.59      | 108.83   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | D     | 304 | EPE  | C5-N4-C3 | 2.11 | 113.58      | 108.83   |
| 2   | M     | 313 | EPE  | C5-N4-C3 | 2.11 | 113.58      | 108.83   |
| 2   | G     | 307 | EPE  | C5-N4-C3 | 2.11 | 113.58      | 108.83   |
| 2   | P     | 316 | EPE  | C5-N4-C3 | 2.11 | 113.58      | 108.83   |
| 2   | F     | 306 | EPE  | C5-N4-C3 | 2.10 | 113.56      | 108.83   |
| 2   | I     | 309 | EPE  | C5-N4-C3 | 2.10 | 113.56      | 108.83   |
| 2   | C     | 303 | EPE  | C5-N4-C3 | 2.10 | 113.55      | 108.83   |
| 2   | L     | 312 | EPE  | C5-N4-C3 | 2.10 | 113.55      | 108.83   |
| 2   | R     | 318 | EPE  | C5-N4-C3 | 2.10 | 113.55      | 108.83   |
| 2   | O     | 315 | EPE  | C5-N4-C3 | 2.09 | 113.52      | 108.83   |
| 2   | B     | 302 | EPE  | C5-N4-C3 | 2.08 | 113.52      | 108.83   |
| 2   | K     | 311 | EPE  | C5-N4-C3 | 2.08 | 113.52      | 108.83   |
| 2   | E     | 305 | EPE  | C5-N4-C3 | 2.08 | 113.51      | 108.83   |
| 2   | N     | 314 | EPE  | C5-N4-C3 | 2.08 | 113.51      | 108.83   |
| 2   | H     | 308 | EPE  | C5-N4-C3 | 2.08 | 113.50      | 108.83   |
| 2   | Q     | 317 | EPE  | C5-N4-C3 | 2.08 | 113.50      | 108.83   |

There are no chirality outliers.

