



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:39 PM UTC

PDB ID : 9DCB / pdb\_00009dcb  
EMDB ID : EMD-46748  
Title : The Structure of AAV5 at 4 Degrees  
Authors : Bennett, A.B.; McKenna, R.  
Deposited on : 2024-08-25  
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

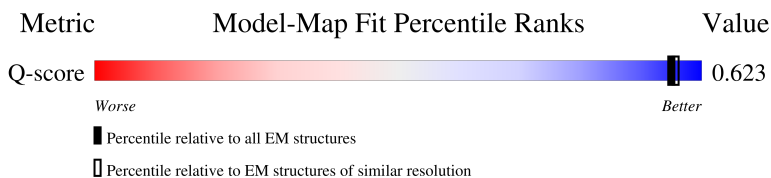
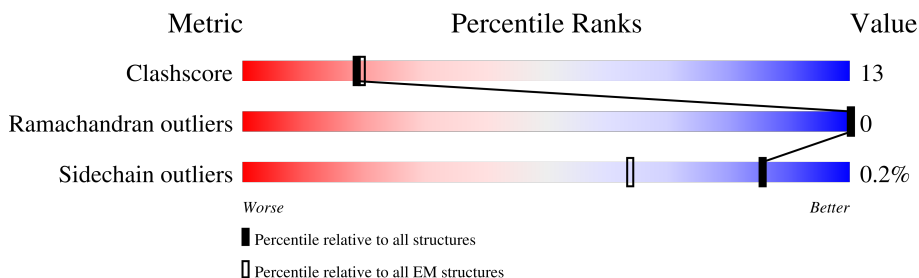
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









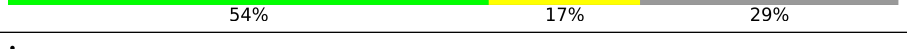
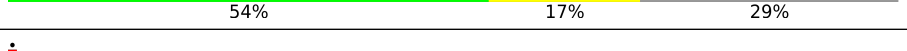
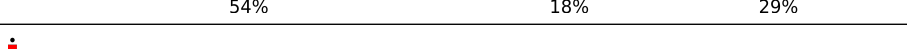
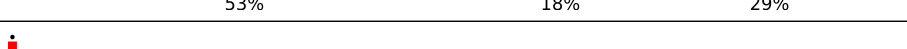
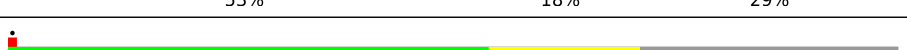

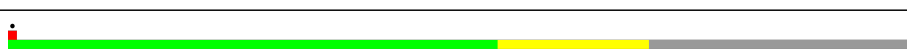

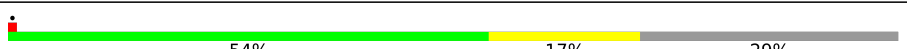





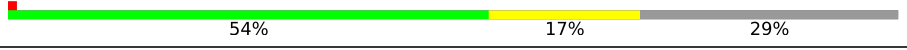
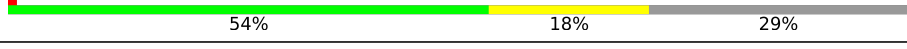



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| Q-score               | -                           | 25397                       | 12148 ( 2.39 - 3.39 )                                    |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 1     | 724    | <br>53% 18% 29% |
| 1   | 2     | 724    | <br>54% 17% 29% |
| 1   | 3     | 724    | <br>54% 17% 29% |
| 1   | 4     | 724    | <br>53% 18% 29% |



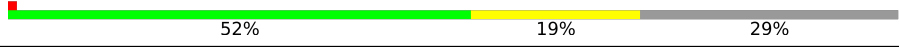




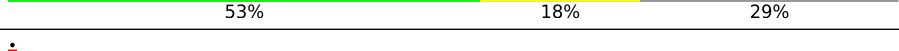
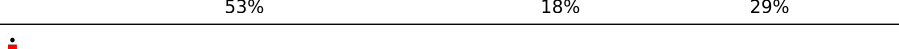
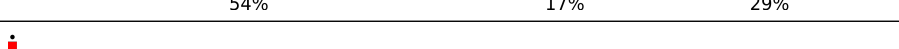
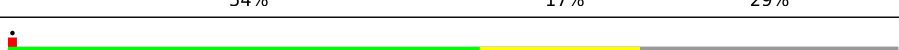

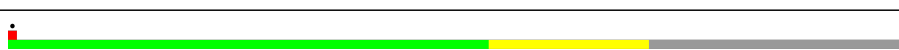

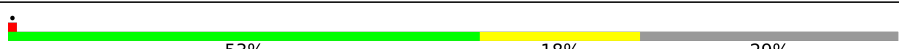





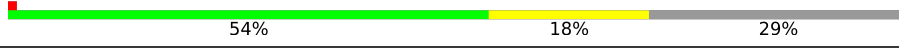
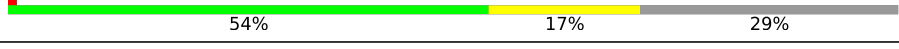



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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 5     | 724    |    |
| 1   | 6     | 724    |    |
| 1   | 7     | 724    |    |
| 1   | 8     | 724    |    |
| 1   | A     | 724    |    |
| 1   | B     | 724    |    |
| 1   | C     | 724    |    |
| 1   | D     | 724    |    |
| 1   | E     | 724    |    |
| 1   | F     | 724    |    |
| 1   | G     | 724    |    |
| 1   | H     | 724    |  |
| 1   | I     | 724    |  |
| 1   | J     | 724    |  |
| 1   | K     | 724    |  |
| 1   | L     | 724    |  |
| 1   | M     | 724    |  |
| 1   | N     | 724    |  |
| 1   | O     | 724    |  |
| 1   | P     | 724    |  |
| 1   | Q     | 724    |  |
| 1   | R     | 724    |  |
| 1   | S     | 724    |  |
| 1   | T     | 724    |  |
| 1   | U     | 724    |  |







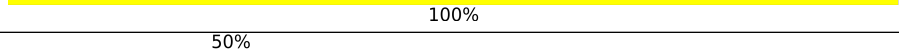
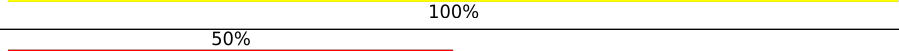
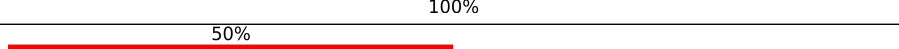
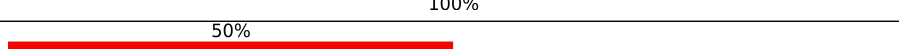
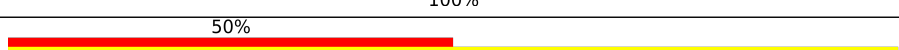
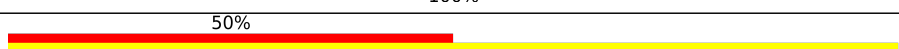

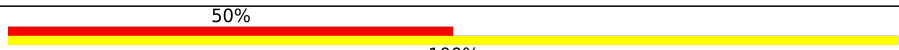
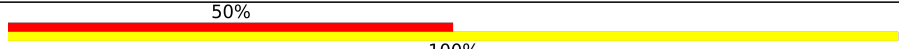


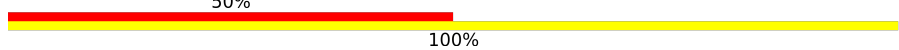
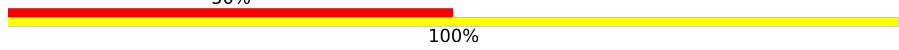

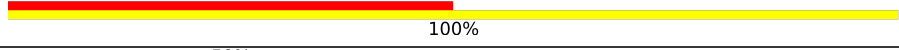
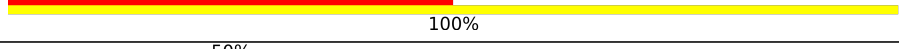
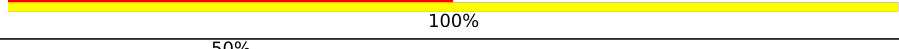
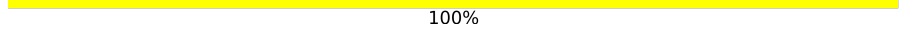

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | V     | 724    |    |
| 1   | W     | 724    |    |
| 1   | X     | 724    |    |
| 1   | Y     | 724    |    |
| 1   | Z     | 724    |    |
| 1   | a     | 724    |    |
| 1   | b     | 724    |    |
| 1   | c     | 724    |    |
| 1   | d     | 724    |    |
| 1   | e     | 724    |    |
| 1   | f     | 724    |    |
| 1   | g     | 724    |  |
| 1   | h     | 724    |  |
| 1   | i     | 724    |  |
| 1   | j     | 724    |  |
| 1   | k     | 724    |  |
| 1   | l     | 724    |  |
| 1   | m     | 724    |  |
| 1   | n     | 724    |  |
| 1   | o     | 724    |  |
| 1   | p     | 724    |  |
| 1   | q     | 724    |  |
| 1   | r     | 724    |  |
| 1   | s     | 724    |  |
| 1   | t     | 724    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | u     | 724    |    |
| 1   | v     | 724    |    |
| 1   | w     | 724    |    |
| 1   | x     | 724    |    |
| 1   | y     | 724    |    |
| 1   | z     | 724    |    |
| 2   | 0     | 2      |    |
| 2   | 0A    | 2      |    |
| 2   | 1A    | 2      |    |
| 2   | 2A    | 2      |    |
| 2   | 3A    | 2      |    |
| 2   | 4A    | 2      |  |
| 2   | 5A    | 2      |  |
| 2   | 9     | 2      |  |
| 2   | AA    | 2      |  |
| 2   | BA    | 2      |  |
| 2   | CA    | 2      |  |
| 2   | DA    | 2      |  |
| 2   | EA    | 2      |  |
| 2   | FA    | 2      |  |
| 2   | GA    | 2      |  |
| 2   | HA    | 2      |  |
| 2   | IA    | 2      |  |
| 2   | JA    | 2      |  |
| 2   | KA    | 2      |  |

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| Mol | Chain | Length | Quality of chain |      |
|-----|-------|--------|------------------|------|
| 2   | LA    | 2      | 50%              | 100% |
| 2   | MA    | 2      | 50%              | 100% |
| 2   | NA    | 2      | 50%              | 100% |
| 2   | OA    | 2      | 50%              | 100% |
| 2   | PA    | 2      | 50%              | 100% |
| 2   | QA    | 2      | 50%              | 100% |
| 2   | RA    | 2      | 50%              | 100% |
| 2   | SA    | 2      | 50%              | 100% |
| 2   | TA    | 2      | 50%              | 100% |
| 2   | UA    | 2      | 50%              | 100% |
| 2   | VA    | 2      | 50%              | 100% |
| 2   | WA    | 2      | 50%              | 100% |
| 2   | XA    | 2      | 50%              | 100% |
| 2   | YA    | 2      | 50%              | 100% |
| 2   | ZA    | 2      | 50%              | 100% |
| 2   | aA    | 2      | 50%              | 100% |
| 2   | bA    | 2      | 50%              | 100% |
| 2   | cA    | 2      | 50%              | 100% |
| 2   | dA    | 2      | 50%              | 100% |
| 2   | eA    | 2      | 50%              | 100% |
| 2   | fA    | 2      | 50%              | 100% |
| 2   | gA    | 2      | 50%              | 100% |
| 2   | hA    | 2      | 50%              | 100% |
| 2   | iA    | 2      | 50%              | 100% |
| 2   | jA    | 2      | 50%              | 100% |

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| Mol | Chain | Length | Quality of chain                            |
|-----|-------|--------|---|
| 2   | kA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | lA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | mA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | nA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | oA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | pA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | qA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | rA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | sA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | tA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | uA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | vA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | wA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | xA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | yA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |
| 2   | zA    | 2      | <div> <div>50%</div> <div>100%</div> </div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 249480 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 Capsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | B     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | C     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | D     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | E     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | F     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | G     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | H     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | I     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | J     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | K     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | L     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | M     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | N     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | O     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | P     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |
| 1   | Q     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | R     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | S     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | T     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | U     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | V     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | W     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | X     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | Y     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | Z     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | a     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | b     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | c     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | d     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | e     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | f     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | g     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | h     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | i     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | j     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | k     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | l     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | m     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | n     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | o     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | p     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | q     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | r     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | s     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | t     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | u     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | v     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | w     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | x     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | y     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | z     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 1     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 2     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 3     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 4     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 5     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 6     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |
| 1   | 7     | 517      | Total<br>4116 | C<br>2603 | N<br>706 | O<br>791 | S<br>16 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 8     | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4116  | 2603 | 706 | 791 | 16 |         |       |

- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 2   | 0     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | JA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | UA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | fA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | qA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | 1A    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | 3A    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | 4A    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | 5A    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | 9     | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | AA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | BA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | CA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | DA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | EA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | FA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | GA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |
| 2   | HA    | 2        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 42    | 20 | 10 | 10 | 2 |         |       |

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| Mol | Chain | Residues | Atoms       |         |         |         |        | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|--------|---------|-------|
| 2   | IA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | KA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | LA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | MA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | NA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | OA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | PA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | QA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | RA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | SA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | TA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | VA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | WA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | XA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | YA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | ZA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | aA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | bA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | cA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | dA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | eA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |

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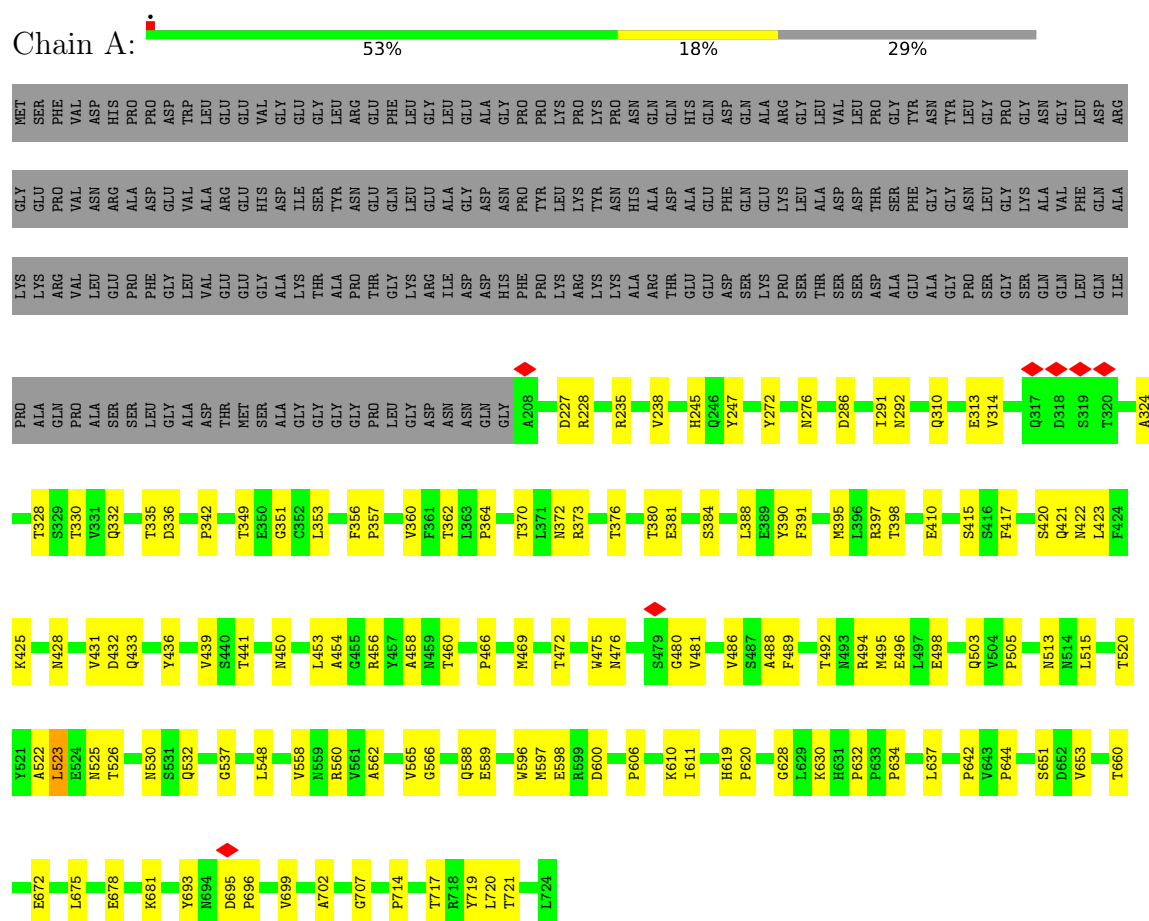
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| Mol | Chain | Residues | Atoms       |         |         |         |        | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|--------|---------|-------|
| 2   | gA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | hA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | iA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | jA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | kA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | lA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | mA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | nA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | oA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | pA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | rA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | sA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | tA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | uA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | vA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | wA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | xA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | yA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | zA    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | 0A    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |
| 2   | 2A    | 2        | Total<br>42 | C<br>20 | N<br>10 | O<br>10 | P<br>2 | 0       | 0     |

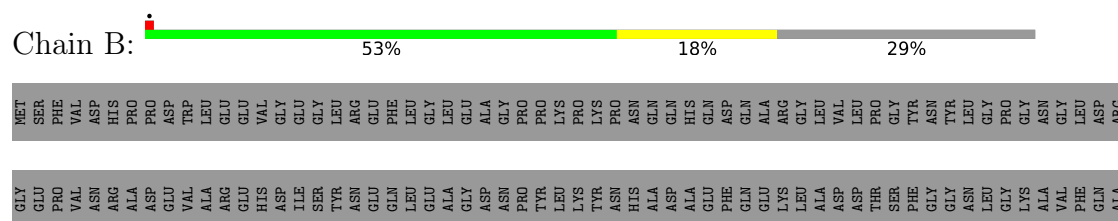
### 3 Residue-property plots

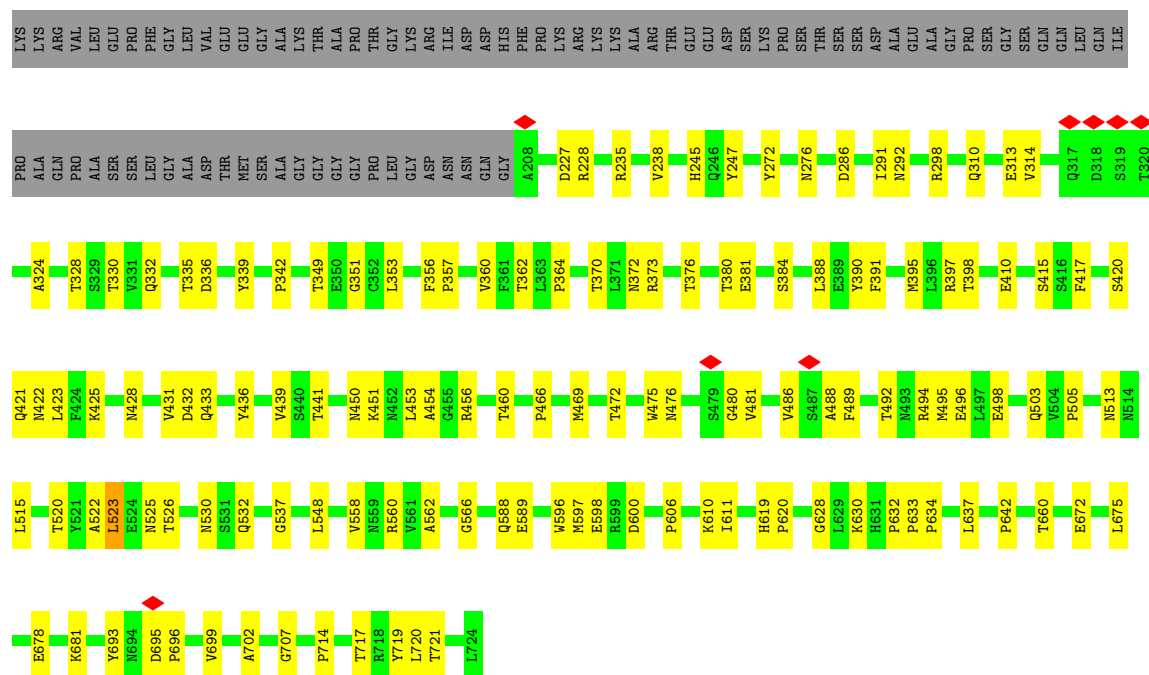
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Capsid protein