All (108) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | A     | 301 | EPE  | C9-C10-S-O1S |
| 2   | B     | 302 | EPE  | C9-C10-S-O1S |
| 2   | C     | 303 | EPE  | C9-C10-S-O1S |
| 2   | D     | 304 | EPE  | C9-C10-S-O1S |
| 2   | E     | 305 | EPE  | C9-C10-S-O1S |
| 2   | F     | 306 | EPE  | C9-C10-S-O1S |
| 2   | G     | 307 | EPE  | C9-C10-S-O1S |
| 2   | H     | 308 | EPE  | C9-C10-S-O1S |
| 2   | I     | 309 | EPE  | C9-C10-S-O1S |
| 2   | J     | 310 | EPE  | C9-C10-S-O1S |
| 2   | K     | 311 | EPE  | C9-C10-S-O1S |
| 2   | L     | 312 | EPE  | C9-C10-S-O1S |
| 2   | M     | 313 | EPE  | C9-C10-S-O1S |
| 2   | N     | 314 | EPE  | C9-C10-S-O1S |
| 2   | O     | 315 | EPE  | C9-C10-S-O1S |
| 2   | P     | 316 | EPE  | C9-C10-S-O1S |
| 2   | Q     | 317 | EPE  | C9-C10-S-O1S |
| 2   | R     | 318 | EPE  | C9-C10-S-O1S |
| 2   | A     | 301 | EPE  | N4-C7-C8-O8  |
| 2   | B     | 302 | EPE  | N4-C7-C8-O8  |
| 2   | C     | 303 | EPE  | N4-C7-C8-O8  |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | D     | 304 | EPE  | N4-C7-C8-O8  |
| 2   | E     | 305 | EPE  | N4-C7-C8-O8  |
| 2   | F     | 306 | EPE  | N4-C7-C8-O8  |
| 2   | G     | 307 | EPE  | N4-C7-C8-O8  |
| 2   | H     | 308 | EPE  | N4-C7-C8-O8  |
| 2   | I     | 309 | EPE  | N4-C7-C8-O8  |
| 2   | J     | 310 | EPE  | N4-C7-C8-O8  |
| 2   | K     | 311 | EPE  | N4-C7-C8-O8  |
| 2   | L     | 312 | EPE  | N4-C7-C8-O8  |
| 2   | M     | 313 | EPE  | N4-C7-C8-O8  |
| 2   | N     | 314 | EPE  | N4-C7-C8-O8  |
| 2   | O     | 315 | EPE  | N4-C7-C8-O8  |
| 2   | P     | 316 | EPE  | N4-C7-C8-O8  |
| 2   | Q     | 317 | EPE  | N4-C7-C8-O8  |
| 2   | R     | 318 | EPE  | N4-C7-C8-O8  |
| 2   | A     | 301 | EPE  | C9-C10-S-O3S |
| 2   | B     | 302 | EPE  | C9-C10-S-O3S |
| 2   | C     | 303 | EPE  | C9-C10-S-O3S |
| 2   | D     | 304 | EPE  | C9-C10-S-O3S |
| 2   | E     | 305 | EPE  | C9-C10-S-O3S |
| 2   | F     | 306 | EPE  | C9-C10-S-O3S |
| 2   | G     | 307 | EPE  | C9-C10-S-O3S |
| 2   | H     | 308 | EPE  | C9-C10-S-O3S |
| 2   | I     | 309 | EPE  | C9-C10-S-O3S |
| 2   | J     | 310 | EPE  | C9-C10-S-O3S |
| 2   | K     | 311 | EPE  | C9-C10-S-O3S |
| 2   | L     | 312 | EPE  | C9-C10-S-O3S |
| 2   | M     | 313 | EPE  | C9-C10-S-O3S |
| 2   | N     | 314 | EPE  | C9-C10-S-O3S |
| 2   | O     | 315 | EPE  | C9-C10-S-O3S |
| 2   | P     | 316 | EPE  | C9-C10-S-O3S |
| 2   | Q     | 317 | EPE  | C9-C10-S-O3S |
| 2   | R     | 318 | EPE  | C9-C10-S-O3S |
| 2   | A     | 301 | EPE  | C10-C9-N1-C6 |
| 2   | B     | 302 | EPE  | C10-C9-N1-C6 |
| 2   | C     | 303 | EPE  | C10-C9-N1-C6 |
| 2   | D     | 304 | EPE  | C10-C9-N1-C6 |
| 2   | E     | 305 | EPE  | C10-C9-N1-C6 |
| 2   | F     | 306 | EPE  | C10-C9-N1-C6 |
| 2   | G     | 307 | EPE  | C10-C9-N1-C6 |
| 2   | H     | 308 | EPE  | C10-C9-N1-C6 |
| 2   | I     | 309 | EPE  | C10-C9-N1-C6 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | J     | 310 | EPE  | C10-C9-N1-C6 |
| 2   | K     | 311 | EPE  | C10-C9-N1-C6 |
| 2   | L     | 312 | EPE  | C10-C9-N1-C6 |
| 2   | M     | 313 | EPE  | C10-C9-N1-C6 |
| 2   | N     | 314 | EPE  | C10-C9-N1-C6 |
| 2   | O     | 315 | EPE  | C10-C9-N1-C6 |
| 2   | P     | 316 | EPE  | C10-C9-N1-C6 |
| 2   | Q     | 317 | EPE  | C10-C9-N1-C6 |
| 2   | R     | 318 | EPE  | C10-C9-N1-C6 |
| 2   | A     | 301 | EPE  | C9-C10-S-O2S |
| 2   | B     | 302 | EPE  | C9-C10-S-O2S |
| 2   | C     | 303 | EPE  | C9-C10-S-O2S |
| 2   | D     | 304 | EPE  | C9-C10-S-O2S |
| 2   | E     | 305 | EPE  | C9-C10-S-O2S |
| 2   | F     | 306 | EPE  | C9-C10-S-O2S |
| 2   | G     | 307 | EPE  | C9-C10-S-O2S |
| 2   | H     | 308 | EPE  | C9-C10-S-O2S |
| 2   | I     | 309 | EPE  | C9-C10-S-O2S |
| 2   | J     | 310 | EPE  | C9-C10-S-O2S |
| 2   | K     | 311 | EPE  | C9-C10-S-O2S |
| 2   | L     | 312 | EPE  | C9-C10-S-O2S |
| 2   | M     | 313 | EPE  | C9-C10-S-O2S |
| 2   | N     | 314 | EPE  | C9-C10-S-O2S |
| 2   | O     | 315 | EPE  | C9-C10-S-O2S |
| 2   | P     | 316 | EPE  | C9-C10-S-O2S |
| 2   | Q     | 317 | EPE  | C9-C10-S-O2S |
| 2   | R     | 318 | EPE  | C9-C10-S-O2S |
| 2   | A     | 301 | EPE  | C8-C7-N4-C3  |
| 2   | B     | 302 | EPE  | C8-C7-N4-C3  |
| 2   | C     | 303 | EPE  | C8-C7-N4-C3  |
| 2   | D     | 304 | EPE  | C8-C7-N4-C3  |
| 2   | E     | 305 | EPE  | C8-C7-N4-C3  |
| 2   | F     | 306 | EPE  | C8-C7-N4-C3  |
| 2   | G     | 307 | EPE  | C8-C7-N4-C3  |
| 2   | H     | 308 | EPE  | C8-C7-N4-C3  |
| 2   | I     | 309 | EPE  | C8-C7-N4-C3  |
| 2   | J     | 310 | EPE  | C8-C7-N4-C3  |
| 2   | K     | 311 | EPE  | C8-C7-N4-C3  |
| 2   | L     | 312 | EPE  | C8-C7-N4-C3  |
| 2   | M     | 313 | EPE  | C8-C7-N4-C3  |
| 2   | N     | 314 | EPE  | C8-C7-N4-C3  |
| 2   | O     | 315 | EPE  | C8-C7-N4-C3  |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | P     | 316 | EPE  | C8-C7-N4-C3 |
| 2   | Q     | 317 | EPE  | C8-C7-N4-C3 |
| 2   | R     | 318 | EPE  | C8-C7-N4-C3 |