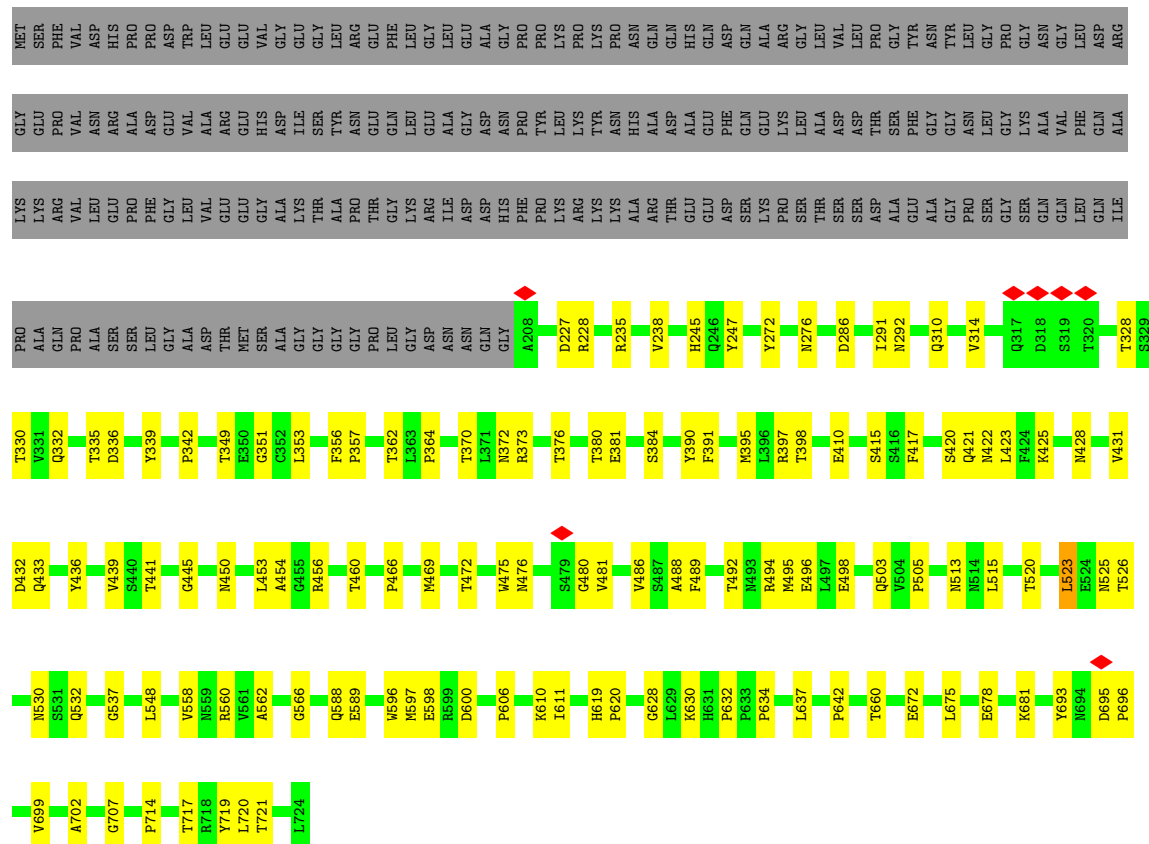


#### • Molecule 1: Capsid protein

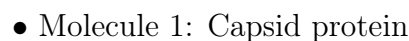




### • Molecule 1: Capsid protein

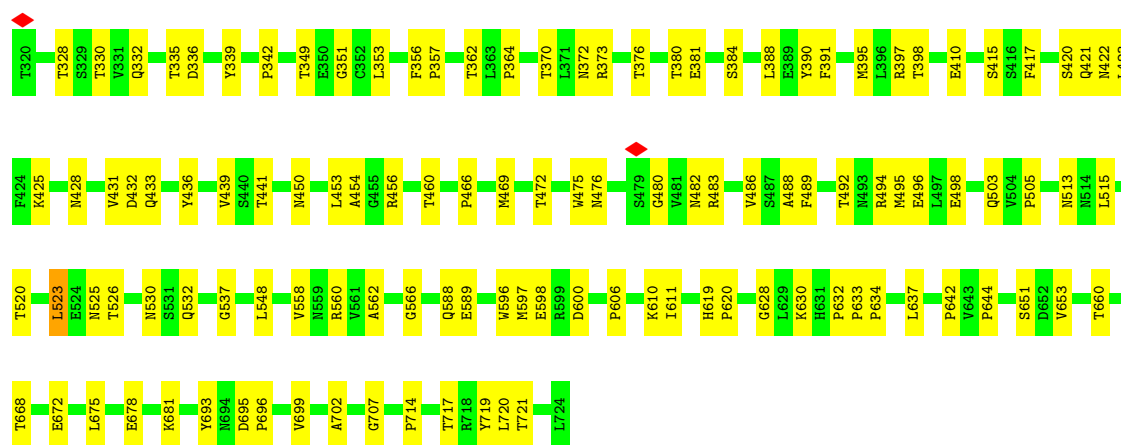


### • Molecule 1: Capsid protein

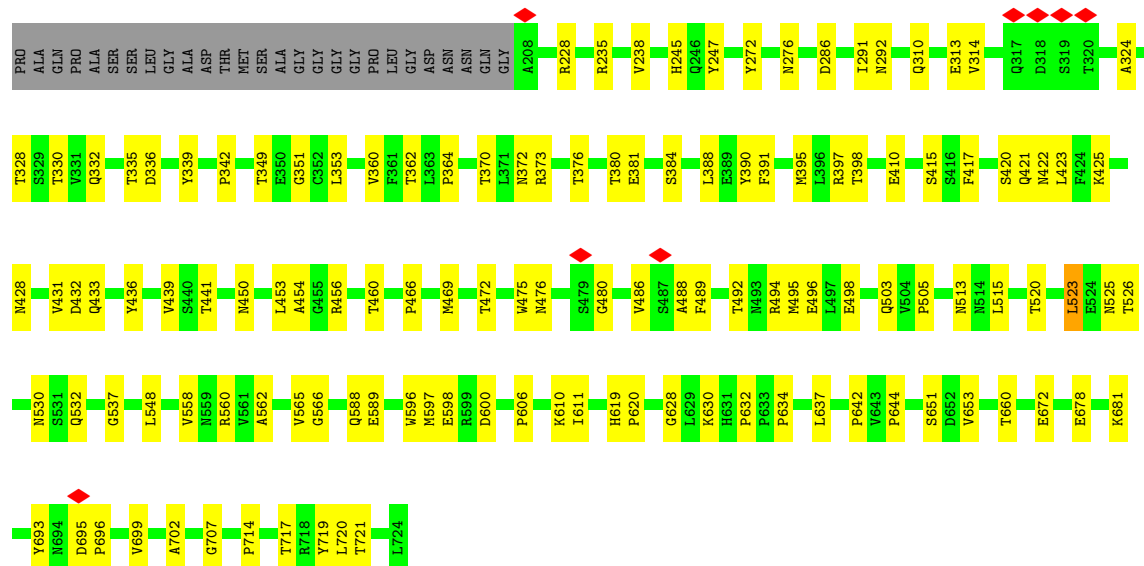
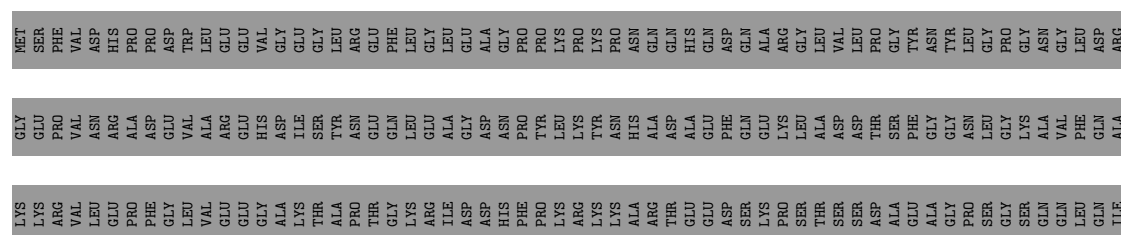




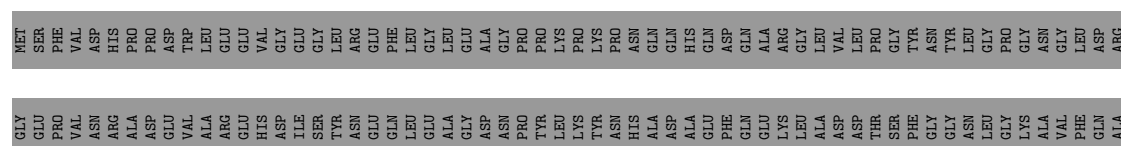


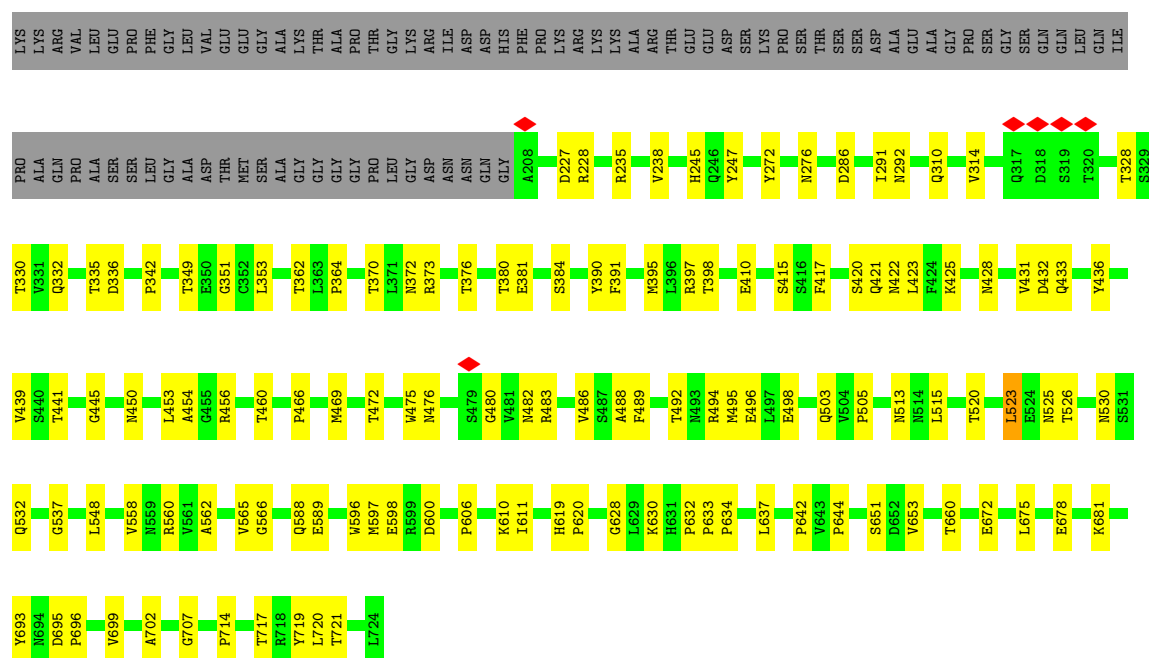


• Molecule 1: Capsid protein

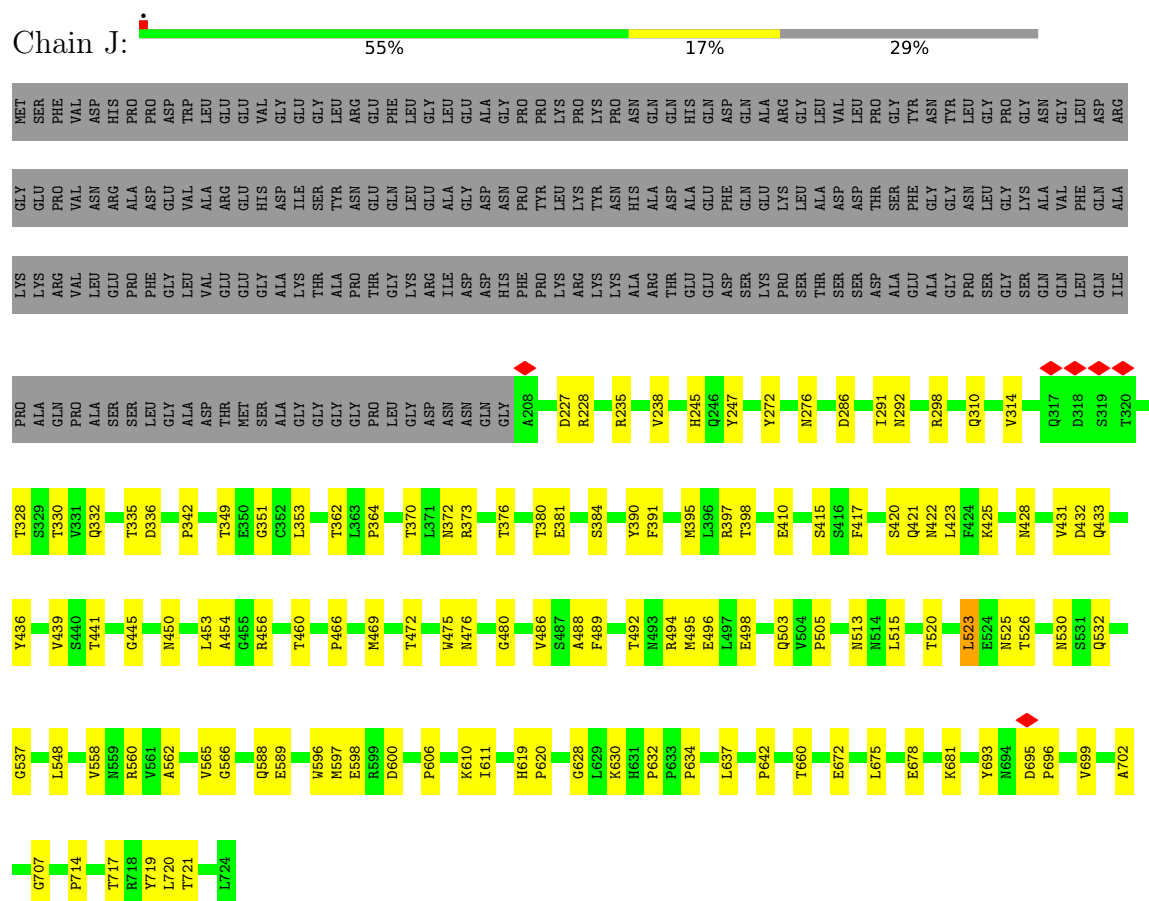


• Molecule 1: Capsid protein





- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

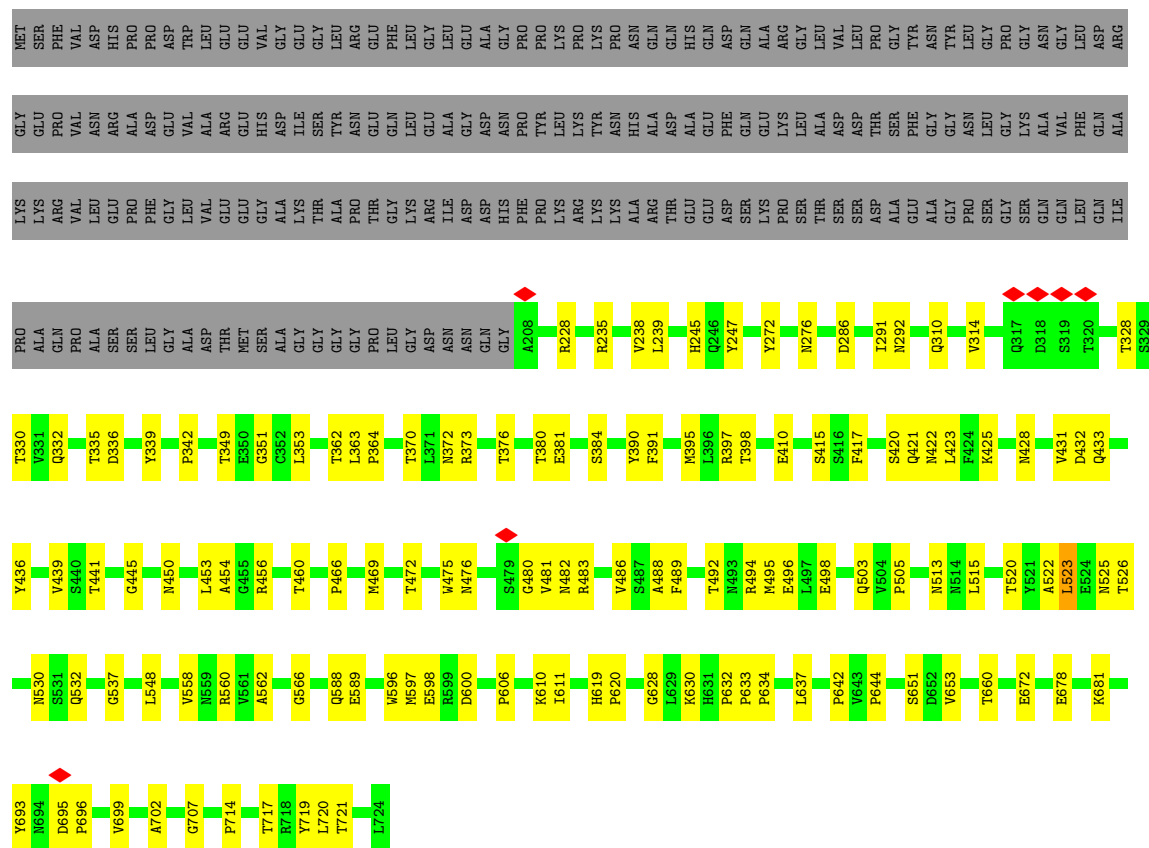






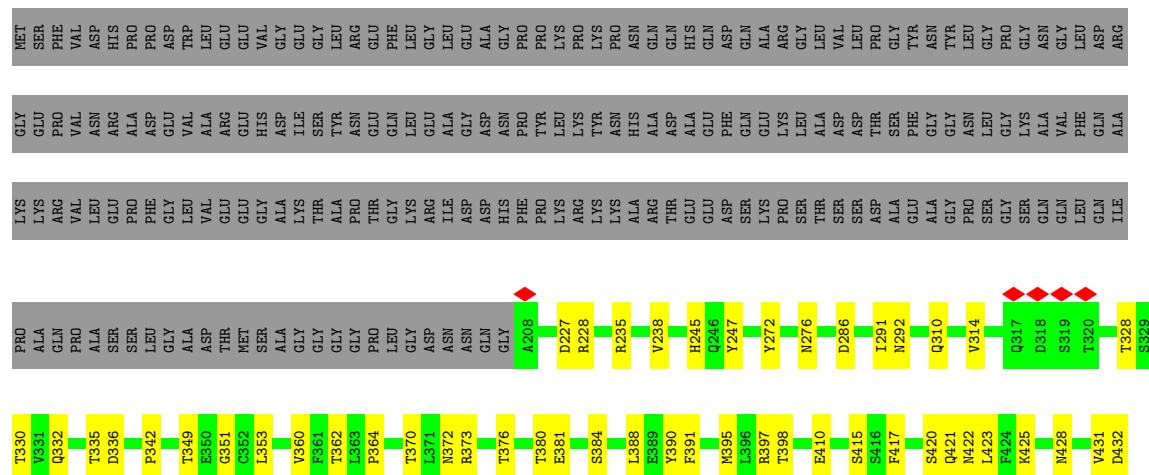
• Molecule 1: Capsid protein

Chain M: 54% 18% 29%

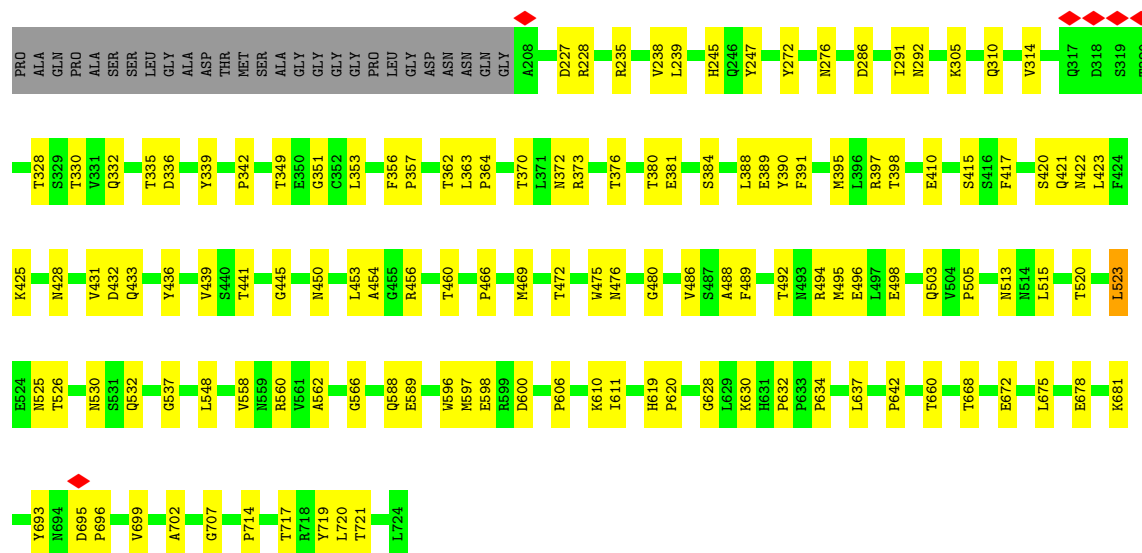


• Molecule 1: Capsid protein

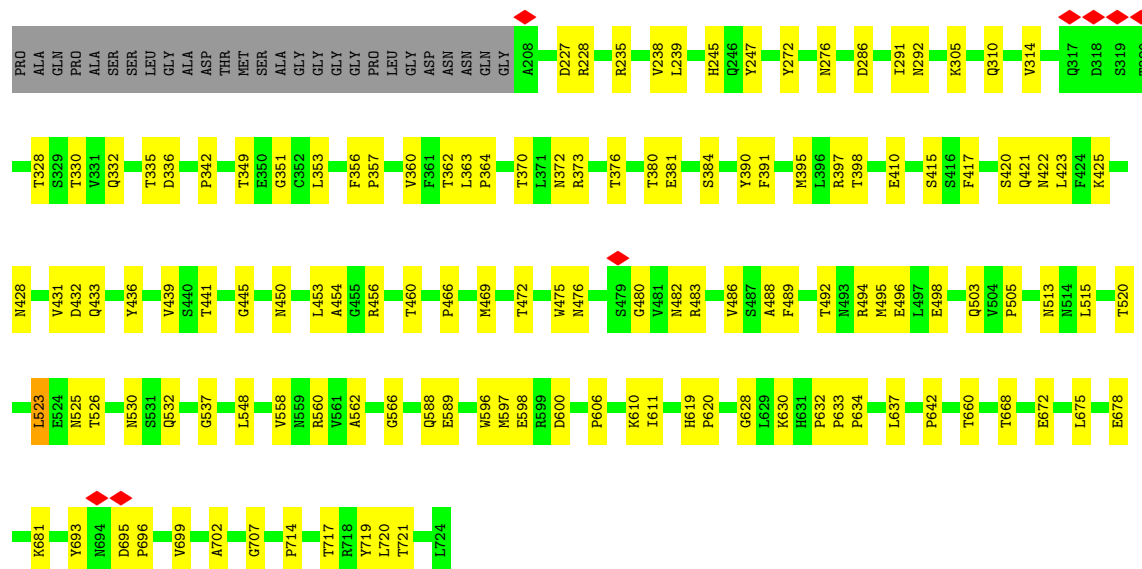
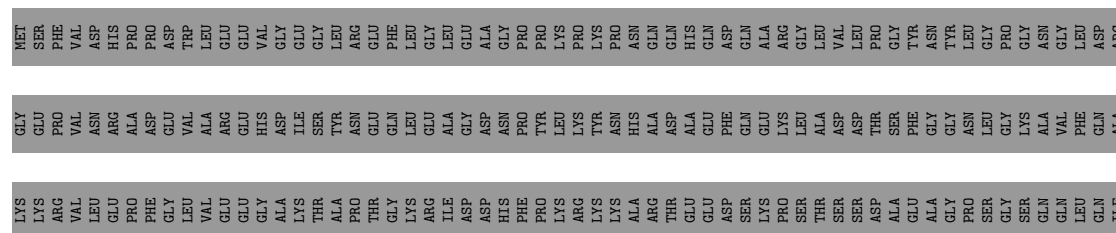
Chain N: 54% 17% 29%