There are no ring outliers.

18 monomers are involved in 55 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | E     | 305 | EPE  | 3       | 0            |
| 2   | N     | 314 | EPE  | 3       | 0            |
| 2   | F     | 306 | EPE  | 3       | 0            |
| 2   | D     | 304 | EPE  | 4       | 0            |
| 2   | H     | 308 | EPE  | 3       | 0            |
| 2   | A     | 301 | EPE  | 3       | 0            |
| 2   | K     | 311 | EPE  | 3       | 0            |
| 2   | O     | 315 | EPE  | 3       | 0            |
| 2   | L     | 312 | EPE  | 3       | 0            |
| 2   | B     | 302 | EPE  | 3       | 0            |
| 2   | P     | 316 | EPE  | 3       | 0            |
| 2   | Q     | 317 | EPE  | 3       | 0            |
| 2   | I     | 309 | EPE  | 3       | 0            |
| 2   | J     | 310 | EPE  | 3       | 0            |
| 2   | M     | 313 | EPE  | 3       | 0            |
| 2   | G     | 307 | EPE  | 3       | 0            |
| 2   | C     | 303 | EPE  | 3       | 0            |
| 2   | R     | 318 | EPE  | 3       | 0            |

## 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.

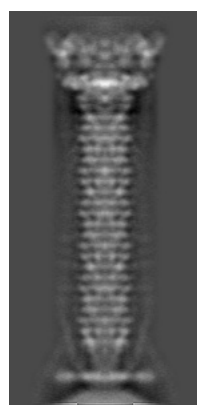
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1126. These allow visual inspection of the internal detail of the map and identification of artifacts.

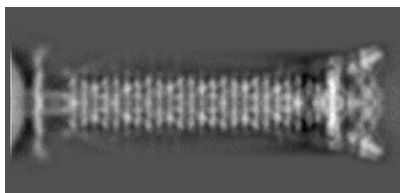
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