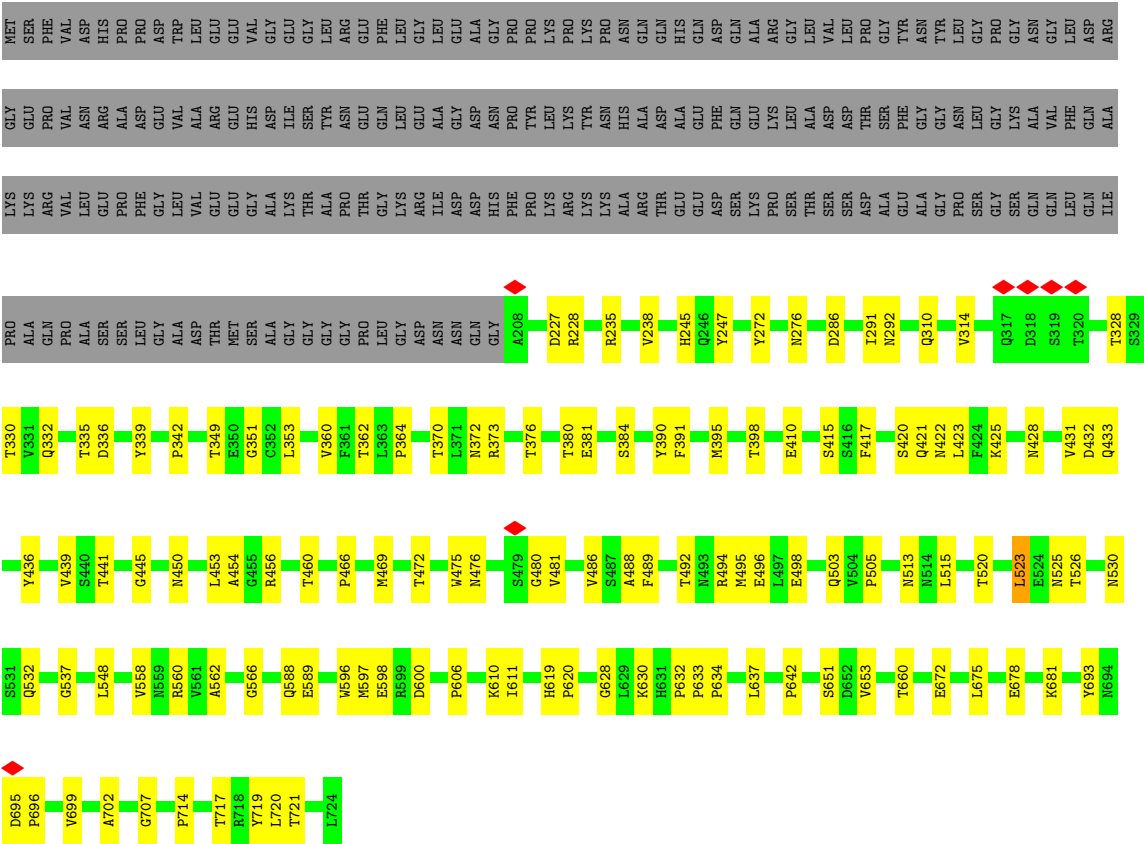


• Molecule 1: Capsid protein

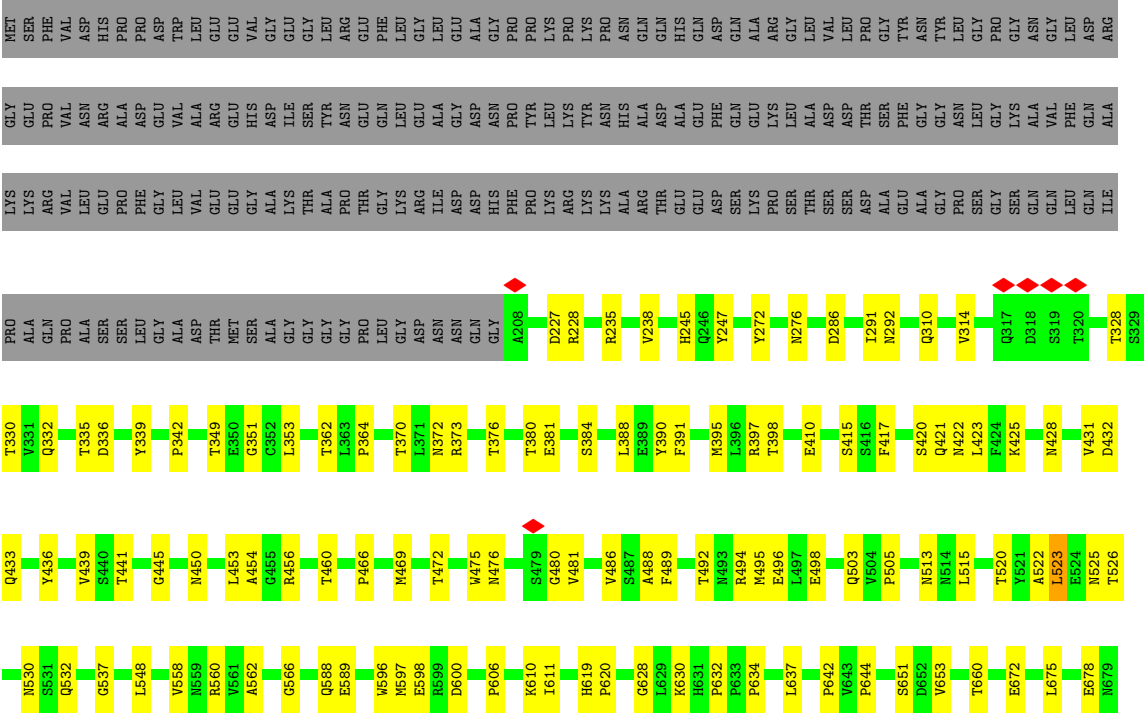


• Molecule 1: Capsid protein



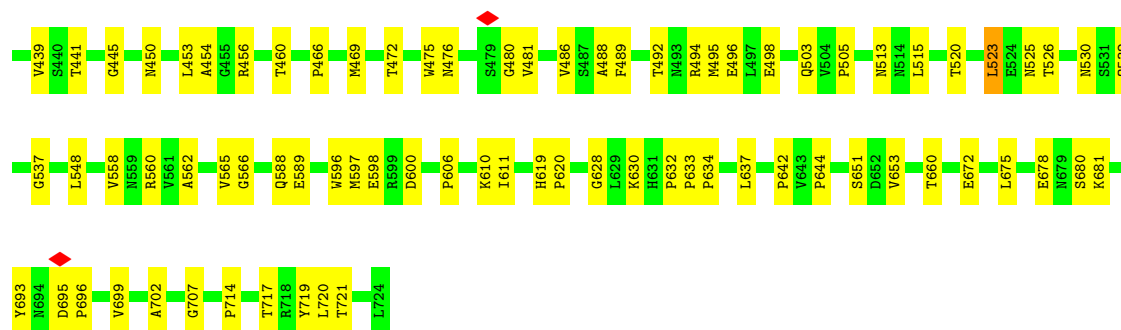


● Molecule 1: Capsid protein

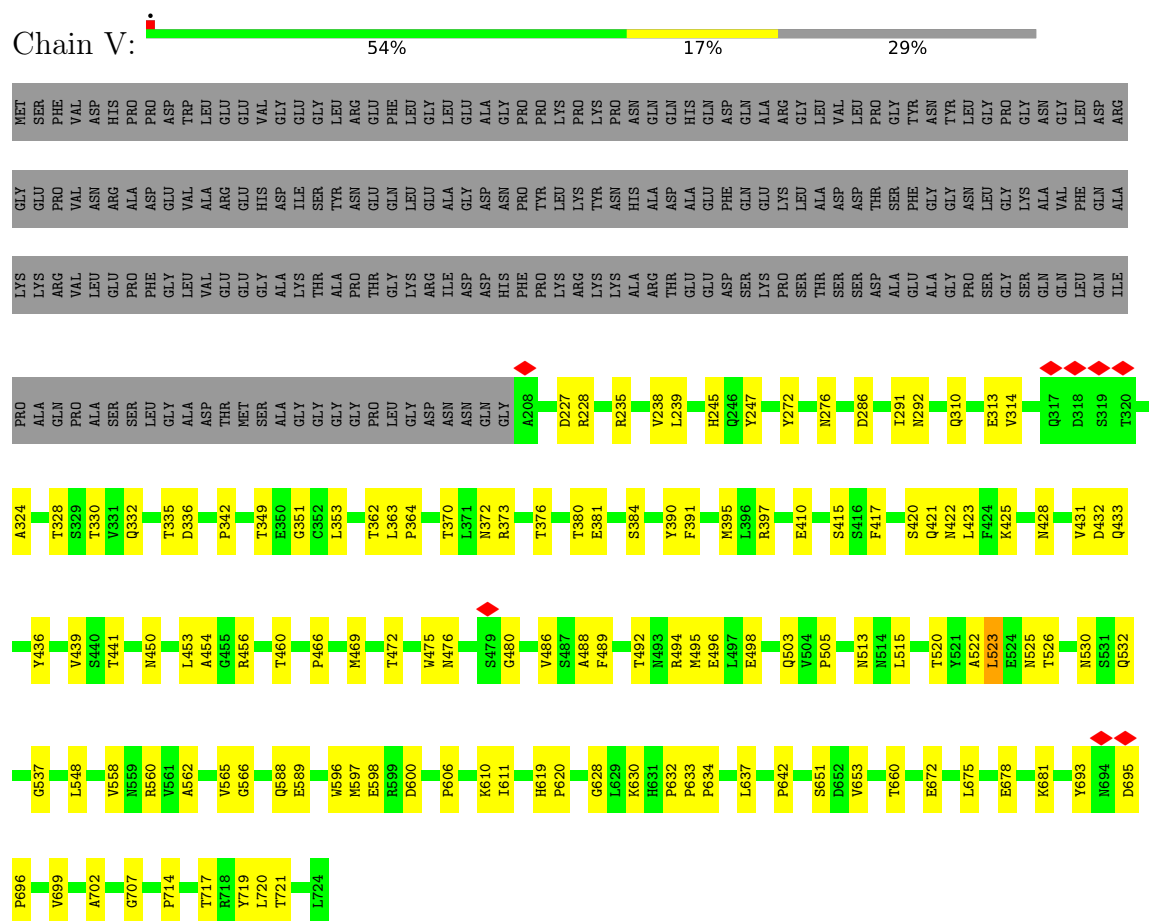




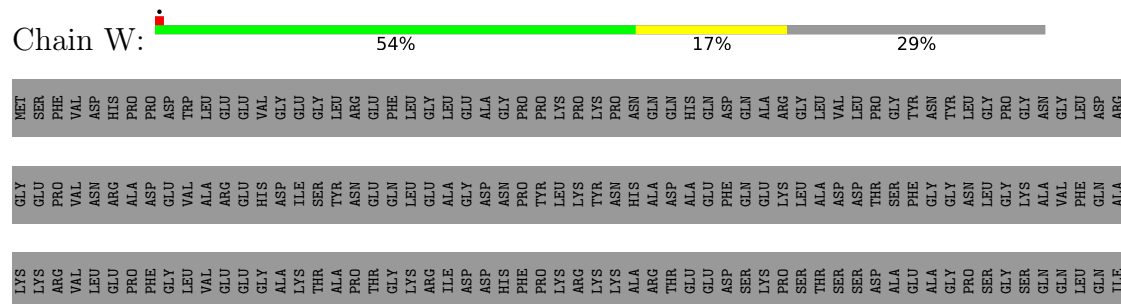


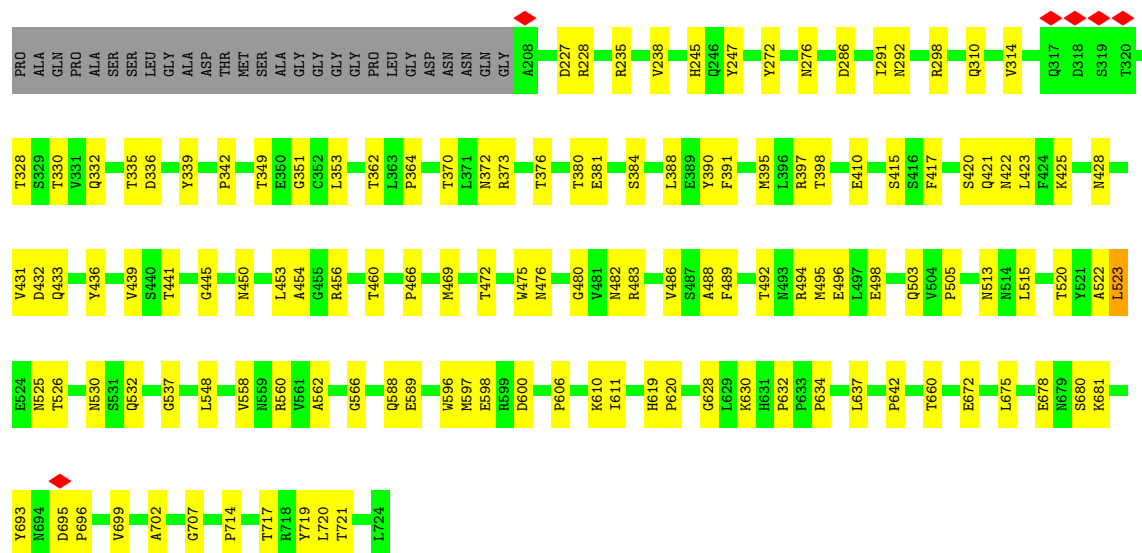


- Molecule 1: Capsid protein

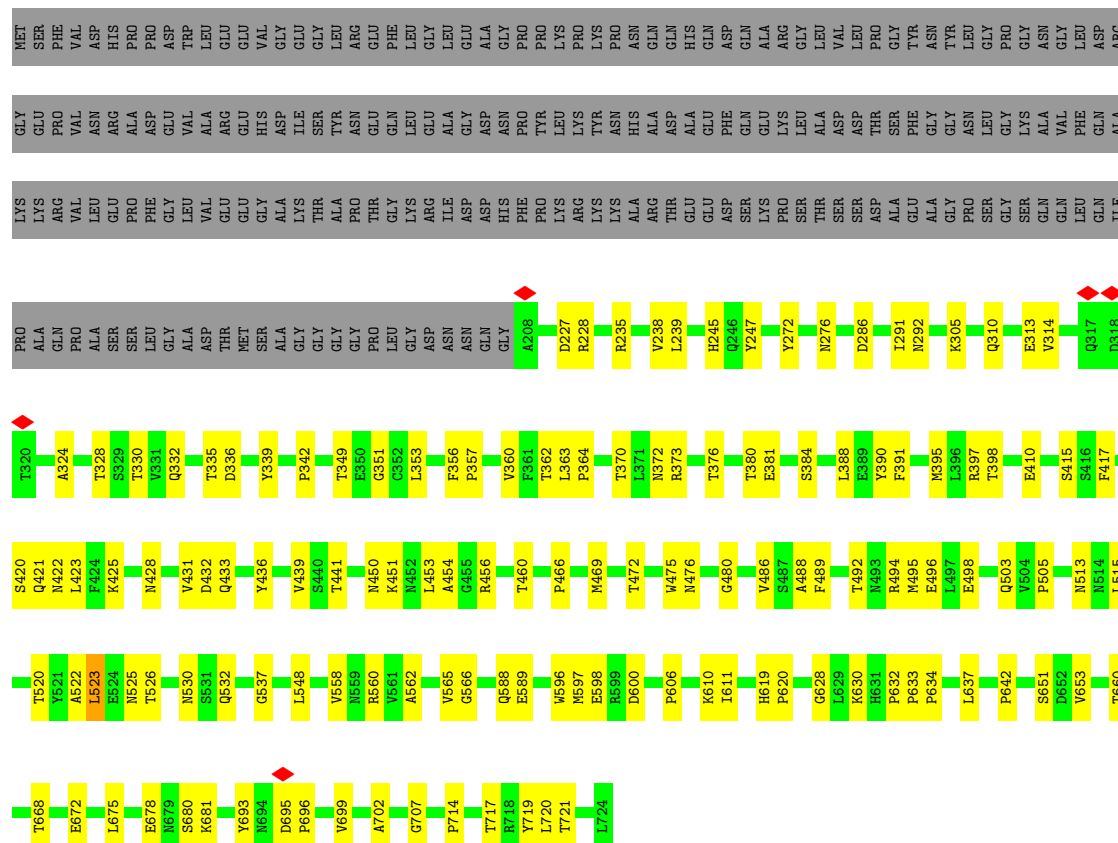


- Molecule 1: Capsid protein



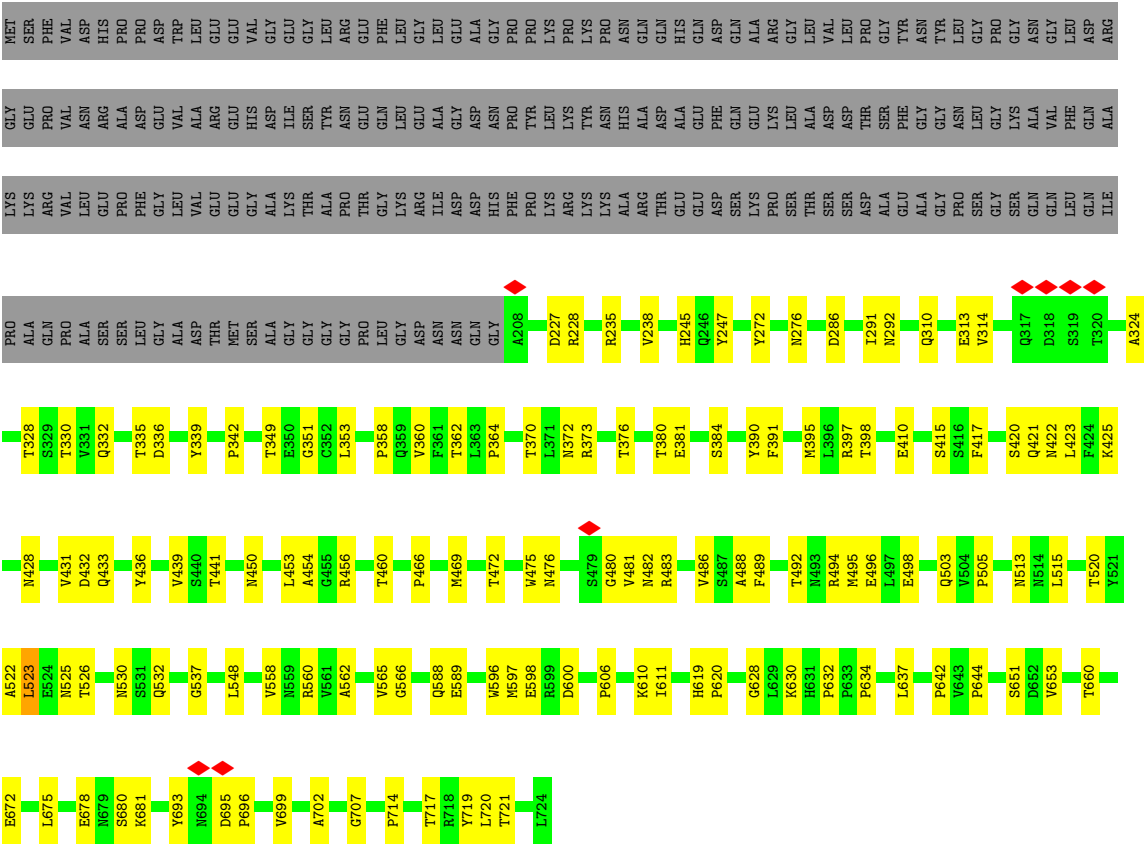


- Molecule 1: Capsid protein

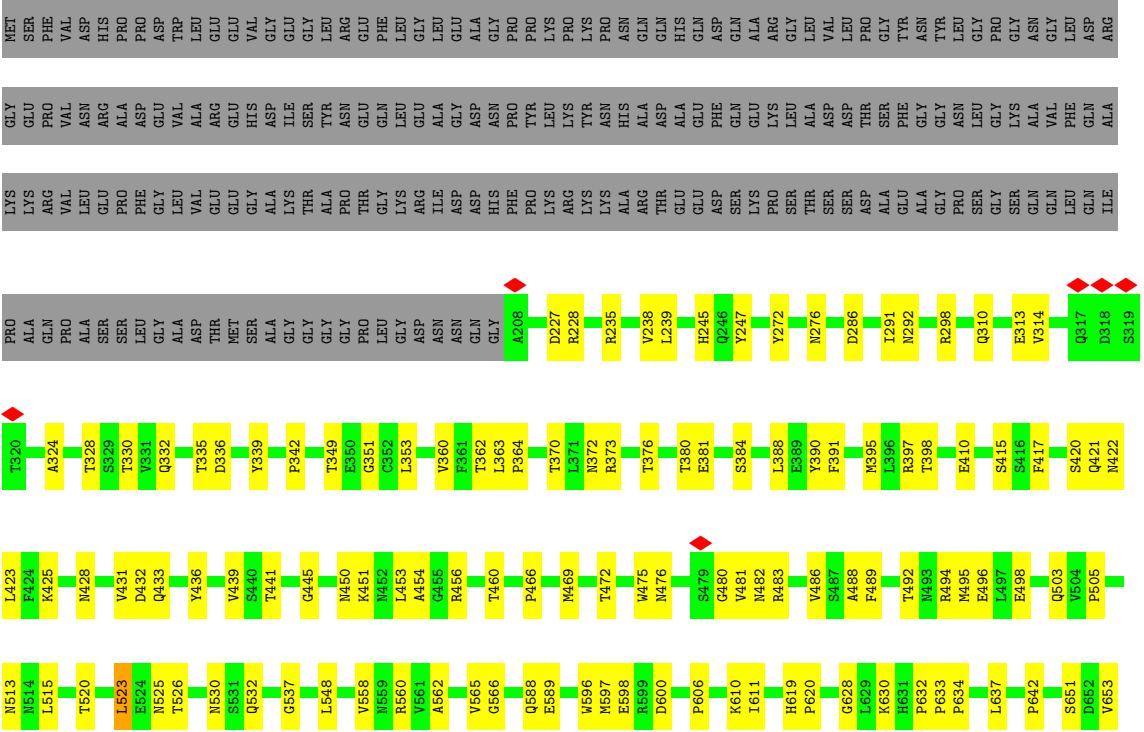


- Molecule 1: Capsid protein

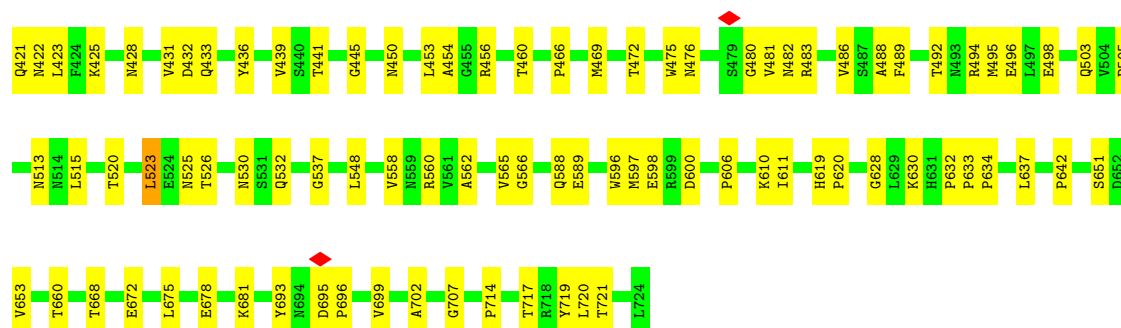




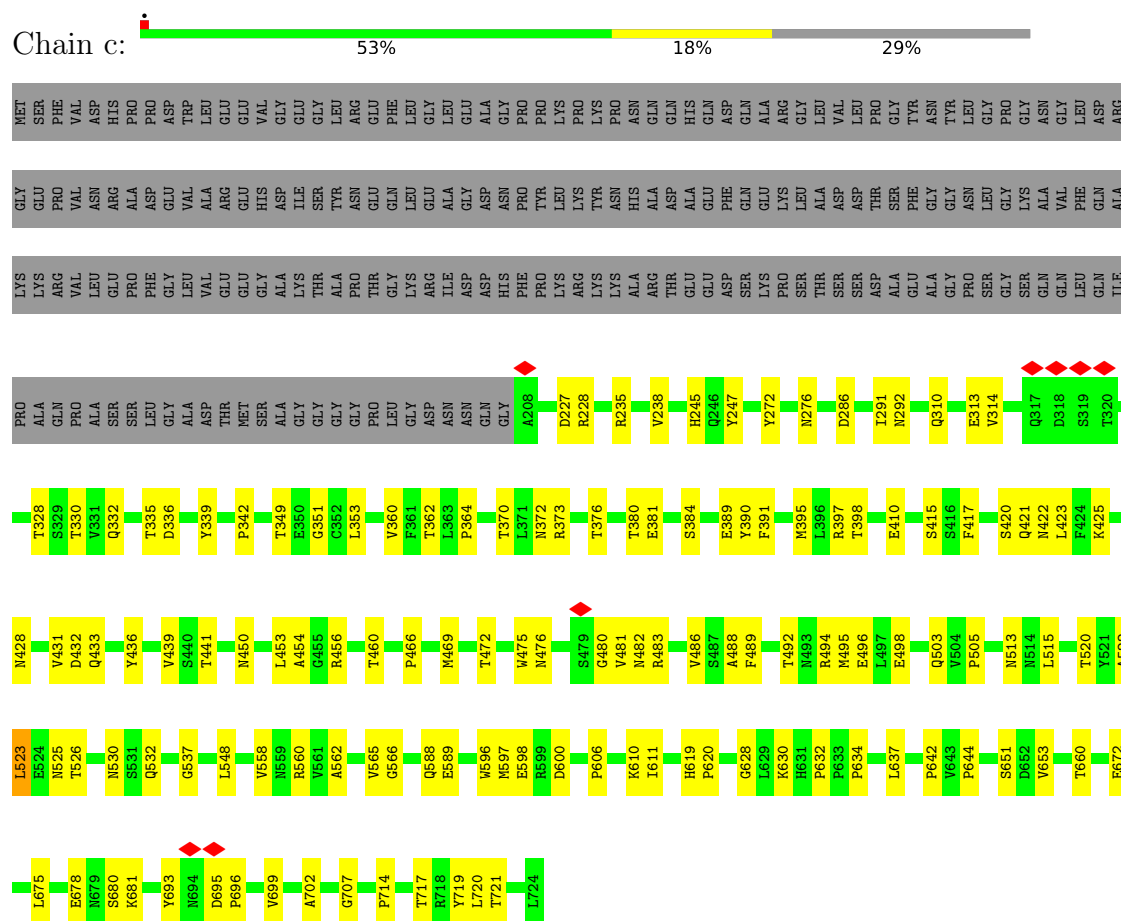
• Molecule 1: Capsid protein



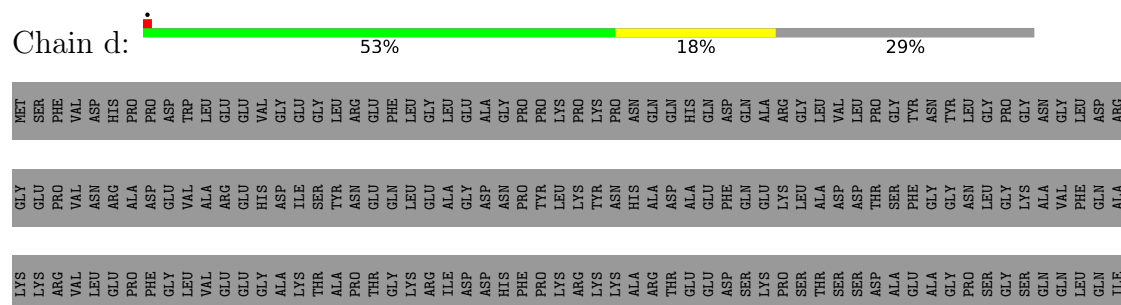


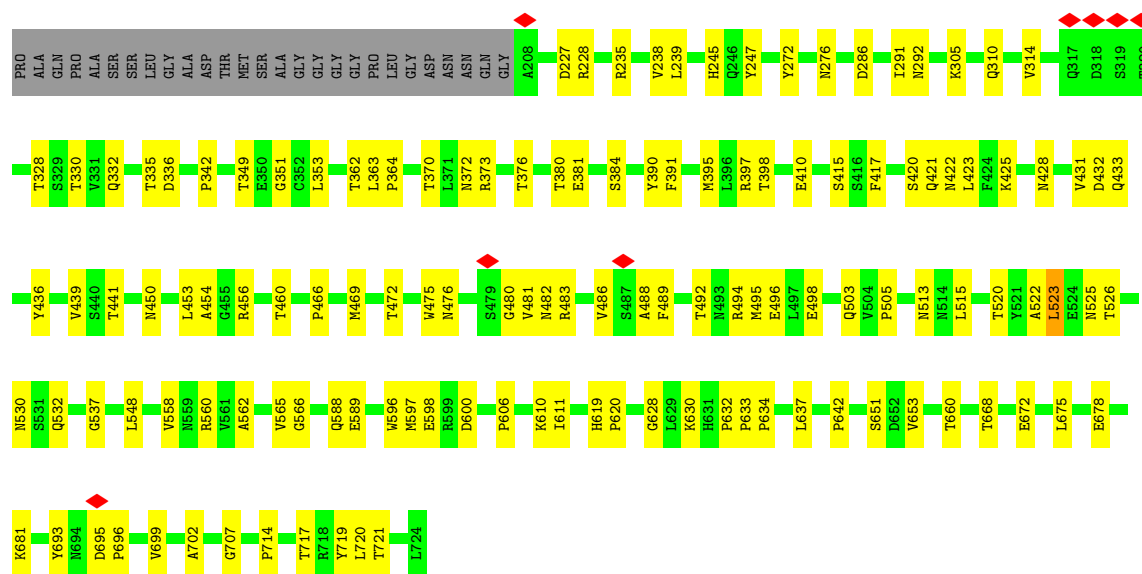


- Molecule 1: Capsid protein

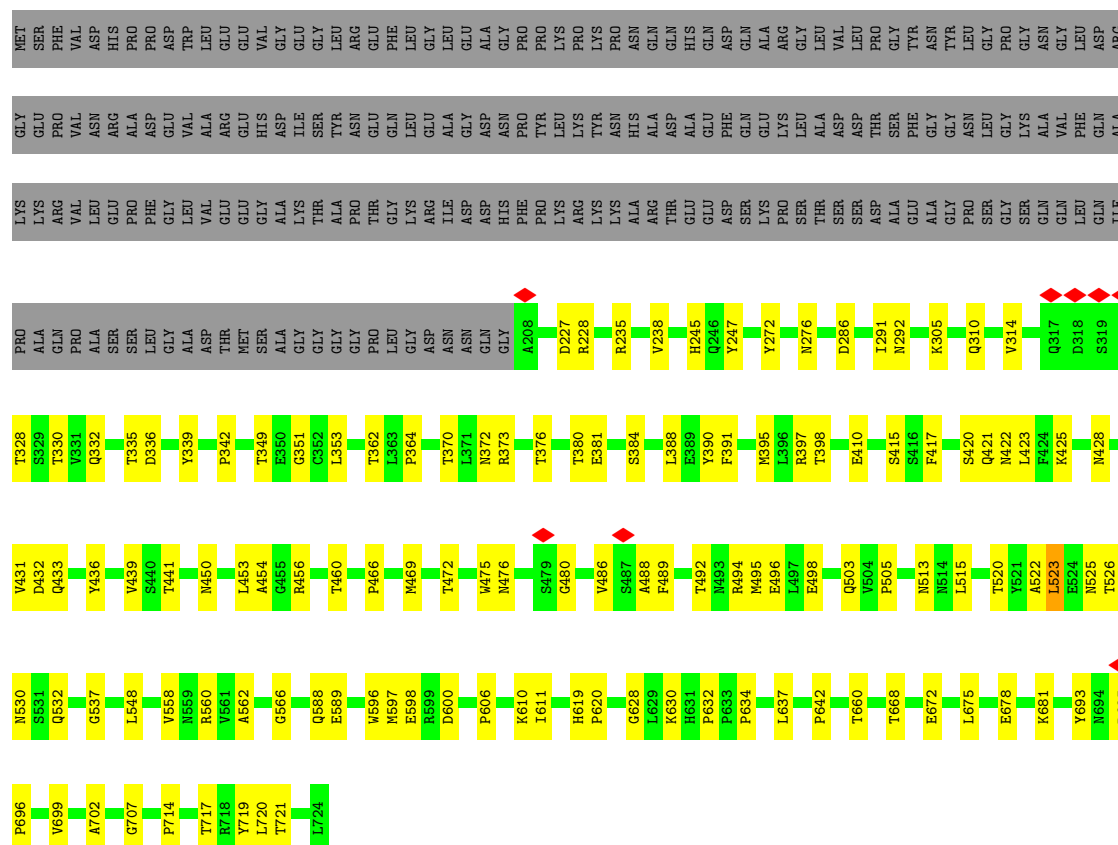