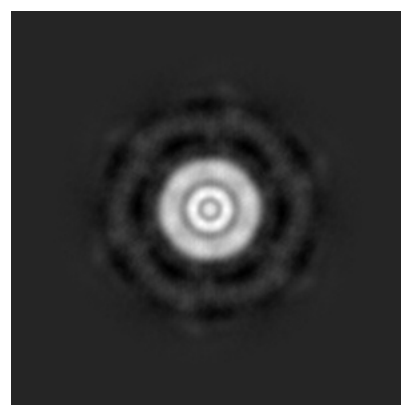
#### 6.1.1 Primary map



X



Y

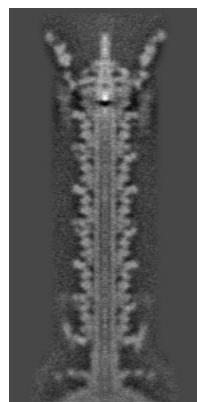


Z

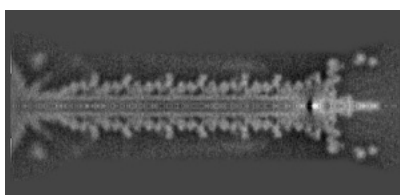
The images above show the map projected in three orthogonal directions.

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

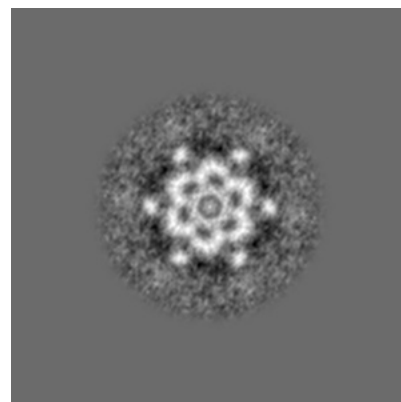
#### 6.2.1 Primary map



X Index: 90



Y Index: 90



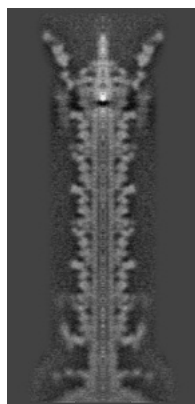
Z Index: 190



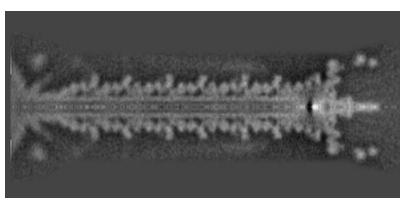
The images above show central slices of the map in three orthogonal directions.

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

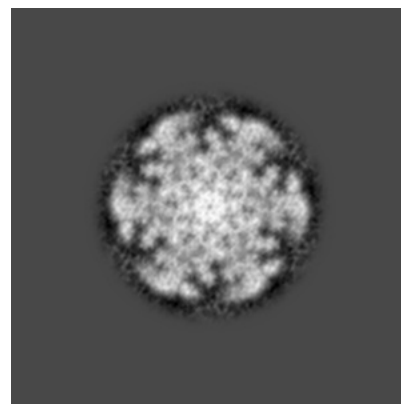
### 6.3.1 Primary map



X Index: 89



Y Index: 90



Z Index: 310

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

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

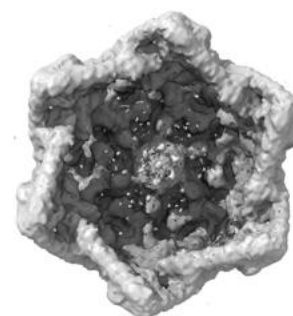
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

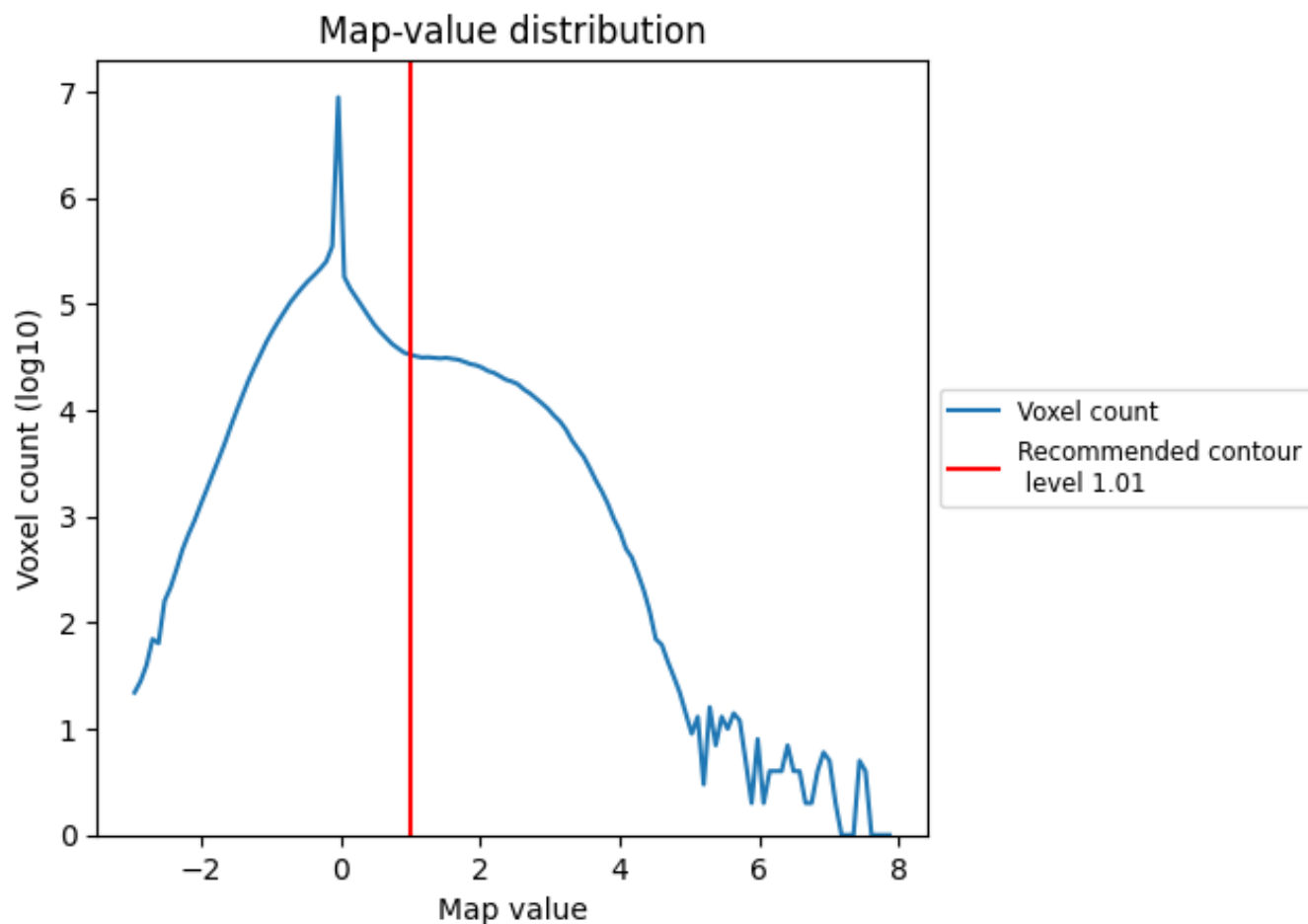
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