- Molecule 1: Capsid protein



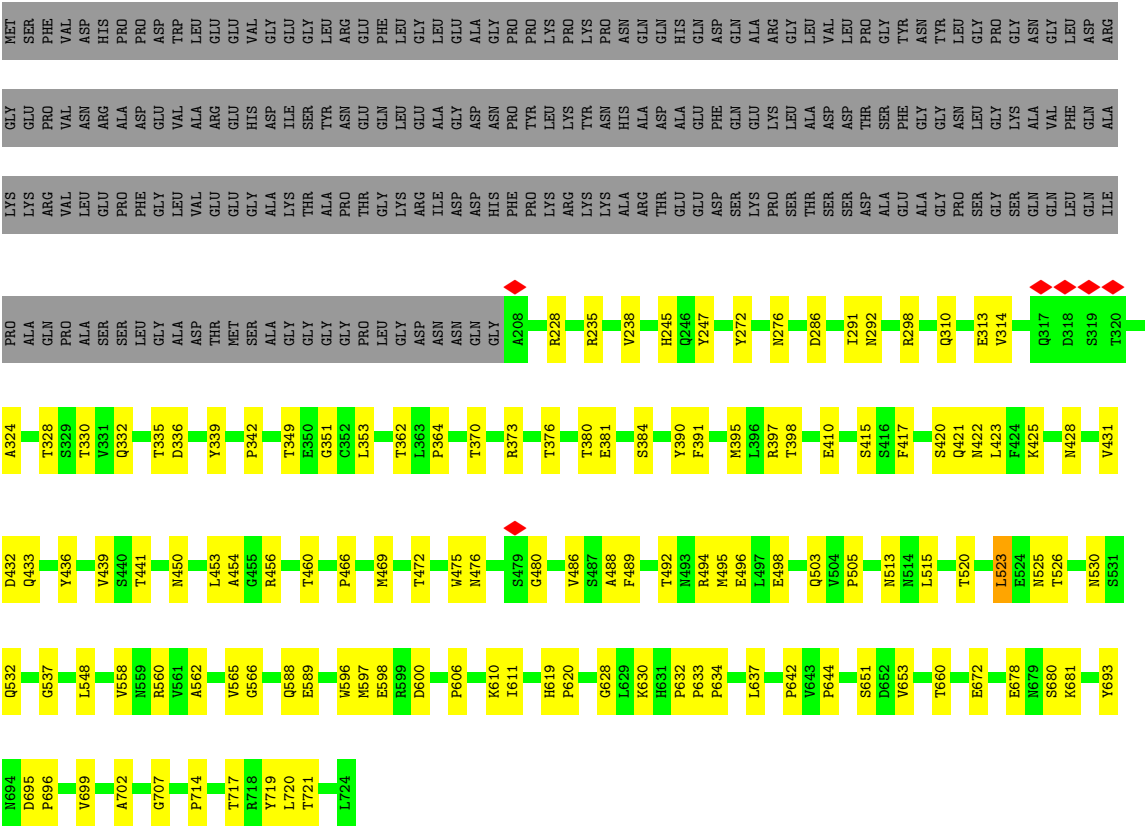


• Molecule 1: Capsid protein

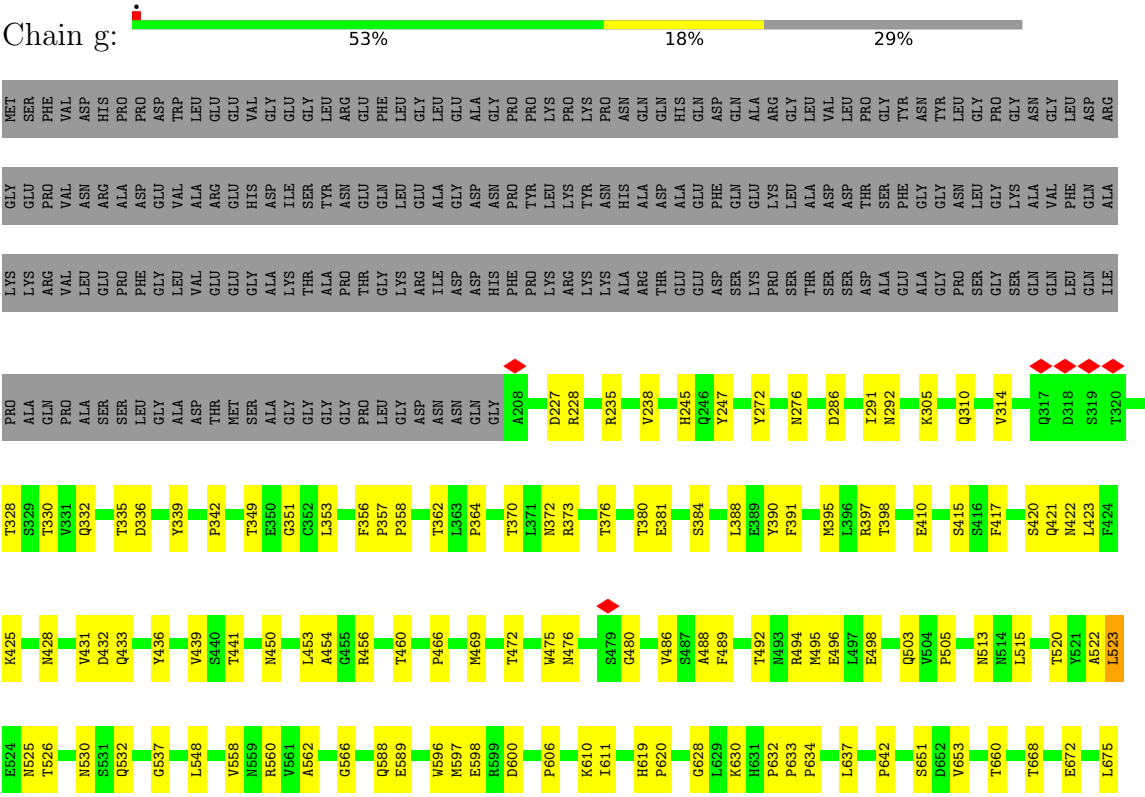


• Molecule 1: Capsid protein



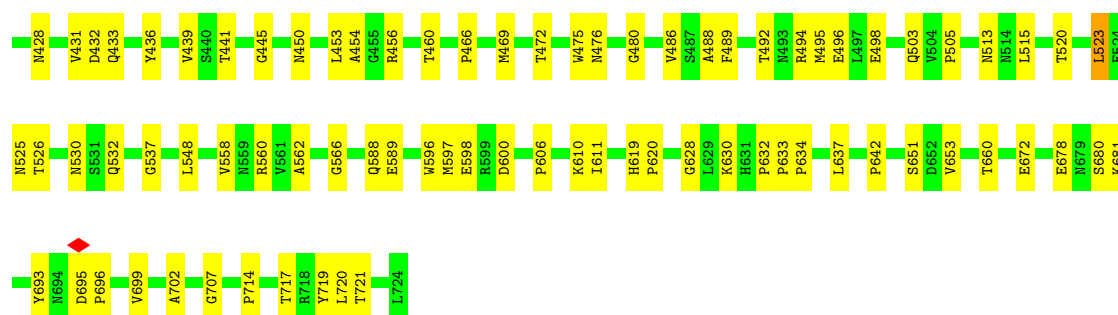


• Molecule 1: Capsid protein

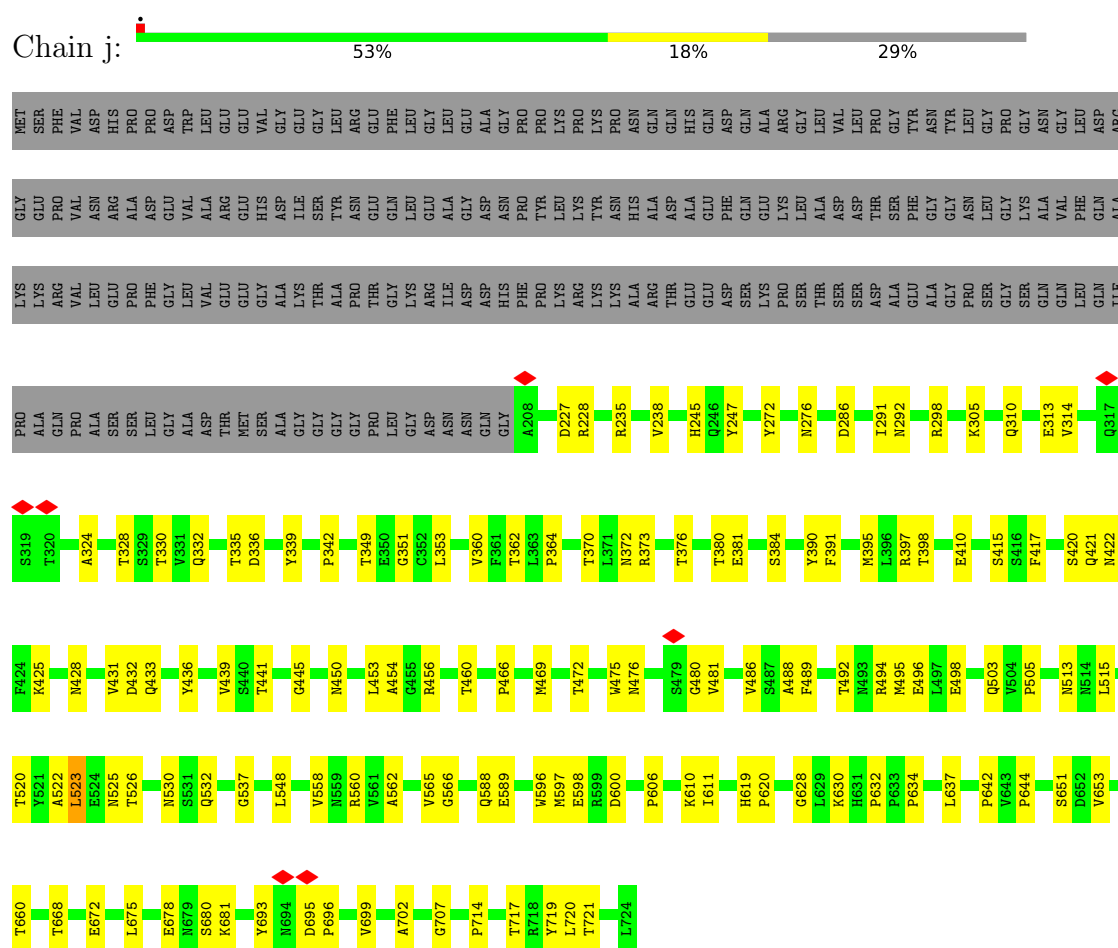




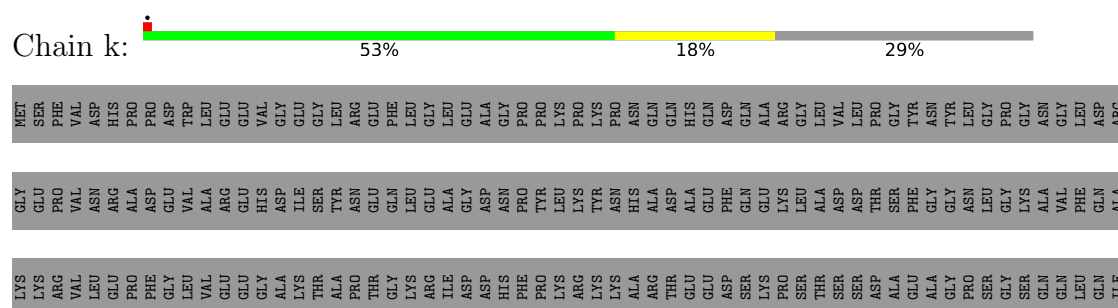




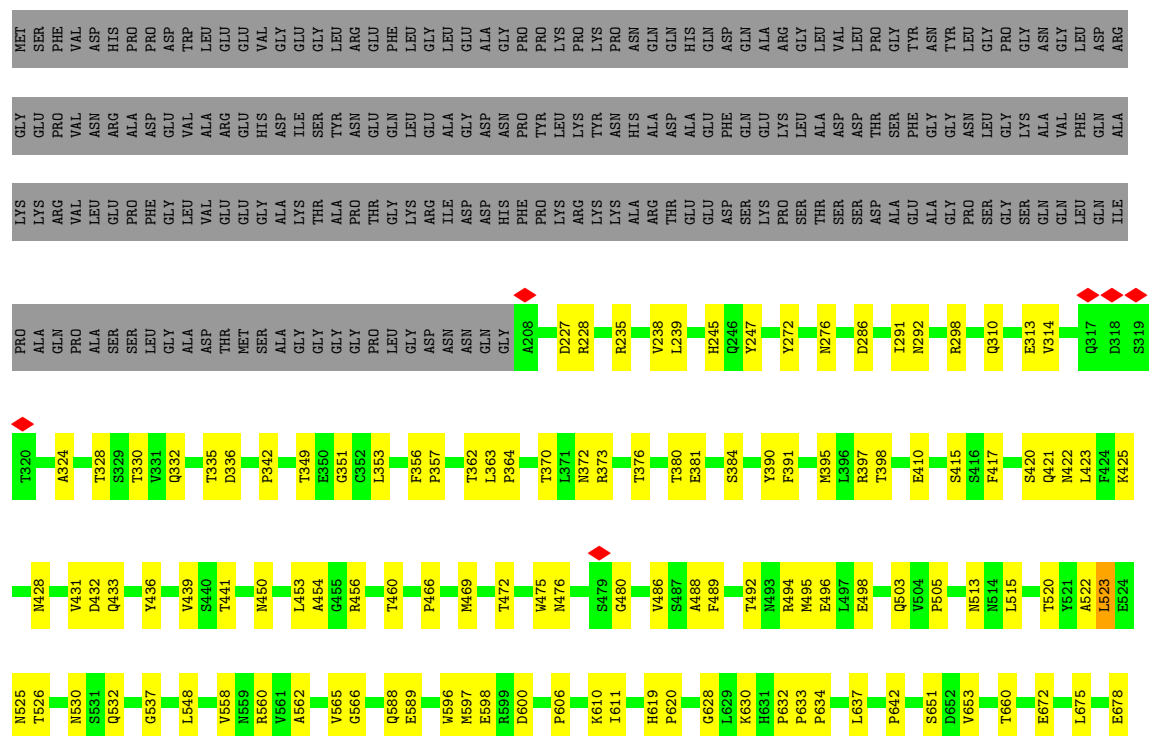
• Molecule 1: Capsid protein



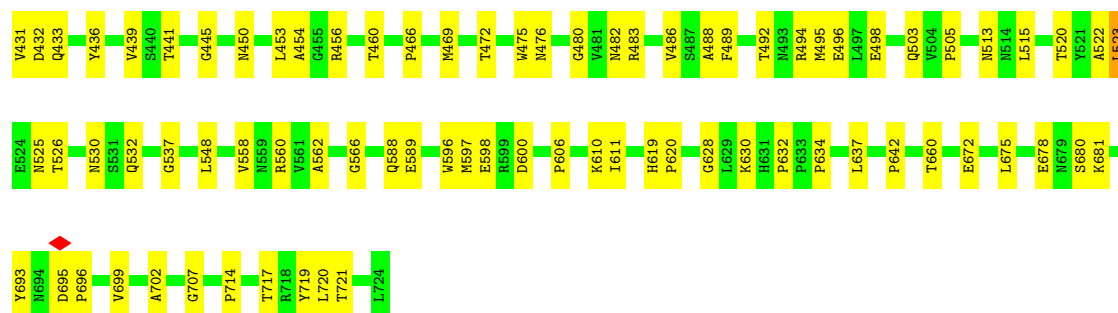
• Molecule 1: Capsid protein



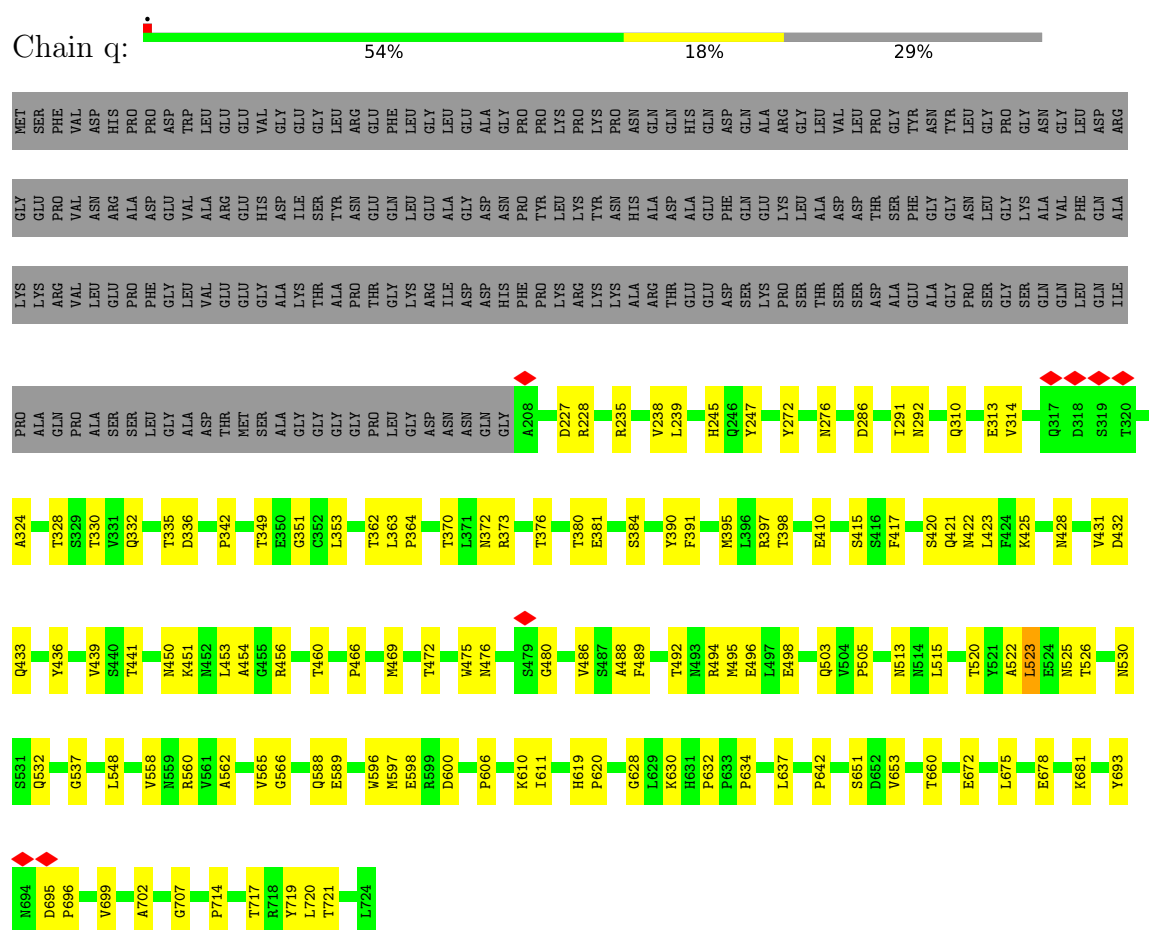




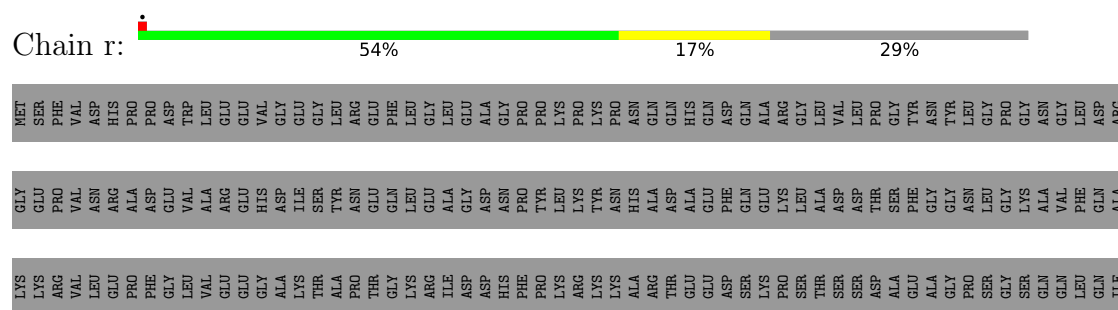




### • Molecule 1: Capsid protein



### • Molecule 1: Capsid protein









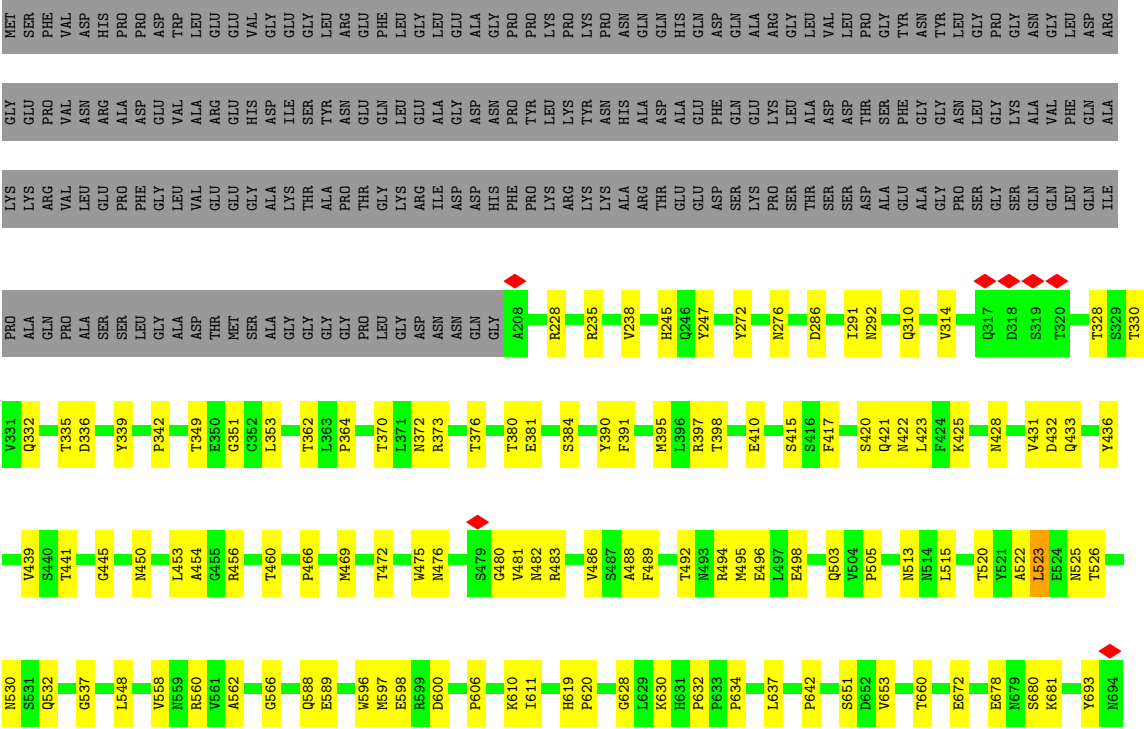








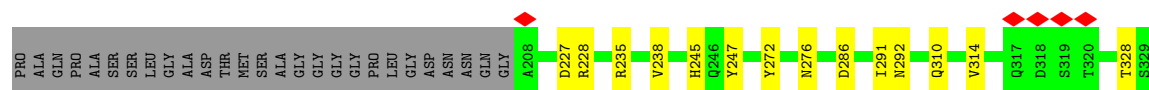
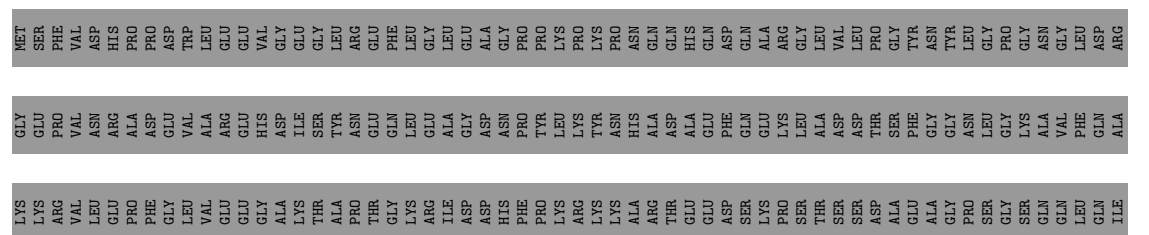
● Molecule 1: Capsid protein





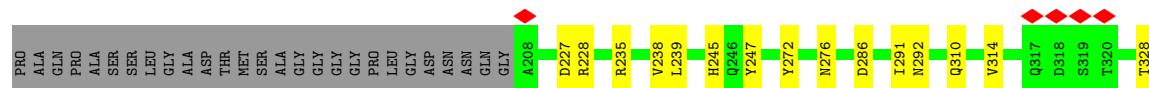
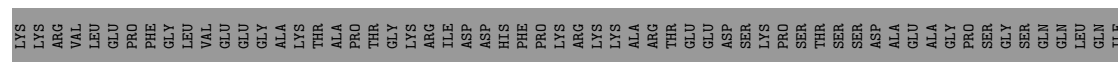