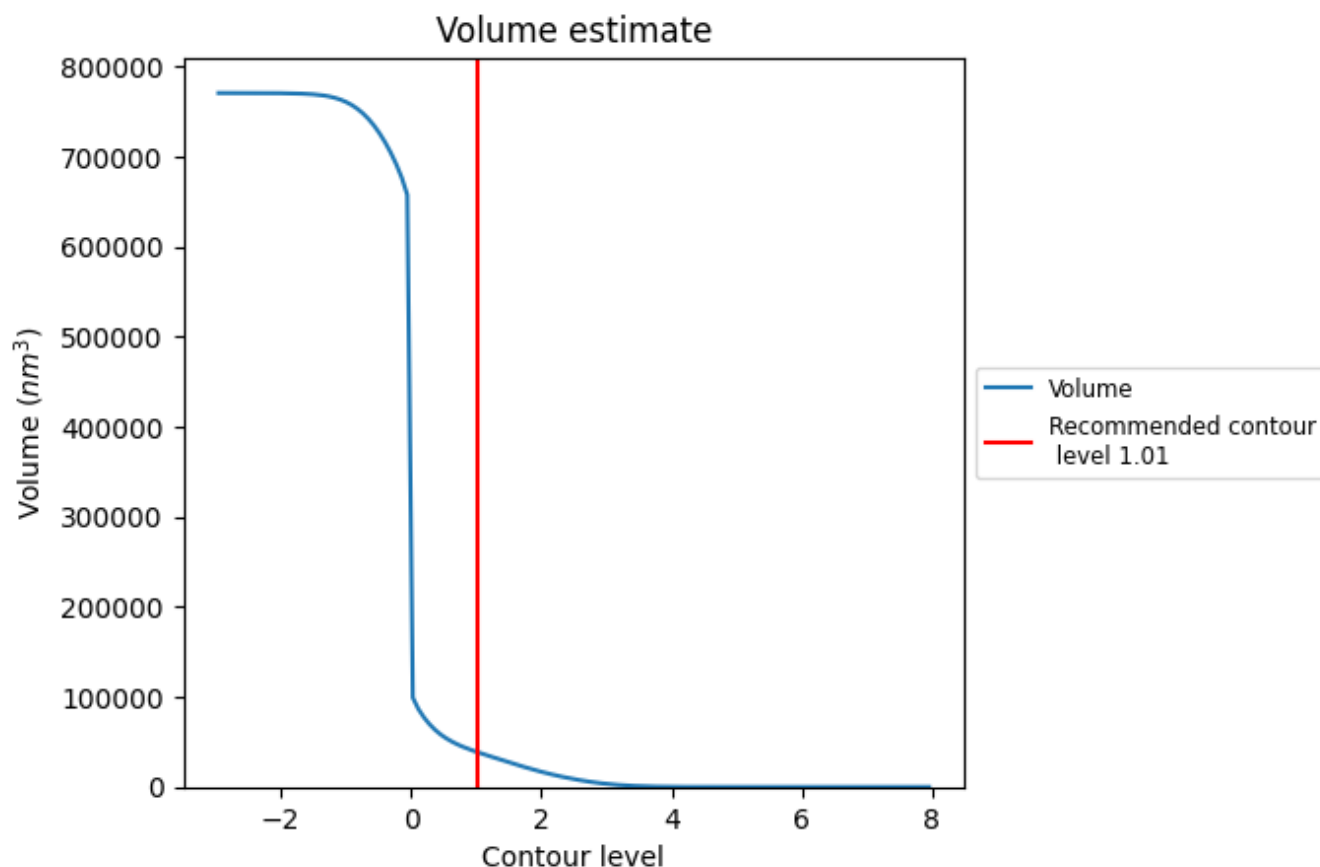
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38892 nm<sup>3</sup>; this corresponds to an approximate mass of 35132 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