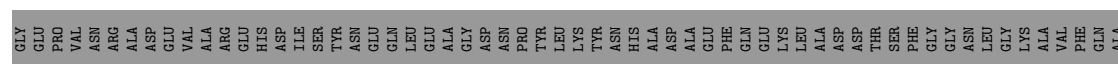
• Molecule 1: Capsid protein

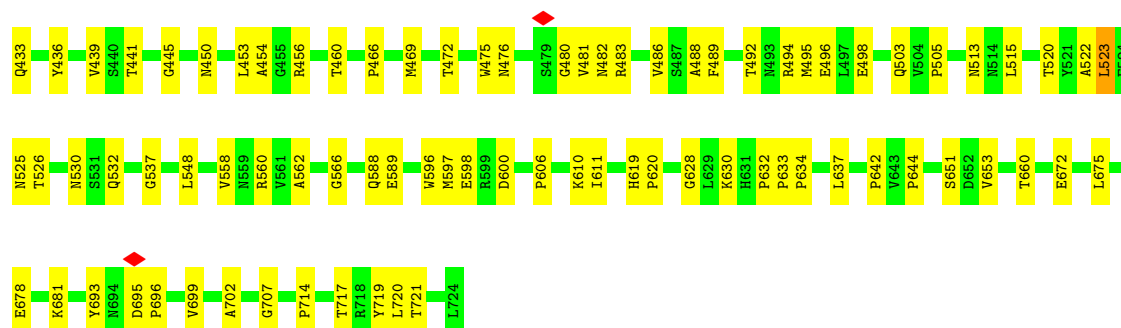
Chain 3: 54% 17% 29%



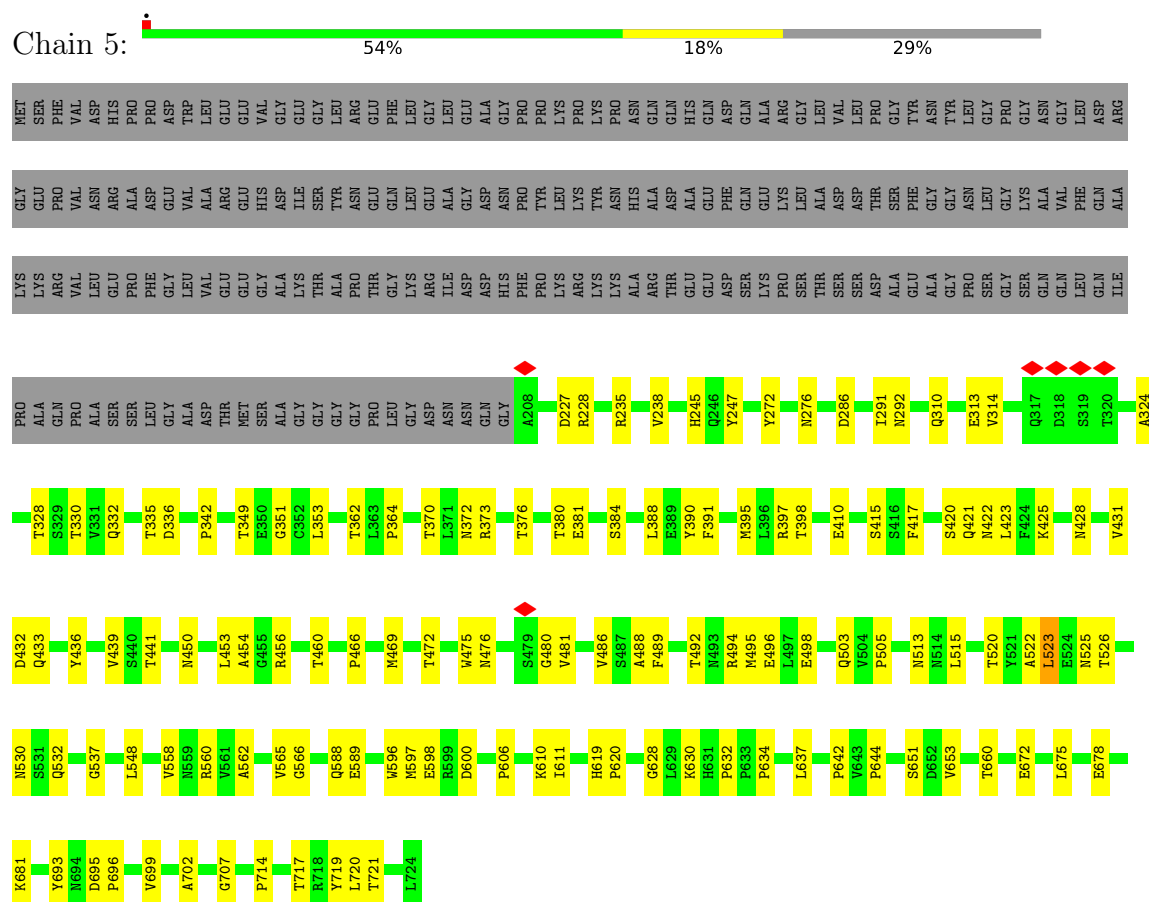
• Molecule 1: Capsid protein

Chain 4: 53% 18% 29%

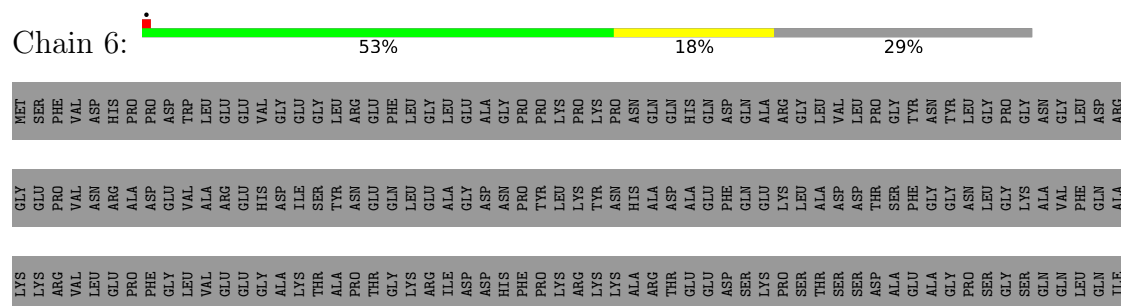


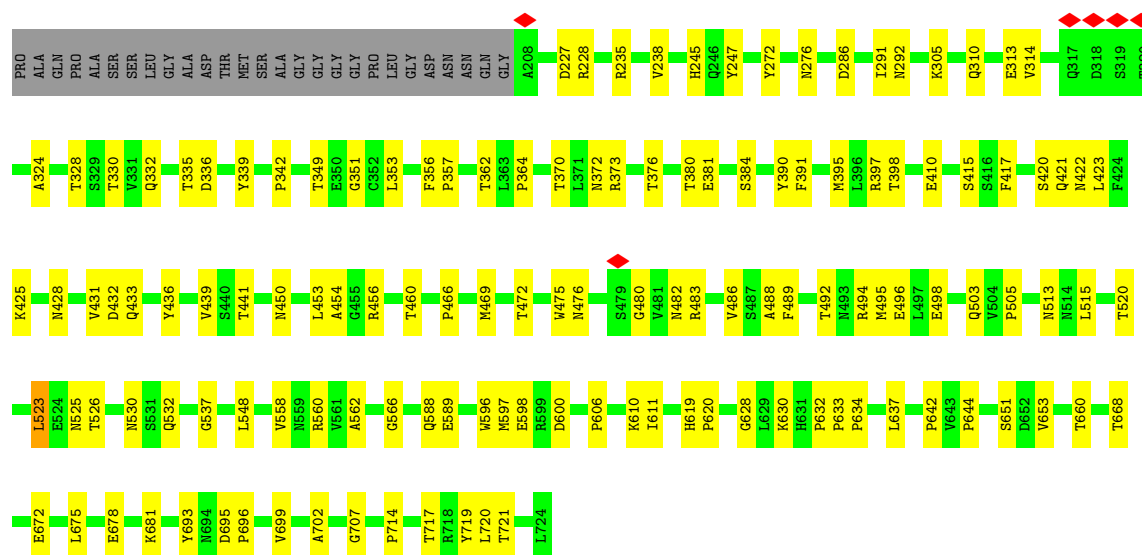


- Molecule 1: Capsid protein

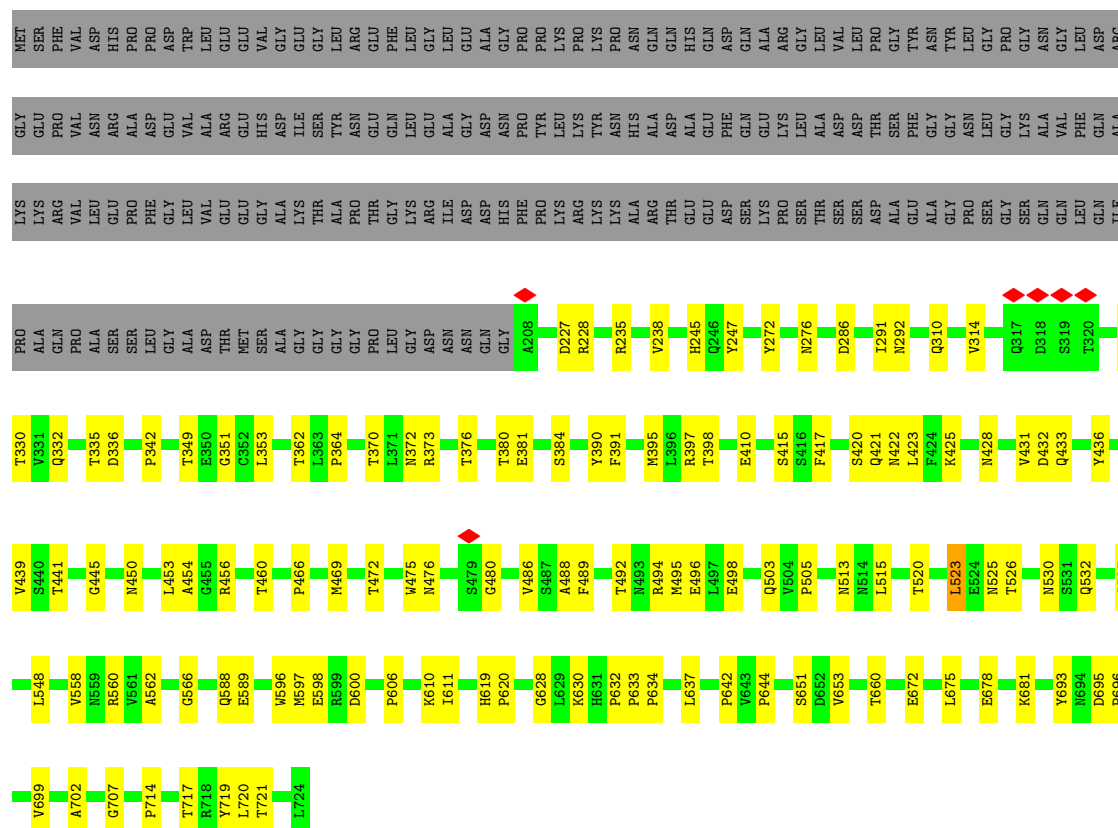


- Molecule 1: Capsid protein

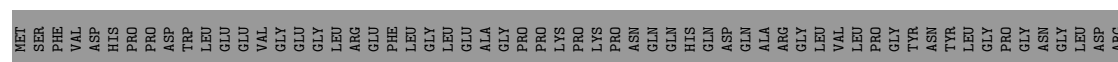




- Molecule 1: Capsid protein



- Molecule 1: Capsid protein







A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')





- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')





- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')





- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



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- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')







- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 23000                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45                                      | Depositor |
| Minimum defocus (nm)                 | 1289                                    | Depositor |
| Maximum defocus (nm)                 | 3967                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 22.666                                  | Depositor |
| Minimum map value                    | -18.405                                 | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 2                                       | Depositor |
| Map size (Å)                         | 467.5, 467.5, 467.5                     | wwPDB     |
| Map dimensions                       | 500, 500, 500                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.935, 0.935, 0.935                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 1     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 2     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 3     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 4     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 5     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 6     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 7     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | 8     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | A     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | B     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | C     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | D     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | E     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | F     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | G     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | H     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | I     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | J     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | K     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | L     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | M     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | N     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | O     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | P     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | Q     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | R     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | S     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | T     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | U     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | V     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | W     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | X     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | Y     | 0.41         | 0/4244      | 0.59        | 0/5800      |
| 1   | Z     | 0.41         | 0/4244      | 0.59        | 0/5800      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | a     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | b     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | c     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | d     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | e     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | f     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | g     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | h     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | i     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | j     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | k     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | l     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | m     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | n     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | o     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | p     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | q     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | r     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | s     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | t     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | u     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | v     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | w     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | x     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | y     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 1   | z     | 0.41         | 0/4244  | 0.59        | 0/5800  |
| 2   | 0     | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | 0A    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | 1A    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | 2A    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | 3A    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | 4A    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | 5A    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | 9     | 0.27         | 0/47    | 0.42        | 0/70    |
| 2   | AA    | 0.27         | 0/47    | 0.42        | 0/70    |
| 2   | BA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | CA    | 0.27         | 0/47    | 0.42        | 0/70    |
| 2   | DA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | EA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | FA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | GA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | HA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | IA    | 0.26         | 0/47    | 0.42        | 0/70    |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 2   | JA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | KA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | LA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | MA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | NA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | OA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | PA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | QA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | RA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | SA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | TA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | UA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | VA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | WA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | XA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | YA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | ZA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | aA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | bA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | cA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | dA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | eA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | fA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | gA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | hA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | iA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | jA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | kA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | lA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | mA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | nA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | oA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | pA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | qA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | rA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | sA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | tA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | uA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | vA    | 0.25         | 0/47    | 0.42        | 0/70    |
| 2   | wA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | xA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | yA    | 0.26         | 0/47    | 0.42        | 0/70    |
| 2   | zA    | 0.26         | 0/47    | 0.42        | 0/70    |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| All | All   | 0.41         | 0/257460 | 0.59        | 0/352200 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | 2     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | 3     | 4116  | 0        | 3863     | 121     | 0            |
| 1   | 4     | 4116  | 0        | 3863     | 128     | 0            |
| 1   | 5     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | 6     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | 7     | 4116  | 0        | 3863     | 119     | 0            |
| 1   | 8     | 4116  | 0        | 3863     | 124     | 0            |
| 1   | A     | 4116  | 0        | 3863     | 127     | 0            |
| 1   | B     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | C     | 4116  | 0        | 3863     | 119     | 0            |
| 1   | D     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | E     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | F     | 4116  | 0        | 3863     | 127     | 0            |
| 1   | G     | 4116  | 0        | 3863     | 126     | 0            |
| 1   | H     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | I     | 4116  | 0        | 3863     | 121     | 0            |
| 1   | J     | 4116  | 0        | 3863     | 119     | 0            |
| 1   | K     | 4116  | 0        | 3863     | 120     | 0            |
| 1   | L     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | M     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | N     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | O     | 4116  | 0        | 3863     | 126     | 0            |
| 1   | P     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | Q     | 4116  | 0        | 3863     | 121     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | R     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | S     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | T     | 4116  | 0        | 3863     | 128     | 0            |
| 1   | U     | 4116  | 0        | 3863     | 124     | 0            |
| 1   | V     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | W     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | X     | 4116  | 0        | 3863     | 130     | 0            |
| 1   | Y     | 4116  | 0        | 3863     | 128     | 0            |
| 1   | Z     | 4116  | 0        | 3863     | 129     | 0            |
| 1   | a     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | b     | 4116  | 0        | 3863     | 129     | 0            |
| 1   | c     | 4116  | 0        | 3863     | 129     | 0            |
| 1   | d     | 4116  | 0        | 3863     | 124     | 0            |
| 1   | e     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | f     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | g     | 4116  | 0        | 3863     | 126     | 0            |
| 1   | h     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | i     | 4116  | 0        | 3863     | 124     | 0            |
| 1   | j     | 4116  | 0        | 3863     | 128     | 0            |
| 1   | k     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | l     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | m     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | n     | 4116  | 0        | 3863     | 126     | 0            |
| 1   | o     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | p     | 4116  | 0        | 3863     | 124     | 0            |
| 1   | q     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | r     | 4116  | 0        | 3863     | 123     | 0            |
| 1   | s     | 4116  | 0        | 3863     | 132     | 0            |
| 1   | t     | 4116  | 0        | 3863     | 125     | 0            |
| 1   | u     | 4116  | 0        | 3863     | 121     | 0            |
| 1   | v     | 4116  | 0        | 3863     | 122     | 0            |
| 1   | w     | 4116  | 0        | 3863     | 126     | 0            |
| 1   | x     | 4116  | 0        | 3863     | 126     | 0            |
| 1   | y     | 4116  | 0        | 3863     | 124     | 0            |
| 1   | z     | 4116  | 0        | 3863     | 122     | 0            |
| 2   | 0     | 42    | 0        | 23       | 28      | 0            |
| 2   | 0A    | 42    | 0        | 23       | 28      | 0            |
| 2   | 1A    | 42    | 0        | 23       | 30      | 0            |
| 2   | 2A    | 42    | 0        | 23       | 28      | 0            |
| 2   | 3A    | 42    | 0        | 23       | 29      | 0            |
| 2   | 4A    | 42    | 0        | 23       | 27      | 0            |
| 2   | 5A    | 42    | 0        | 23       | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 9     | 42    | 0        | 23       | 29      | 0            |
| 2   | AA    | 42    | 0        | 23       | 29      | 0            |
| 2   | BA    | 42    | 0        | 23       | 30      | 0            |
| 2   | CA    | 42    | 0        | 23       | 28      | 0            |
| 2   | DA    | 42    | 0        | 23       | 28      | 0            |
| 2   | EA    | 42    | 0        | 23       | 28      | 0            |
| 2   | FA    | 42    | 0        | 23       | 28      | 0            |
| 2   | GA    | 42    | 0        | 23       | 26      | 0            |
| 2   | HA    | 42    | 0        | 23       | 28      | 0            |
| 2   | IA    | 42    | 0        | 23       | 28      | 0            |
| 2   | JA    | 42    | 0        | 23       | 28      | 0            |
| 2   | KA    | 42    | 0        | 23       | 30      | 0            |
| 2   | LA    | 42    | 0        | 23       | 29      | 0            |
| 2   | MA    | 42    | 0        | 23       | 27      | 0            |
| 2   | NA    | 42    | 0        | 23       | 29      | 0            |
| 2   | OA    | 42    | 0        | 23       | 28      | 0            |
| 2   | PA    | 42    | 0        | 23       | 28      | 0            |
| 2   | QA    | 42    | 0        | 23       | 28      | 0            |
| 2   | RA    | 42    | 0        | 23       | 30      | 0            |
| 2   | SA    | 42    | 0        | 23       | 28      | 0            |
| 2   | TA    | 42    | 0        | 23       | 28      | 0            |
| 2   | UA    | 42    | 0        | 23       | 26      | 0            |
| 2   | VA    | 42    | 0        | 23       | 27      | 0            |
| 2   | WA    | 42    | 0        | 23       | 28      | 0            |
| 2   | XA    | 42    | 0        | 23       | 29      | 0            |
| 2   | YA    | 42    | 0        | 23       | 28      | 0            |
| 2   | ZA    | 42    | 0        | 23       | 29      | 0            |
| 2   | aA    | 42    | 0        | 23       | 29      | 0            |
| 2   | bA    | 42    | 0        | 23       | 30      | 0            |
| 2   | cA    | 42    | 0        | 23       | 27      | 0            |
| 2   | dA    | 42    | 0        | 23       | 28      | 0            |
| 2   | eA    | 42    | 0        | 23       | 29      | 0            |
| 2   | fA    | 42    | 0        | 23       | 27      | 0            |
| 2   | gA    | 42    | 0        | 23       | 29      | 0            |
| 2   | hA    | 42    | 0        | 23       | 27      | 0            |
| 2   | iA    | 42    | 0        | 23       | 29      | 0            |
| 2   | jA    | 42    | 0        | 23       | 27      | 0            |
| 2   | kA    | 42    | 0        | 23       | 28      | 0            |
| 2   | lA    | 42    | 0        | 23       | 28      | 0            |
| 2   | mA    | 42    | 0        | 23       | 30      | 0            |
| 2   | nA    | 42    | 0        | 23       | 28      | 0            |
| 2   | oA    | 42    | 0        | 23       | 26      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | pA    | 42     | 0        | 23       | 28      | 0            |
| 2   | qA    | 42     | 0        | 23       | 27      | 0            |
| 2   | rA    | 42     | 0        | 23       | 28      | 0            |
| 2   | sA    | 42     | 0        | 23       | 28      | 0            |
| 2   | tA    | 42     | 0        | 23       | 28      | 0            |
| 2   | uA    | 42     | 0        | 23       | 28      | 0            |
| 2   | vA    | 42     | 0        | 23       | 27      | 0            |
| 2   | wA    | 42     | 0        | 23       | 26      | 0            |
| 2   | xA    | 42     | 0        | 23       | 28      | 0            |
| 2   | yA    | 42     | 0        | 23       | 28      | 0            |
| 2   | zA    | 42     | 0        | 23       | 28      | 0            |
| All | All   | 249480 | 0        | 233160   | 6225    | 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 13.

All (6225) 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:h:620:PRO:HD2 | 2:ZA:997:DA:C2' | 1.00                     | 1.48              |
| 1:n:620:PRO:HD2 | 2:gA:997:DA:C2' | 1.00                     | 1.48              |
| 1:z:620:PRO:HD2 | 2:tA:997:DA:C2' | 1.00                     | 1.48              |
| 1:N:620:PRO:HD2 | 2:DA:997:DA:C2' | 1.00                     | 1.48              |
| 1:f:620:PRO:HD2 | 2:XA:997:DA:C2' | 1.00                     | 1.48              |
| 1:m:620:PRO:HD2 | 2:eA:997:DA:C2' | 1.00                     | 1.48              |
| 1:P:620:PRO:HD2 | 2:FA:997:DA:C2' | 1.00                     | 1.47              |
| 1:x:620:PRO:HD2 | 2:rA:997:DA:C2' | 1.00                     | 1.47              |
| 1:l:620:PRO:HD2 | 2:uA:997:DA:C2' | 1.00                     | 1.47              |
| 1:B:620:PRO:HD2 | 2:JA:997:DA:C2' | 1.00                     | 1.47              |
| 1:L:620:PRO:HD2 | 2:BA:997:DA:C2' | 1.00                     | 1.47              |
| 1:U:620:PRO:HD2 | 2:LA:997:DA:C2' | 1.00                     | 1.47              |
| 1:a:620:PRO:HD2 | 2:RA:997:DA:C2' | 1.00                     | 1.47              |
| 1:8:620:PRO:HD2 | 2:2A:997:DA:C2' | 1.00                     | 1.47              |
| 1:w:620:PRO:HD2 | 2:pA:997:DA:C2' | 1.00                     | 1.47              |
| 1:D:620:PRO:HD2 | 2:fA:997:DA:C2' | 1.00                     | 1.47              |
| 1:I:620:PRO:HD2 | 2:5A:997:DA:C2' | 1.00                     | 1.47              |
| 1:K:620:PRO:CD  | 2:AA:997:DA:C2' | 1.93                     | 1.47              |
| 1:M:620:PRO:HD2 | 2:CA:997:DA:C2' | 1.00                     | 1.47              |
| 1:S:620:PRO:CD  | 2:IA:997:DA:C2' | 1.93                     | 1.47              |
| 1:S:620:PRO:HD2 | 2:IA:997:DA:C2' | 1.00                     | 1.47              |
| 1:w:620:PRO:CD  | 2:pA:997:DA:C2' | 1.93                     | 1.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:7:620:PRO:HD2 | 2:0A:997:DA:C2' | 1.00                     | 1.47              |
| 1:J:620:PRO:CD  | 2:9:997:DA:C2'  | 1.93                     | 1.47              |
| 1:X:620:PRO:CD  | 2:0A:997:DA:C2' | 1.93                     | 1.47              |
| 1:s:620:PRO:CD  | 2:lA:997:DA:C2' | 1.93                     | 1.47              |
| 1:2:620:PRO:HD2 | 2:vA:997:DA:C2' | 1.00                     | 1.47              |
| 1:Z:620:PRO:HD2 | 2:QA:997:DA:C2' | 1.00                     | 1.46              |
| 1:c:620:PRO:HD2 | 2:TA:997:DA:C2' | 1.00                     | 1.46              |
| 1:4:620:PRO:HD2 | 2:xA:997:DA:C2' | 1.00                     | 1.46              |
| 1:X:620:PRO:HD2 | 2:0A:997:DA:C2' | 1.00                     | 1.46              |
| 1:Y:620:PRO:HD2 | 2:PA:997:DA:C2' | 1.00                     | 1.46              |
| 1:b:620:PRO:HD2 | 2:SA:997:DA:C2' | 1.00                     | 1.46              |
| 1:c:620:PRO:CD  | 2:TA:997:DA:C2' | 1.93                     | 1.46              |
| 1:s:620:PRO:HD2 | 2:lA:997:DA:C2' | 1.00                     | 1.46              |
| 1:O:620:PRO:HD2 | 2:EA:997:DA:C2' | 1.00                     | 1.46              |
| 1:U:620:PRO:CD  | 2:LA:997:DA:C2' | 1.93                     | 1.46              |
| 1:Y:620:PRO:CD  | 2:PA:997:DA:C2' | 1.93                     | 1.46              |
| 1:g:620:PRO:CD  | 2:YA:997:DA:C2' | 1.93                     | 1.46              |
| 1:k:620:PRO:HD2 | 2:cA:997:DA:C2' | 1.00                     | 1.46              |
| 1:x:620:PRO:CD  | 2:rA:997:DA:C2' | 1.93                     | 1.46              |
| 1:A:620:PRO:HD2 | 2:0:997:DA:C2'  | 1.00                     | 1.46              |
| 1:H:620:PRO:CD  | 2:4A:997:DA:C2' | 1.93                     | 1.46              |
| 1:I:620:PRO:CD  | 2:5A:997:DA:C2' | 1.93                     | 1.46              |
| 1:O:620:PRO:CD  | 2:EA:997:DA:C2' | 1.93                     | 1.46              |
| 1:d:620:PRO:HD2 | 2:VA:997:DA:C2' | 1.00                     | 1.46              |
| 1:7:620:PRO:CD  | 2:0A:997:DA:C2' | 1.93                     | 1.46              |
| 1:F:620:PRO:HD2 | 2:1A:997:DA:C2' | 1.00                     | 1.46              |
| 1:W:620:PRO:HD2 | 2:NA:997:DA:C2' | 1.00                     | 1.46              |
| 1:g:620:PRO:HD2 | 2:YA:997:DA:C2' | 1.00                     | 1.46              |
| 1:o:620:PRO:CD  | 2:hA:997:DA:C2' | 1.93                     | 1.46              |
| 1:u:620:PRO:HD2 | 2:nA:997:DA:C2' | 1.00                     | 1.46              |
| 1:C:620:PRO:HD2 | 2:UA:997:DA:C2' | 1.00                     | 1.45              |
| 1:K:620:PRO:HD2 | 2:AA:997:DA:C2' | 1.00                     | 1.45              |
| 1:n:620:PRO:CD  | 2:gA:997:DA:C2' | 1.93                     | 1.45              |
| 1:t:620:PRO:HD2 | 2:mA:997:DA:C2' | 1.00                     | 1.45              |
| 1:v:620:PRO:HD2 | 2:oA:997:DA:C2' | 1.00                     | 1.45              |
| 1:v:620:PRO:CD  | 2:oA:997:DA:C2' | 1.93                     | 1.45              |
| 1:5:620:PRO:HD2 | 2:yA:997:DA:C2' | 1.00                     | 1.45              |
| 1:6:620:PRO:HD2 | 2:zA:997:DA:C2' | 1.00                     | 1.45              |
| 1:E:620:PRO:HD2 | 2:qA:997:DA:C2' | 1.00                     | 1.45              |
| 1:J:620:PRO:HD2 | 2:9:997:DA:C2'  | 1.00                     | 1.45              |
| 1:Q:620:PRO:HD2 | 2:GA:997:DA:C2' | 1.00                     | 1.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:h:620:PRO:CD  | 2:ZA:997:DA:C2' | 1.93                     | 1.45              |
| 1:j:620:PRO:HD2 | 2:bA:997:DA:C2' | 1.00                     | 1.45              |
| 1:l:620:PRO:HD2 | 2:dA:997:DA:C2' | 1.00                     | 1.45              |
| 1:p:620:PRO:HD2 | 2:iA:997:DA:C2' | 1.00                     | 1.45              |
| 1:3:620:PRO:HD2 | 2:wA:997:DA:C2' | 1.00                     | 1.45              |
| 1:G:620:PRO:CD  | 2:3A:997:DA:C2' | 1.93                     | 1.45              |
| 1:G:620:PRO:HD2 | 2:3A:997:DA:C2' | 1.00                     | 1.45              |
| 1:H:620:PRO:HD2 | 2:4A:997:DA:C2' | 1.00                     | 1.45              |
| 1:Q:620:PRO:CD  | 2:GA:997:DA:C2' | 1.93                     | 1.45              |
| 1:R:620:PRO:HD2 | 2:HA:997:DA:C2' | 1.00                     | 1.45              |
| 1:T:620:PRO:HD2 | 2:KA:997:DA:C2' | 1.00                     | 1.45              |
| 1:1:620:PRO:CD  | 2:uA:997:DA:C2' | 1.93                     | 1.45              |
| 1:F:620:PRO:CD  | 2:1A:997:DA:C2' | 1.93                     | 1.45              |
| 1:V:620:PRO:HD2 | 2:MA:997:DA:C2' | 1.00                     | 1.45              |
| 1:b:620:PRO:CD  | 2:SA:997:DA:C2' | 1.93                     | 1.45              |
| 1:i:620:PRO:HD2 | 2:aA:997:DA:C2' | 1.00                     | 1.45              |
| 1:j:620:PRO:CD  | 2:bA:997:DA:C2' | 1.93                     | 1.45              |
| 1:o:620:PRO:HD2 | 2:hA:997:DA:C2' | 1.00                     | 1.45              |
| 1:t:620:PRO:CD  | 2:mA:997:DA:C2' | 1.93                     | 1.45              |
| 1:u:620:PRO:CD  | 2:nA:997:DA:C2' | 1.93                     | 1.45              |
| 1:y:620:PRO:HD2 | 2:sA:997:DA:C2' | 1.00                     | 1.45              |
| 1:E:620:PRO:CD  | 2:qA:997:DA:C2' | 1.93                     | 1.45              |
| 1:P:620:PRO:CD  | 2:FA:997:DA:C2' | 1.93                     | 1.45              |
| 1:T:620:PRO:CD  | 2:KA:997:DA:C2' | 1.93                     | 1.45              |
| 1:q:620:PRO:HD2 | 2:jA:997:DA:C2' | 1.00                     | 1.45              |
| 1:y:620:PRO:CD  | 2:sA:997:DA:C2' | 1.93                     | 1.45              |
| 1:z:620:PRO:CD  | 2:tA:997:DA:C2' | 1.93                     | 1.45              |
| 1:6:620:PRO:CD  | 2:zA:997:DA:C2' | 1.93                     | 1.45              |
| 1:B:620:PRO:CD  | 2:JA:997:DA:C2' | 1.93                     | 1.44              |
| 1:Z:620:PRO:CD  | 2:QA:997:DA:C2' | 1.93                     | 1.44              |
| 1:N:620:PRO:CD  | 2:DA:997:DA:C2' | 1.93                     | 1.44              |
| 1:R:620:PRO:CD  | 2:HA:997:DA:C2' | 1.93                     | 1.44              |
| 1:8:620:PRO:CD  | 2:2A:997:DA:C2' | 1.93                     | 1.44              |
| 1:m:620:PRO:CD  | 2:eA:997:DA:C2' | 1.93                     | 1.44              |
| 1:L:620:PRO:CD  | 2:BA:997:DA:C2' | 1.93                     | 1.44              |
| 1:W:620:PRO:CD  | 2:NA:997:DA:C2' | 1.93                     | 1.44              |
| 1:f:620:PRO:CD  | 2:XA:997:DA:C2' | 1.93                     | 1.44              |
| 1:C:620:PRO:CD  | 2:UA:997:DA:C2' | 1.93                     | 1.43              |
| 1:p:620:PRO:CD  | 2:iA:997:DA:C2' | 1.93                     | 1.43              |
| 1:A:620:PRO:CD  | 2:O:997:DA:H2'' | 1.49                     | 1.43              |
| 1:a:620:PRO:CD  | 2:RA:997:DA:C2' | 1.93                     | 1.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:e:620:PRO:CD  | 2:WA:997:DA:C2'  | 1.93                     | 1.43              |
| 1:e:620:PRO:HD2 | 2:WA:997:DA:C2'  | 1.00                     | 1.43              |
| 1:5:620:PRO:CD  | 2:yA:997:DA:H2'' | 1.49                     | 1.43              |
| 1:r:620:PRO:HD2 | 2:kA:997:DA:C2'  | 1.00                     | 1.43              |
| 1:G:620:PRO:CD  | 2:3A:997:DA:H2'' | 1.49                     | 1.43              |
| 1:M:620:PRO:CD  | 2:CA:997:DA:H2'' | 1.49                     | 1.43              |
| 1:V:620:PRO:CD  | 2:MA:997:DA:C2'  | 1.93                     | 1.43              |
| 1:r:620:PRO:CD  | 2:kA:997:DA:C2'  | 1.93                     | 1.43              |
| 1:4:620:PRO:CD  | 2:xA:997:DA:H2'' | 1.49                     | 1.43              |
| 1:q:620:PRO:CD  | 2:jA:997:DA:C2'  | 1.93                     | 1.43              |
| 1:6:620:PRO:CD  | 2:zA:997:DA:H2'' | 1.49                     | 1.43              |
| 1:n:620:PRO:CD  | 2:gA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:q:620:PRO:CD  | 2:jA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:4:620:PRO:CD  | 2:xA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:D:620:PRO:CD  | 2:fA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:M:620:PRO:CD  | 2:CA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:V:620:PRO:CD  | 2:MA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:d:620:PRO:CD  | 2:VA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:h:620:PRO:CD  | 2:ZA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:2:620:PRO:CD  | 2:vA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:Y:620:PRO:CD  | 2:PA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:k:620:PRO:CD  | 2:cA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:5:620:PRO:CD  | 2:yA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:c:620:PRO:CD  | 2:TA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:d:620:PRO:CD  | 2:VA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:f:620:PRO:CD  | 2:XA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:i:620:PRO:CD  | 2:aA:997:DA:C2'  | 1.93                     | 1.42              |
| 1:k:620:PRO:CD  | 2:cA:997:DA:H2'' | 1.49                     | 1.42              |
| 1:A:620:PRO:CD  | 2:O:997:DA:C2'   | 1.93                     | 1.41              |
| 1:l:620:PRO:CD  | 2:dA:997:DA:C2'  | 1.93                     | 1.41              |
| 1:m:620:PRO:CD  | 2:eA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:3:620:PRO:CD  | 2:wA:997:DA:C2'  | 1.93                     | 1.41              |
| 1:L:620:PRO:CD  | 2:BA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:Q:620:PRO:CD  | 2:GA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:v:620:PRO:CD  | 2:oA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:D:620:PRO:CD  | 2:fA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:U:620:PRO:CD  | 2:LA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:a:620:PRO:CD  | 2:RA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:x:620:PRO:CD  | 2:rA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:2:620:PRO:CD  | 2:vA:997:DA:H2'' | 1.49                     | 1.41              |
| 1:g:620:PRO:CD  | 2:YA:997:DA:H2'' | 1.49                     | 1.40              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:w:620:PRO:CD | 2:pA:997:DA:H2'' | 1.49                     | 1.40              |
| 1:O:620:PRO:CD | 2:EA:997:DA:H2'' | 1.49                     | 1.40              |
| 1:T:620:PRO:CD | 2:KA:997:DA:H2'' | 1.49                     | 1.40              |
| 1:j:620:PRO:CD | 2:bA:997:DA:H2'' | 1.49                     | 1.40              |
| 1:S:620:PRO:CD | 2:IA:997:DA:H2'' | 1.49                     | 1.40              |
| 1:I:620:PRO:CD | 2:5A:997:DA:H2'' | 1.49                     | 1.40              |
| 1:Z:620:PRO:CD | 2:QA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:e:620:PRO:CD | 2:WA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:l:620:PRO:CD | 2:dA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:7:620:PRO:CD | 2:0A:997:DA:H2'' | 1.49                     | 1.39              |
| 1:X:620:PRO:CD | 2:OA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:b:620:PRO:CD | 2:SA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:r:620:PRO:CD | 2:kA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:y:620:PRO:CD | 2:sA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:N:620:PRO:CD | 2:DA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:i:620:PRO:CD | 2:aA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:s:620:PRO:CD | 2:lA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:R:620:PRO:CD | 2:HA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:o:620:PRO:CD | 2:hA:997:DA:H2'' | 1.49                     | 1.39              |
| 1:H:620:PRO:CD | 2:4A:997:DA:H2'' | 1.49                     | 1.38              |
| 1:p:620:PRO:CD | 2:iA:997:DA:H2'' | 1.49                     | 1.38              |
| 1:z:620:PRO:CD | 2:tA:997:DA:H2'' | 1.49                     | 1.38              |
| 1:W:620:PRO:CD | 2:NA:997:DA:H2'' | 1.49                     | 1.38              |
| 1:E:620:PRO:CD | 2:qA:997:DA:H2'' | 1.49                     | 1.36              |
| 1:u:620:PRO:CD | 2:nA:997:DA:H2'' | 1.49                     | 1.36              |
| 1:C:620:PRO:CD | 2:UA:997:DA:H2'' | 1.49                     | 1.35              |
| 1:3:620:PRO:CD | 2:wA:997:DA:H2'' | 1.49                     | 1.35              |
| 1:F:620:PRO:CD | 2:1A:997:DA:H2'' | 1.49                     | 1.34              |
| 1:8:620:PRO:CD | 2:2A:997:DA:H2'' | 1.49                     | 1.34              |
| 1:B:620:PRO:CD | 2:JA:997:DA:H2'' | 1.49                     | 1.34              |
| 1:t:620:PRO:CD | 2:mA:997:DA:H2'' | 1.49                     | 1.33              |
| 1:J:620:PRO:CD | 2:9:997:DA:H2''  | 1.49                     | 1.33              |
| 1:K:620:PRO:CD | 2:AA:997:DA:H2'' | 1.49                     | 1.33              |
| 1:P:620:PRO:CD | 2:FA:997:DA:H2'' | 1.49                     | 1.32              |
| 1:1:620:PRO:CD | 2:uA:997:DA:H2'' | 1.49                     | 1.32              |
| 1:B:628:GLY:O  | 2:JA:997:DA:N1   | 1.79                     | 1.15              |
| 1:C:628:GLY:O  | 2:UA:997:DA:N1   | 1.80                     | 1.15              |
| 1:K:628:GLY:O  | 2:AA:997:DA:N1   | 1.80                     | 1.15              |
| 1:R:628:GLY:O  | 2:HA:997:DA:N1   | 1.80                     | 1.15              |
| 1:S:628:GLY:O  | 2:IA:997:DA:N1   | 1.80                     | 1.15              |
| 1:s:628:GLY:O  | 2:lA:997:DA:N1   | 1.80                     | 1.15              |