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

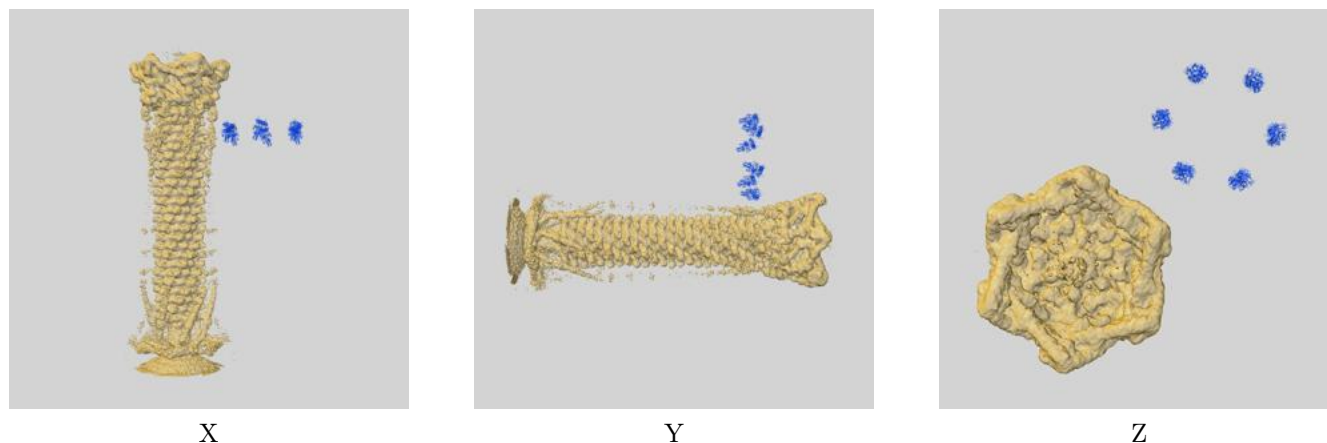
## 8 Fourier-Shell correlation

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

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

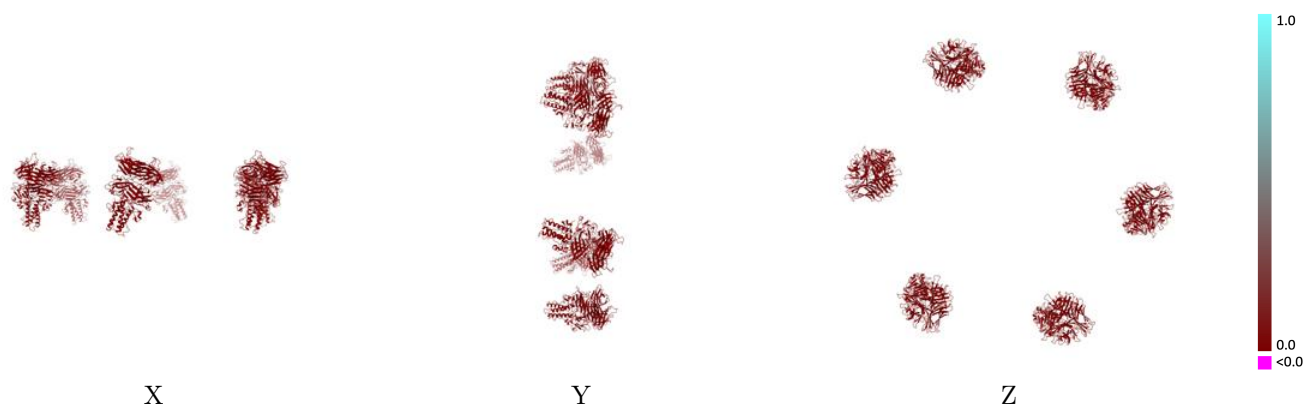
This section contains information regarding the fit between EMDB map EMD-1126 and PDB model 1ZKU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



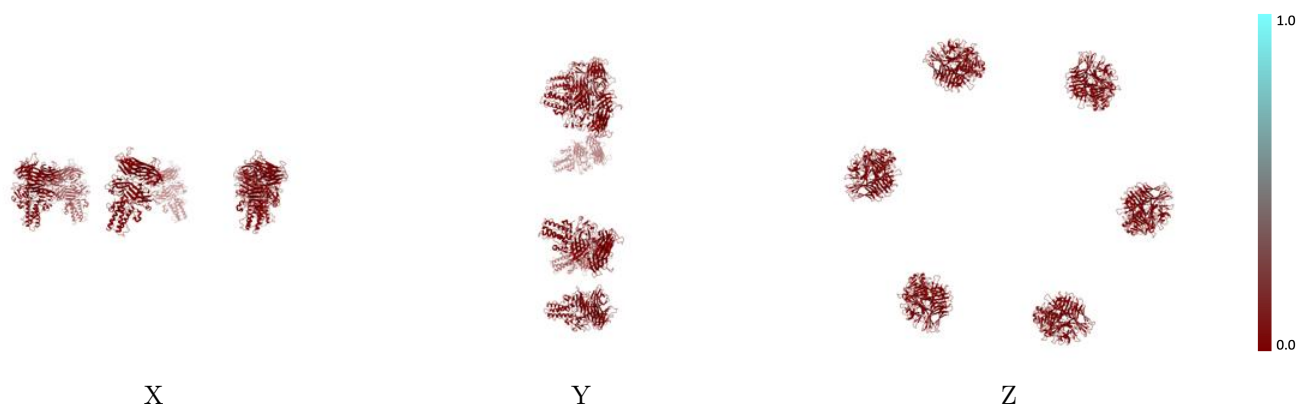
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