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| Atom-1        | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------|--------------------------|-------------------|
| 1:w:628:GLY:O | 2:pA:997:DA:N1 | 1.80                     | 1.15              |
| 1:y:628:GLY:O | 2:sA:997:DA:N1 | 1.80                     | 1.15              |
| 1:5:628:GLY:O | 2:yA:997:DA:N1 | 1.80                     | 1.15              |
| 1:A:628:GLY:O | 2:0:997:DA:N1  | 1.80                     | 1.15              |
| 1:J:628:GLY:O | 2:9:997:DA:N1  | 1.80                     | 1.15              |
| 1:X:628:GLY:O | 2:OA:997:DA:N1 | 1.80                     | 1.15              |
| 1:n:628:GLY:O | 2:gA:997:DA:N1 | 1.80                     | 1.15              |
| 1:3:628:GLY:O | 2:wA:997:DA:N1 | 1.80                     | 1.15              |
| 1:8:628:GLY:O | 2:2A:997:DA:N1 | 1.79                     | 1.15              |
| 1:U:628:GLY:O | 2:LA:997:DA:N1 | 1.80                     | 1.15              |
| 1:d:628:GLY:O | 2:VA:997:DA:N1 | 1.80                     | 1.15              |
| 1:h:628:GLY:O | 2:ZA:997:DA:N1 | 1.80                     | 1.15              |
| 1:j:628:GLY:O | 2:bA:997:DA:N1 | 1.80                     | 1.15              |
| 1:k:628:GLY:O | 2:cA:997:DA:N1 | 1.79                     | 1.15              |
| 1:x:628:GLY:O | 2:rA:997:DA:N1 | 1.80                     | 1.15              |
| 1:T:628:GLY:O | 2:KA:997:DA:N1 | 1.80                     | 1.15              |
| 1:a:628:GLY:O | 2:RA:997:DA:N1 | 1.80                     | 1.15              |
| 1:e:628:GLY:O | 2:WA:997:DA:N1 | 1.80                     | 1.15              |
| 1:H:628:GLY:O | 2:4A:997:DA:N1 | 1.79                     | 1.15              |
| 1:L:628:GLY:O | 2:BA:997:DA:N1 | 1.80                     | 1.15              |
| 1:o:628:GLY:O | 2:hA:997:DA:N1 | 1.80                     | 1.15              |
| 1:p:628:GLY:O | 2:iA:997:DA:N1 | 1.80                     | 1.15              |
| 1:r:628:GLY:O | 2:kA:997:DA:N1 | 1.80                     | 1.15              |
| 1:7:628:GLY:O | 2:0A:997:DA:N1 | 1.80                     | 1.15              |
| 1:I:628:GLY:O | 2:5A:997:DA:N1 | 1.80                     | 1.14              |
| 1:W:628:GLY:O | 2:NA:997:DA:N1 | 1.80                     | 1.14              |
| 1:Y:628:GLY:O | 2:PA:997:DA:N1 | 1.80                     | 1.14              |
| 1:c:628:GLY:O | 2:TA:997:DA:N1 | 1.79                     | 1.14              |
| 1:O:628:GLY:O | 2:EA:997:DA:N1 | 1.80                     | 1.14              |
| 1:F:628:GLY:O | 2:1A:997:DA:N1 | 1.80                     | 1.14              |
| 1:Q:628:GLY:O | 2:GA:997:DA:N1 | 1.80                     | 1.14              |
| 1:g:628:GLY:O | 2:YA:997:DA:N1 | 1.80                     | 1.14              |
| 1:z:628:GLY:O | 2:tA:997:DA:N1 | 1.79                     | 1.14              |
| 1:V:628:GLY:O | 2:MA:997:DA:N1 | 1.80                     | 1.14              |
| 1:t:628:GLY:O | 2:mA:997:DA:N1 | 1.80                     | 1.14              |
| 1:v:628:GLY:O | 2:oA:997:DA:N1 | 1.80                     | 1.14              |
| 1:D:628:GLY:O | 2:fA:997:DA:N1 | 1.80                     | 1.14              |
| 1:E:628:GLY:O | 2:qA:997:DA:N1 | 1.80                     | 1.14              |
| 1:N:628:GLY:O | 2:DA:997:DA:N1 | 1.80                     | 1.14              |
| 1:Z:628:GLY:O | 2:QA:997:DA:N1 | 1.80                     | 1.14              |
| 1:i:628:GLY:O | 2:aA:997:DA:N1 | 1.80                     | 1.14              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:q:628:GLY:O   | 2:jA:997:DA:N1  | 1.80                     | 1.14              |
| 1:u:628:GLY:O   | 2:nA:997:DA:N1  | 1.80                     | 1.14              |
| 1:2:628:GLY:O   | 2:vA:997:DA:N1  | 1.80                     | 1.14              |
| 1:4:628:GLY:O   | 2:xA:997:DA:N1  | 1.80                     | 1.14              |
| 1:M:628:GLY:O   | 2:CA:997:DA:N1  | 1.80                     | 1.13              |
| 1:b:628:GLY:O   | 2:SA:997:DA:N1  | 1.80                     | 1.13              |
| 1:l:628:GLY:O   | 2:dA:997:DA:N1  | 1.80                     | 1.13              |
| 1:f:628:GLY:O   | 2:XA:997:DA:N1  | 1.80                     | 1.12              |
| 1:m:628:GLY:O   | 2:eA:997:DA:N1  | 1.80                     | 1.12              |
| 1:1:628:GLY:O   | 2:uA:997:DA:N1  | 1.80                     | 1.12              |
| 1:P:628:GLY:O   | 2:FA:997:DA:N1  | 1.80                     | 1.12              |
| 1:6:628:GLY:O   | 2:zA:997:DA:N1  | 1.80                     | 1.12              |
| 1:G:628:GLY:O   | 2:3A:997:DA:N1  | 1.80                     | 1.11              |
| 1:8:620:PRO:CD  | 2:2A:997:DA:H2' | 1.72                     | 1.08              |
| 1:7:620:PRO:CD  | 2:0A:997:DA:H2' | 1.72                     | 1.08              |
| 1:H:620:PRO:CD  | 2:4A:997:DA:H2' | 1.72                     | 1.08              |
| 1:X:620:PRO:CD  | 2:OA:997:DA:H2' | 1.72                     | 1.07              |
| 1:o:620:PRO:CD  | 2:hA:997:DA:H2' | 1.72                     | 1.07              |
| 1:I:620:PRO:CD  | 2:5A:997:DA:H2' | 1.72                     | 1.07              |
| 1:z:620:PRO:CD  | 2:tA:997:DA:H2' | 1.72                     | 1.06              |
| 1:M:620:PRO:CD  | 2:CA:997:DA:H2' | 1.72                     | 1.06              |
| 1:4:620:PRO:CD  | 2:xA:997:DA:H2' | 1.72                     | 1.06              |
| 1:K:620:PRO:CD  | 2:AA:997:DA:H2' | 1.72                     | 1.05              |
| 1:N:620:PRO:CD  | 2:DA:997:DA:H2' | 1.72                     | 1.05              |
| 1:a:620:PRO:CD  | 2:RA:997:DA:H2' | 1.72                     | 1.05              |
| 1:J:620:PRO:CD  | 2:9:997:DA:H2'  | 1.72                     | 1.05              |
| 1:O:620:PRO:CD  | 2:EA:997:DA:H2' | 1.72                     | 1.05              |
| 1:L:620:PRO:CD  | 2:BA:997:DA:H2' | 1.72                     | 1.05              |
| 1:g:620:PRO:CD  | 2:YA:997:DA:H2' | 1.72                     | 1.05              |
| 1:c:620:PRO:CD  | 2:TA:997:DA:H2' | 1.72                     | 1.04              |
| 1:6:620:PRO:CD  | 2:zA:997:DA:H2' | 1.72                     | 1.04              |
| 1:Y:620:PRO:CD  | 2:PA:997:DA:H2' | 1.72                     | 1.04              |
| 1:j:620:PRO:CD  | 2:bA:997:DA:H2' | 1.72                     | 1.04              |
| 1:G:620:PRO:CD  | 2:3A:997:DA:H2' | 1.72                     | 1.03              |
| 1:T:620:PRO:CD  | 2:KA:997:DA:H2' | 1.72                     | 1.03              |
| 1:W:620:PRO:CD  | 2:NA:997:DA:H2' | 1.72                     | 1.03              |
| 1:h:620:PRO:CD  | 2:ZA:997:DA:H2' | 1.72                     | 1.02              |
| 1:k:620:PRO:CD  | 2:cA:997:DA:H2' | 1.71                     | 1.02              |
| 1:p:620:PRO:CD  | 2:iA:997:DA:H2' | 1.72                     | 1.02              |
| 1:d:620:PRO:CD  | 2:VA:997:DA:H2' | 1.72                     | 1.02              |
| 1:H:620:PRO:HD2 | 2:4A:997:DA:H2' | 1.02                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:620:PRO:HD2  | 2:LA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:o:620:PRO:HD2  | 2:hA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:x:620:PRO:HD2  | 2:rA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:Z:620:PRO:CD   | 2:QA:997:DA:H2'  | 1.72                     | 1.02              |
| 1:n:620:PRO:CD   | 2:gA:997:DA:H2'  | 1.72                     | 1.02              |
| 1:A:620:PRO:HD2  | 2:O:997:DA:H2'   | 1.02                     | 1.02              |
| 1:Q:620:PRO:HD2  | 2:GA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:W:620:PRO:HD2  | 2:NA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:p:620:PRO:HD2  | 2:iA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:5:620:PRO:HD2  | 2:yA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:6:620:PRO:HD2  | 2:zA:997:DA:H2'  | 1.02                     | 1.02              |
| 1:8:620:PRO:HD2  | 2:2A:997:DA:H2'  | 1.02                     | 1.02              |
| 1:B:620:PRO:HD2  | 2:JA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:C:620:PRO:HD2  | 2:UA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:P:620:PRO:CD   | 2:FA:997:DA:H2'  | 1.72                     | 1.01              |
| 1:v:620:PRO:HD2  | 2:oA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:G:620:PRO:HD2  | 2:3A:997:DA:H2'  | 1.02                     | 1.01              |
| 1:b:620:PRO:CD   | 2:SA:997:DA:H2'  | 1.72                     | 1.01              |
| 1:3:620:PRO:HD2  | 2:wA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:1:620:PRO:CD   | 2:uA:997:DA:H2'  | 1.72                     | 1.01              |
| 1:B:513:ASN:HD22 | 1:B:526:THR:HG22 | 1.26                     | 1.01              |
| 1:K:620:PRO:HD2  | 2:AA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:V:620:PRO:CD   | 2:MA:997:DA:H2'  | 1.72                     | 1.01              |
| 1:8:513:ASN:HD22 | 1:8:526:THR:HG22 | 1.26                     | 1.01              |
| 1:F:620:PRO:HD2  | 2:1A:997:DA:H2'  | 1.02                     | 1.01              |
| 1:H:513:ASN:HD22 | 1:H:526:THR:HG22 | 1.26                     | 1.01              |
| 1:J:620:PRO:HD2  | 2:9:997:DA:H2'   | 1.02                     | 1.01              |
| 1:V:620:PRO:HD2  | 2:MA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:o:513:ASN:HD22 | 1:o:526:THR:HG22 | 1.26                     | 1.01              |
| 1:t:620:PRO:HD2  | 2:mA:997:DA:H2'  | 1.02                     | 1.01              |
| 1:5:620:PRO:CD   | 2:yA:997:DA:H2'  | 1.72                     | 1.01              |
| 1:A:620:PRO:CD   | 2:O:997:DA:H2'   | 1.72                     | 1.00              |
| 1:E:513:ASN:HD22 | 1:E:526:THR:HG22 | 1.26                     | 1.00              |
| 1:S:620:PRO:HD2  | 2:IA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:Y:513:ASN:HD22 | 1:Y:526:THR:HG22 | 1.26                     | 1.00              |
| 1:i:620:PRO:CD   | 2:aA:997:DA:H2'  | 1.72                     | 1.00              |
| 1:n:513:ASN:HD22 | 1:n:526:THR:HG22 | 1.26                     | 1.00              |
| 1:n:620:PRO:HD2  | 2:gA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:r:620:PRO:HD2  | 2:kA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:u:513:ASN:HD22 | 1:u:526:THR:HG22 | 1.26                     | 1.00              |
| 1:u:620:PRO:CD   | 2:nA:997:DA:H2'  | 1.72                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:620:PRO:HD2  | 2:xA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:M:620:PRO:HD2  | 2:CA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:c:513:ASN:HD22 | 1:c:526:THR:HG22 | 1.26                     | 1.00              |
| 1:e:620:PRO:HD2  | 2:WA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:h:513:ASN:HD22 | 1:h:526:THR:HG22 | 1.26                     | 1.00              |
| 1:h:620:PRO:HD2  | 2:ZA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:l:620:PRO:CD   | 2:dA:997:DA:H2'  | 1.72                     | 1.00              |
| 1:q:620:PRO:HD2  | 2:jA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:q:620:PRO:CD   | 2:jA:997:DA:H2'  | 1.72                     | 1.00              |
| 1:E:620:PRO:HD2  | 2:qA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:E:620:PRO:CD   | 2:qA:997:DA:H2'  | 1.72                     | 1.00              |
| 1:S:620:PRO:CD   | 2:IA:997:DA:H2'  | 1.71                     | 1.00              |
| 1:l:620:PRO:HD2  | 2:dA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:v:620:PRO:CD   | 2:oA:997:DA:H2'  | 1.72                     | 1.00              |
| 1:w:620:PRO:HD2  | 2:pA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:w:620:PRO:CD   | 2:pA:997:DA:H2'  | 1.71                     | 1.00              |
| 1:R:513:ASN:HD22 | 1:R:526:THR:HG22 | 1.26                     | 1.00              |
| 1:u:620:PRO:HD2  | 2:nA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:y:513:ASN:HD22 | 1:y:526:THR:HG22 | 1.26                     | 1.00              |
| 1:i:620:PRO:HD2  | 2:aA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:2:620:PRO:HD2  | 2:vA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:J:513:ASN:HD22 | 1:J:526:THR:HG22 | 1.26                     | 1.00              |
| 1:a:620:PRO:HD2  | 2:RA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:3:620:PRO:CD   | 2:wA:997:DA:H2'  | 1.71                     | 1.00              |
| 1:P:620:PRO:HD2  | 2:FA:997:DA:H2'  | 1.02                     | 1.00              |
| 1:C:620:PRO:CD   | 2:UA:997:DA:H2'  | 1.71                     | 0.99              |
| 1:D:620:PRO:HD2  | 2:fA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:R:620:PRO:HD2  | 2:HA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:r:620:PRO:CD   | 2:kA:997:DA:H2'  | 1.72                     | 0.99              |
| 1:L:620:PRO:HD2  | 2:BA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:N:620:PRO:HD2  | 2:DA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:Q:620:PRO:CD   | 2:GA:997:DA:H2'  | 1.72                     | 0.99              |
| 1:y:620:PRO:HD2  | 2:sA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:c:620:PRO:HD2  | 2:TA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:K:513:ASN:HD22 | 1:K:526:THR:HG22 | 1.26                     | 0.99              |
| 1:m:620:PRO:HD2  | 2:eA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:1:620:PRO:HD2  | 2:uA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:e:620:PRO:CD   | 2:WA:997:DA:H2'  | 1.72                     | 0.99              |
| 1:z:620:PRO:HD2  | 2:tA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:X:620:PRO:HD2  | 2:OA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:Y:620:PRO:HD2  | 2:PA:997:DA:H2'  | 1.02                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:620:PRO:HD2  | 2:lA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:f:620:PRO:HD2  | 2:XA:997:DA:H2'  | 1.02                     | 0.99              |
| 1:p:513:ASN:HD22 | 1:p:526:THR:HG22 | 1.26                     | 0.99              |
| 1:W:513:ASN:HD22 | 1:W:526:THR:HG22 | 1.26                     | 0.99              |
| 1:Z:620:PRO:HD2  | 2:QA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:d:620:PRO:HD2  | 2:VA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:j:513:ASN:HD22 | 1:j:526:THR:HG22 | 1.26                     | 0.98              |
| 1:7:620:PRO:HD2  | 2:0A:997:DA:H2'  | 1.02                     | 0.98              |
| 1:I:620:PRO:HD2  | 2:5A:997:DA:H2'  | 1.02                     | 0.98              |
| 1:P:513:ASN:HD22 | 1:P:526:THR:HG22 | 1.26                     | 0.98              |
| 1:O:620:PRO:HD2  | 2:EA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:S:513:ASN:HD22 | 1:S:526:THR:HG22 | 1.26                     | 0.98              |
| 1:T:513:ASN:HD22 | 1:T:526:THR:HG22 | 1.26                     | 0.98              |
| 1:b:620:PRO:HD2  | 2:SA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:g:620:PRO:HD2  | 2:YA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:k:513:ASN:HD22 | 1:k:526:THR:HG22 | 1.26                     | 0.98              |
| 1:v:513:ASN:HD22 | 1:v:526:THR:HG22 | 1.26                     | 0.98              |
| 1:k:620:PRO:HD2  | 2:cA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:b:513:ASN:HD22 | 1:b:526:THR:HG22 | 1.26                     | 0.98              |
| 1:w:513:ASN:HD22 | 1:w:526:THR:HG22 | 1.26                     | 0.98              |
| 1:l:513:ASN:HD22 | 1:l:526:THR:HG22 | 1.26                     | 0.98              |
| 1:C:513:ASN:HD22 | 1:C:526:THR:HG22 | 1.26                     | 0.98              |
| 1:T:620:PRO:HD2  | 2:KA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:Z:513:ASN:HD22 | 1:Z:526:THR:HG22 | 1.26                     | 0.98              |
| 1:Q:513:ASN:HD22 | 1:Q:526:THR:HG22 | 1.26                     | 0.98              |
| 1:d:513:ASN:HD22 | 1:d:526:THR:HG22 | 1.26                     | 0.98              |
| 1:7:513:ASN:HD22 | 1:7:526:THR:HG22 | 1.26                     | 0.98              |
| 1:Z:620:PRO:HD2  | 2:QA:997:DA:C1'  | 1.94                     | 0.98              |
| 1:b:620:PRO:HD2  | 2:SA:997:DA:C1'  | 1.94                     | 0.98              |
| 1:j:620:PRO:HD2  | 2:bA:997:DA:H2'  | 1.02                     | 0.98              |
| 1:G:620:PRO:HD2  | 2:3A:997:DA:C1'  | 1.94                     | 0.98              |
| 1:6:620:PRO:HD2  | 2:zA:997:DA:C1'  | 1.94                     | 0.98              |
| 1:B:620:PRO:HD2  | 2:JA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:i:513:ASN:HD22 | 1:i:526:THR:HG22 | 1.26                     | 0.97              |
| 1:2:513:ASN:HD22 | 1:2:526:THR:HG22 | 1.26                     | 0.97              |
| 1:3:513:ASN:HD22 | 1:3:526:THR:HG22 | 1.26                     | 0.97              |
| 1:8:620:PRO:HD2  | 2:2A:997:DA:C1'  | 1.94                     | 0.97              |
| 1:D:620:PRO:HD2  | 2:fA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:N:620:PRO:HD2  | 2:DA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:V:513:ASN:HD22 | 1:V:526:THR:HG22 | 1.26                     | 0.97              |
| 1:r:620:PRO:HD2  | 2:kA:997:DA:C1'  | 1.94                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:620:PRO:HD2  | 2:vA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:D:513:ASN:HD22 | 1:D:526:THR:HG22 | 1.26                     | 0.97              |
| 1:I:513:ASN:HD22 | 1:I:526:THR:HG22 | 1.26                     | 0.97              |
| 1:Q:620:PRO:HD2  | 2:GA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:X:513:ASN:HD22 | 1:X:526:THR:HG22 | 1.26                     | 0.97              |
| 1:y:620:PRO:HD2  | 2:sA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:z:620:PRO:HD2  | 2:tA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:O:620:PRO:HD2  | 2:EA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:R:620:PRO:HD2  | 2:HA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:e:620:PRO:HD2  | 2:WA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:f:513:ASN:HD22 | 1:f:526:THR:HG22 | 1.26                     | 0.97              |
| 1:v:620:PRO:HD2  | 2:oA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:C:620:PRO:HD2  | 2:UA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:J:620:PRO:HD2  | 2:9:997:DA:C1'   | 1.94                     | 0.97              |
| 1:d:620:PRO:HD2  | 2:VA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:g:620:PRO:HD2  | 2:YA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:k:620:PRO:HD2  | 2:cA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:l:513:ASN:HD22 | 1:l:526:THR:HG22 | 1.26                     | 0.97              |
| 1:G:513:ASN:HD22 | 1:G:526:THR:HG22 | 1.26                     | 0.97              |
| 1:K:620:PRO:HD2  | 2:AA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:W:620:PRO:HD2  | 2:NA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:e:513:ASN:HD22 | 1:e:526:THR:HG22 | 1.26                     | 0.97              |
| 1:f:620:PRO:HD2  | 2:XA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:q:513:ASN:HD22 | 1:q:526:THR:HG22 | 1.26                     | 0.97              |
| 1:3:620:PRO:HD2  | 2:wA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:Y:620:PRO:HD2  | 2:PA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:m:620:PRO:HD2  | 2:eA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:u:620:PRO:HD2  | 2:nA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:E:620:PRO:HD2  | 2:qA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:c:620:PRO:HD2  | 2:TA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:f:620:PRO:CD   | 2:XA:997:DA:H2'  | 1.72                     | 0.97              |
| 1:p:620:PRO:HD2  | 2:iA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:M:620:PRO:HD2  | 2:CA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:N:513:ASN:HD22 | 1:N:526:THR:HG22 | 1.26                     | 0.97              |
| 1:U:620:PRO:HD2  | 2:LA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:V:620:PRO:HD2  | 2:MA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:m:513:ASN:HD22 | 1:m:526:THR:HG22 | 1.26                     | 0.97              |
| 1:q:620:PRO:HD2  | 2:jA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:A:620:PRO:HD2  | 2:0:997:DA:C1'   | 1.94                     | 0.97              |
| 1:L:620:PRO:HD2  | 2:BA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:s:513:ASN:HD22 | 1:s:526:THR:HG22 | 1.26                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:620:PRO:HD2  | 2:xA:997:DA:C1'  | 1.94                     | 0.97              |
| 1:6:513:ASN:HD22 | 1:6:526:THR:HG22 | 1.26                     | 0.97              |
| 1:a:620:PRO:HD2  | 2:RA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:r:513:ASN:HD22 | 1:r:526:THR:HG22 | 1.26                     | 0.96              |
| 1:x:620:PRO:HD2  | 2:rA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:5:620:PRO:HD2  | 2:yA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:a:513:ASN:HD22 | 1:a:526:THR:HG22 | 1.26                     | 0.96              |
| 1:o:620:PRO:HD2  | 2:hA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:s:620:PRO:HD2  | 2:lA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:z:513:ASN:HD22 | 1:z:526:THR:HG22 | 1.26                     | 0.96              |
| 1:1:620:PRO:HD2  | 2:uA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:L:513:ASN:HD22 | 1:L:526:THR:HG22 | 1.26                     | 0.96              |
| 1:X:620:PRO:HD2  | 2:OA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:t:620:PRO:CD   | 2:mA:997:DA:H2'  | 1.72                     | 0.96              |
| 1:P:620:PRO:HD2  | 2:FA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:m:620:PRO:CD   | 2:eA:997:DA:H2'  | 1.72                     | 0.96              |
| 1:7:620:PRO:HD2  | 2:0A:997:DA:C1'  | 1.94                     | 0.96              |