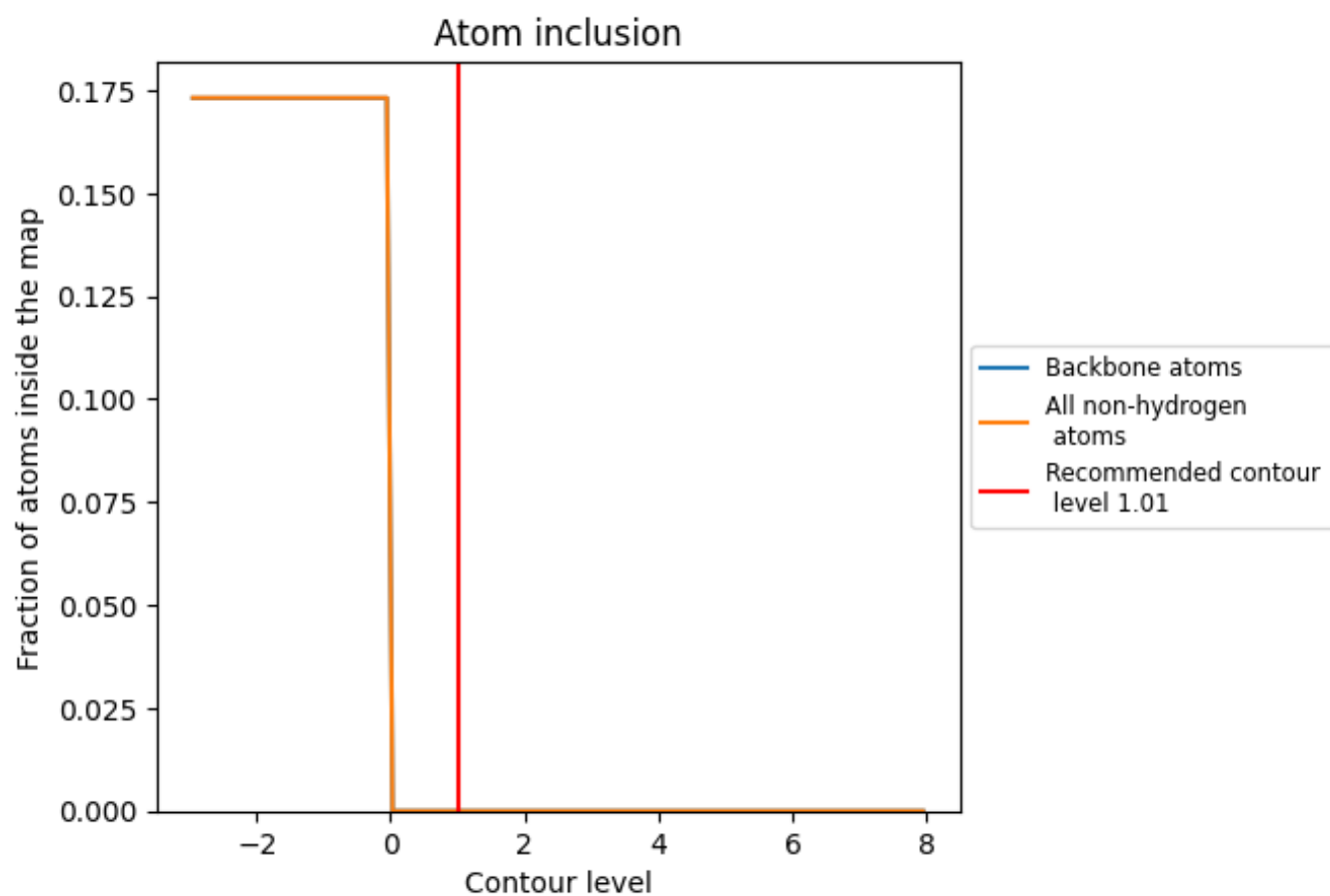
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (1.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| A     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| B     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| C     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| D     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| E     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| F     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| G     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| H     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| I     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| J     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| K     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| L     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| M     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| N     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| O     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| P     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| Q     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |
| R     | <div><div></div>0.0000</div> | <div><div></div>0.0000</div> |

1.0

0.0

<0.0