| 1:F:513:ASN:HD22 | 1:F:526:THR:HG22 | 1.26                     | 0.96              |
| 1:I:620:PRO:HD2  | 2:5A:997:DA:C1'  | 1.94                     | 0.96              |
| 1:i:620:PRO:HD2  | 2:aA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:l:620:PRO:HD2  | 2:dA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:F:620:PRO:HD2  | 2:1A:997:DA:C1'  | 1.94                     | 0.96              |
| 1:H:620:PRO:HD2  | 2:4A:997:DA:C1'  | 1.94                     | 0.96              |
| 1:T:620:PRO:HD2  | 2:KA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:V:620:PRO:HD3  | 2:MA:997:DA:H2'' | 1.48                     | 0.96              |
| 1:j:620:PRO:HD2  | 2:bA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:q:620:PRO:HD3  | 2:jA:997:DA:H2'' | 1.48                     | 0.96              |
| 1:t:513:ASN:HD22 | 1:t:526:THR:HG22 | 1.26                     | 0.96              |
| 1:t:620:PRO:HD2  | 2:mA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:2:620:PRO:CD   | 2:vA:997:DA:H2'  | 1.72                     | 0.96              |
| 1:h:620:PRO:HD2  | 2:ZA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:5:513:ASN:HD22 | 1:5:526:THR:HG22 | 1.26                     | 0.96              |
| 1:A:513:ASN:HD22 | 1:A:526:THR:HG22 | 1.26                     | 0.96              |
| 1:G:620:PRO:HD3  | 2:3A:997:DA:H2'' | 1.48                     | 0.96              |
| 1:Z:620:PRO:HD3  | 2:QA:997:DA:H2'' | 1.48                     | 0.96              |
| 1:n:620:PRO:HD2  | 2:gA:997:DA:C1'  | 1.94                     | 0.96              |
| 1:6:620:PRO:HD3  | 2:zA:997:DA:H2'' | 1.48                     | 0.96              |
| 1:F:620:PRO:CD   | 2:1A:997:DA:H2'  | 1.72                     | 0.95              |
| 1:O:513:ASN:HD22 | 1:O:526:THR:HG22 | 1.26                     | 0.95              |
| 1:b:620:PRO:HD3  | 2:SA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:w:620:PRO:HD2  | 2:pA:997:DA:C1'  | 1.94                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:513:ASN:HD22 | 1:x:526:THR:HG22 | 1.26                     | 0.95              |
| 1:l:620:PRO:HD3  | 2:5A:997:DA:H2'' | 1.48                     | 0.95              |
| 1:d:620:PRO:HD3  | 2:VA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:D:620:PRO:CD   | 2:fA:997:DA:H2'  | 1.72                     | 0.95              |
| 1:D:620:PRO:HD3  | 2:fA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:S:620:PRO:HD2  | 2:IA:997:DA:C1'  | 1.94                     | 0.95              |
| 1:g:513:ASN:HD22 | 1:g:526:THR:HG22 | 1.26                     | 0.95              |
| 1:k:620:PRO:HD3  | 2:cA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:7:620:PRO:HD3  | 2:0A:997:DA:H2'' | 1.48                     | 0.95              |
| 1:F:620:PRO:HD3  | 2:1A:997:DA:H2'' | 1.48                     | 0.95              |
| 1:M:513:ASN:HD22 | 1:M:526:THR:HG22 | 1.26                     | 0.95              |
| 1:U:513:ASN:HD22 | 1:U:526:THR:HG22 | 1.26                     | 0.95              |
| 1:2:620:PRO:HD3  | 2:vA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:X:620:PRO:HD3  | 2:OA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:s:620:PRO:HD3  | 2:lA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:t:620:PRO:HD3  | 2:mA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:4:513:ASN:HD22 | 1:4:526:THR:HG22 | 1.26                     | 0.95              |
| 1:i:620:PRO:HD3  | 2:aA:997:DA:H2'' | 1.48                     | 0.95              |
| 1:F:620:PRO:HG2  | 2:1A:997:DA:N3   | 1.82                     | 0.94              |
| 1:L:620:PRO:HD3  | 2:BA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:q:620:PRO:HG2  | 2:jA:997:DA:N3   | 1.82                     | 0.94              |
| 1:t:620:PRO:HG2  | 2:mA:997:DA:N3   | 1.82                     | 0.94              |
| 1:G:620:PRO:HG2  | 2:3A:997:DA:N3   | 1.82                     | 0.94              |
| 1:M:620:PRO:HG2  | 2:CA:997:DA:N3   | 1.82                     | 0.94              |
| 1:O:620:PRO:HG2  | 2:EA:997:DA:N3   | 1.82                     | 0.94              |
| 1:V:620:PRO:HG2  | 2:MA:997:DA:N3   | 1.82                     | 0.94              |
| 1:a:620:PRO:HD3  | 2:RA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:g:620:PRO:HG2  | 2:YA:997:DA:N3   | 1.82                     | 0.94              |
| 1:l:620:PRO:HD3  | 2:dA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:4:620:PRO:HG2  | 2:xA:997:DA:N3   | 1.82                     | 0.94              |
| 1:C:620:PRO:HG2  | 2:UA:997:DA:N3   | 1.82                     | 0.94              |
| 1:d:620:PRO:HG2  | 2:VA:997:DA:N3   | 1.82                     | 0.94              |
| 1:e:620:PRO:HG2  | 2:WA:997:DA:N3   | 1.82                     | 0.94              |
| 1:k:620:PRO:HG2  | 2:cA:997:DA:N3   | 1.82                     | 0.94              |
| 1:3:620:PRO:HG2  | 2:wA:997:DA:N3   | 1.82                     | 0.94              |
| 1:6:620:PRO:HG2  | 2:zA:997:DA:N3   | 1.82                     | 0.94              |
| 1:j:620:PRO:HG2  | 2:bA:997:DA:N3   | 1.82                     | 0.94              |
| 1:r:620:PRO:HG2  | 2:kA:997:DA:N3   | 1.82                     | 0.94              |
| 1:E:620:PRO:HG2  | 2:qA:997:DA:N3   | 1.82                     | 0.94              |
| 1:U:620:PRO:HD3  | 2:LA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:X:620:PRO:HG2  | 2:OA:997:DA:N3   | 1.82                     | 0.94              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:i:620:PRO:HG2 | 2:aA:997:DA:N3   | 1.82                     | 0.94              |
| 1:l:620:PRO:HG2 | 2:dA:997:DA:N3   | 1.82                     | 0.94              |
| 1:w:620:PRO:HD3 | 2:pA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:D:620:PRO:HG2 | 2:fA:997:DA:N3   | 1.82                     | 0.94              |
| 1:T:620:PRO:HG2 | 2:KA:997:DA:N3   | 1.82                     | 0.94              |
| 1:n:620:PRO:HD3 | 2:gA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:u:620:PRO:HG2 | 2:nA:997:DA:N3   | 1.82                     | 0.94              |
| 1:p:620:PRO:HD3 | 2:iA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:s:620:PRO:HG2 | 2:lA:997:DA:N3   | 1.82                     | 0.94              |
| 1:L:620:PRO:HG2 | 2:BA:997:DA:N3   | 1.82                     | 0.94              |
| 1:R:620:PRO:CD  | 2:HA:997:DA:H2'  | 1.71                     | 0.94              |
| 1:S:620:PRO:HD3 | 2:IA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:b:620:PRO:HG2 | 2:SA:997:DA:N3   | 1.82                     | 0.94              |
| 1:h:620:PRO:HD3 | 2:ZA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:m:620:PRO:HG2 | 2:eA:997:DA:N3   | 1.82                     | 0.94              |
| 1:n:620:PRO:HG2 | 2:gA:997:DA:N3   | 1.82                     | 0.94              |
| 1:o:620:PRO:HG2 | 2:hA:997:DA:N3   | 1.82                     | 0.94              |
| 1:v:620:PRO:HG2 | 2:oA:997:DA:N3   | 1.82                     | 0.94              |
| 1:x:620:PRO:HD3 | 2:rA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:2:620:PRO:HG2 | 2:vA:997:DA:N3   | 1.82                     | 0.94              |
| 1:H:620:PRO:HG2 | 2:4A:997:DA:N3   | 1.82                     | 0.94              |
| 1:J:620:PRO:HD3 | 2:9:997:DA:H2''  | 1.48                     | 0.94              |
| 1:P:620:PRO:HD3 | 2:FA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:Q:620:PRO:HG2 | 2:GA:997:DA:N3   | 1.82                     | 0.94              |
| 1:W:620:PRO:HD3 | 2:NA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:Z:620:PRO:HG2 | 2:QA:997:DA:N3   | 1.82                     | 0.94              |
| 1:a:620:PRO:HG2 | 2:RA:997:DA:N3   | 1.82                     | 0.94              |
| 1:c:620:PRO:HG2 | 2:TA:997:DA:N3   | 1.82                     | 0.94              |
| 1:h:620:PRO:HG2 | 2:ZA:997:DA:N3   | 1.82                     | 0.94              |
| 1:y:620:PRO:CD  | 2:sA:997:DA:H2'  | 1.72                     | 0.94              |
| 1:I:620:PRO:HG2 | 2:5A:997:DA:N3   | 1.82                     | 0.94              |
| 1:K:620:PRO:HG2 | 2:AA:997:DA:N3   | 1.82                     | 0.94              |
| 1:e:620:PRO:HD3 | 2:WA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:f:620:PRO:HG2 | 2:XA:997:DA:N3   | 1.82                     | 0.94              |
| 1:m:620:PRO:HD3 | 2:eA:997:DA:H2'' | 1.48                     | 0.94              |
| 1:5:620:PRO:HG2 | 2:yA:997:DA:N3   | 1.82                     | 0.94              |
| 1:7:620:PRO:HG2 | 2:0A:997:DA:N3   | 1.82                     | 0.94              |
| 1:A:620:PRO:HG2 | 2:0:997:DA:N3    | 1.82                     | 0.93              |
| 1:J:620:PRO:HG2 | 2:9:997:DA:N3    | 1.82                     | 0.93              |
| 1:Y:620:PRO:HG2 | 2:PA:997:DA:N3   | 1.82                     | 0.93              |
| 1:B:620:PRO:CD  | 2:JA:997:DA:H2'  | 1.72                     | 0.93              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:620:PRO:HD3 | 2:JA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:K:620:PRO:HD3 | 2:AA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:r:620:PRO:HD3 | 2:kA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:v:620:PRO:HD3 | 2:oA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:1:620:PRO:HD3 | 2:uA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:Q:620:PRO:HD3 | 2:GA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:N:620:PRO:HG2 | 2:DA:997:DA:N3   | 1.82                     | 0.93              |
| 1:f:620:PRO:HD3 | 2:XA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:8:620:PRO:HD3 | 2:2A:997:DA:H2'' | 1.48                     | 0.93              |
| 1:N:620:PRO:HD3 | 2:DA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:y:620:PRO:HG2 | 2:sA:997:DA:N3   | 1.82                     | 0.93              |
| 1:z:620:PRO:HG2 | 2:tA:997:DA:N3   | 1.82                     | 0.93              |
| 1:R:620:PRO:HG2 | 2:HA:997:DA:N3   | 1.82                     | 0.93              |
| 1:U:620:PRO:HG2 | 2:LA:997:DA:N3   | 1.82                     | 0.93              |
| 1:z:620:PRO:HD3 | 2:tA:997:DA:H2'' | 1.48                     | 0.93              |
| 1:R:620:PRO:HD3 | 2:HA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:j:620:PRO:HD3 | 2:bA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:w:620:PRO:HG2 | 2:pA:997:DA:N3   | 1.82                     | 0.92              |
| 1:x:620:PRO:HG2 | 2:rA:997:DA:N3   | 1.82                     | 0.92              |
| 1:M:620:PRO:HD3 | 2:CA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:S:620:PRO:HG2 | 2:IA:997:DA:N3   | 1.82                     | 0.92              |
| 1:O:620:PRO:HD3 | 2:EA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:o:620:PRO:HD3 | 2:hA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:u:620:PRO:HD3 | 2:nA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:y:620:PRO:HD3 | 2:sA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:4:620:PRO:HD3 | 2:xA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:E:620:PRO:HD3 | 2:qA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:H:620:PRO:HD3 | 2:4A:997:DA:H2'' | 1.48                     | 0.92              |
| 1:T:620:PRO:HD3 | 2:KA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:8:620:PRO:HG2 | 2:2A:997:DA:N3   | 1.82                     | 0.92              |
| 1:g:620:PRO:HD3 | 2:YA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:W:620:PRO:HG2 | 2:NA:997:DA:N3   | 1.82                     | 0.92              |
| 1:B:620:PRO:HG2 | 2:JA:997:DA:N3   | 1.82                     | 0.92              |
| 1:P:620:PRO:HG2 | 2:FA:997:DA:N3   | 1.82                     | 0.92              |
| 1:Y:620:PRO:HD3 | 2:PA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:c:620:PRO:HD3 | 2:TA:997:DA:H2'' | 1.48                     | 0.92              |
| 1:p:620:PRO:HG2 | 2:iA:997:DA:N3   | 1.82                     | 0.91              |
| 1:1:620:PRO:HG2 | 2:uA:997:DA:N3   | 1.82                     | 0.91              |
| 1:B:620:PRO:HD2 | 2:JA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:n:620:PRO:HD2 | 2:gA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:8:620:PRO:HD2 | 2:2A:997:DA:H2'' | 0.91                     | 0.91              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:a:620:PRO:HD2 | 2:RA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:h:620:PRO:HD2 | 2:ZA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:x:620:PRO:CD  | 2:rA:997:DA:H2'  | 1.72                     | 0.91              |
| 1:L:620:PRO:HD2 | 2:BA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:6:620:PRO:HD2 | 2:zA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:I:620:PRO:HD2 | 2:5A:997:DA:H2'' | 0.91                     | 0.91              |
| 1:N:620:PRO:HD2 | 2:DA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:z:620:PRO:HD2 | 2:tA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:C:620:PRO:HD3 | 2:UA:997:DA:H2'' | 1.48                     | 0.91              |
| 1:E:620:PRO:HD2 | 2:qA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:G:620:PRO:HD2 | 2:3A:997:DA:H2'' | 0.91                     | 0.91              |
| 1:u:620:PRO:HD2 | 2:nA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:3:620:PRO:HD3 | 2:wA:997:DA:H2'' | 1.48                     | 0.91              |
| 1:7:620:PRO:HD2 | 2:0A:997:DA:H2'' | 0.91                     | 0.91              |
| 1:Y:620:PRO:HD2 | 2:PA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:4:620:PRO:HD2 | 2:xA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:D:620:PRO:HD2 | 2:fA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:U:620:PRO:CD  | 2:LA:997:DA:H2'  | 1.72                     | 0.91              |
| 1:c:620:PRO:HD2 | 2:TA:997:DA:H2'' | 0.91                     | 0.91              |
| 1:2:620:PRO:HD2 | 2:vA:997:DA:H2'' | 0.91                     | 0.90              |
| 1:n:619:HIS:HA  | 2:gA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:Q:619:HIS:HA  | 2:GA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:h:619:HIS:HA  | 2:ZA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:v:619:HIS:HA  | 2:oA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:U:619:HIS:HA  | 2:LA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:W:619:HIS:HA  | 2:NA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:x:619:HIS:HA  | 2:rA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:z:619:HIS:HA  | 2:tA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:N:619:HIS:HA  | 2:DA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:U:620:PRO:HD2 | 2:LA:997:DA:H2'' | 0.91                     | 0.90              |
| 1:x:620:PRO:HD2 | 2:rA:997:DA:H2'' | 0.91                     | 0.90              |
| 1:C:619:HIS:HA  | 2:UA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:I:619:HIS:HA  | 2:5A:997:DA:C3'  | 2.02                     | 0.90              |
| 1:L:619:HIS:HA  | 2:BA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:m:619:HIS:HA  | 2:eA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:p:619:HIS:HA  | 2:iA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:s:620:PRO:CD  | 2:lA:997:DA:H2'  | 1.71                     | 0.90              |
| 1:3:619:HIS:HA  | 2:wA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:3:620:PRO:HD2 | 2:wA:997:DA:H2'' | 0.91                     | 0.90              |
| 1:7:619:HIS:HA  | 2:0A:997:DA:C3'  | 2.02                     | 0.90              |
| 1:A:620:PRO:HD3 | 2:0:997:DA:H2''  | 1.48                     | 0.90              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:a:619:HIS:HA  | 2:RA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:b:619:HIS:HA  | 2:SA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:f:619:HIS:HA  | 2:XA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:4:619:HIS:HA  | 2:xA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:A:619:HIS:HA  | 2:O:997:DA:C3'   | 2.02                     | 0.90              |
| 1:C:620:PRO:HD2 | 2:UA:997:DA:H2'' | 0.91                     | 0.90              |
| 1:F:620:PRO:HD2 | 2:1A:997:DA:H2'' | 0.91                     | 0.90              |
| 1:H:619:HIS:HA  | 2:4A:997:DA:C3'  | 2.02                     | 0.90              |
| 1:J:620:PRO:HD2 | 2:9:997:DA:H2''  | 0.91                     | 0.90              |
| 1:R:620:PRO:HD2 | 2:HA:997:DA:H2'' | 0.91                     | 0.90              |
| 1:Z:619:HIS:HA  | 2:QA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:c:619:HIS:HA  | 2:TA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:w:619:HIS:HA  | 2:pA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:5:619:HIS:HA  | 2:yA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:8:619:HIS:HA  | 2:2A:997:DA:C3'  | 2.02                     | 0.90              |
| 1:B:619:HIS:HA  | 2:JA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:M:619:HIS:HA  | 2:CA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:S:619:HIS:HA  | 2:IA:997:DA:C3'  | 2.02                     | 0.90              |
| 1:D:619:HIS:HA  | 2:fA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:K:620:PRO:HD2 | 2:AA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:X:619:HIS:HA  | 2:OA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:Y:619:HIS:HA  | 2:PA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:o:619:HIS:HA  | 2:hA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:q:619:HIS:HA  | 2:jA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:t:620:PRO:HD2 | 2:mA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:G:619:HIS:HA  | 2:3A:997:DA:C3'  | 2.02                     | 0.89              |
| 1:S:620:PRO:HD2 | 2:IA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:V:619:HIS:HA  | 2:MA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:V:620:PRO:HD2 | 2:MA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:q:620:PRO:HD2 | 2:jA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:t:619:HIS:HA  | 2:mA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:w:620:PRO:HD2 | 2:pA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:5:620:PRO:HD3 | 2:yA:997:DA:H2'' | 1.48                     | 0.89              |
| 1:6:619:HIS:HA  | 2:zA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:H:620:PRO:HD2 | 2:4A:997:DA:H2'' | 0.91                     | 0.89              |
| 1:J:619:HIS:HA  | 2:9:997:DA:C3'   | 2.02                     | 0.89              |
| 1:O:619:HIS:HA  | 2:EA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:T:619:HIS:HA  | 2:KA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:j:619:HIS:HA  | 2:bA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:o:620:PRO:HD2 | 2:hA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:s:619:HIS:HA  | 2:1A:997:DA:C3'  | 2.02                     | 0.89              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:y:620:PRO:HD2 | 2:sA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:2:619:HIS:HA  | 2:vA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:F:619:HIS:HA  | 2:1A:997:DA:C3'  | 2.02                     | 0.89              |
| 1:K:619:HIS:HA  | 2:AA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:R:619:HIS:HA  | 2:HA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:d:620:PRO:HD2 | 2:VA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:g:619:HIS:HA  | 2:YA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:k:619:HIS:HA  | 2:cA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:d:619:HIS:HA  | 2:VA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:k:620:PRO:HD2 | 2:cA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:u:619:HIS:HA  | 2:nA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:y:619:HIS:HA  | 2:sA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:E:619:HIS:HA  | 2:qA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:X:620:PRO:HD2 | 2:OA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:g:620:PRO:HD2 | 2:YA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:i:619:HIS:HA  | 2:aA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:O:620:PRO:HD2 | 2:EA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:j:620:PRO:HD2 | 2:bA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:l:619:HIS:HA  | 2:dA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:r:620:PRO:HD2 | 2:kA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:1:619:HIS:HA  | 2:uA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:1:620:PRO:HD2 | 2:uA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:P:620:PRO:HD2 | 2:FA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:m:620:PRO:HD2 | 2:eA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:p:620:PRO:HD2 | 2:iA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:s:620:PRO:HD2 | 2:lA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:P:619:HIS:HA  | 2:FA:997:DA:C3'  | 2.02                     | 0.89              |
| 1:W:620:PRO:HD2 | 2:NA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:e:620:PRO:HD2 | 2:WA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:A:620:PRO:HD2 | 2:O:997:DA:H2''  | 0.91                     | 0.89              |
| 1:T:620:PRO:HD2 | 2:KA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:f:620:PRO:HD2 | 2:XA:997:DA:H2'' | 0.91                     | 0.89              |
| 1:i:620:PRO:HD2 | 2:aA:997:DA:H2'' | 0.91                     | 0.88              |
| 1:l:620:PRO:HD2 | 2:dA:997:DA:H2'' | 0.91                     | 0.88              |
| 1:5:620:PRO:HD2 | 2:yA:997:DA:H2'' | 0.91                     | 0.88              |
| 1:r:619:HIS:HA  | 2:kA:997:DA:C3'  | 2.02                     | 0.88              |
| 1:e:619:HIS:HA  | 2:WA:997:DA:C3'  | 2.02                     | 0.88              |
| 1:Q:620:PRO:HD2 | 2:GA:997:DA:H2'' | 0.91                     | 0.87              |
| 1:Z:620:PRO:HD2 | 2:QA:997:DA:H2'' | 0.91                     | 0.87              |
| 1:A:619:HIS:HA  | 2:O:997:DA:C2'   | 2.05                     | 0.87              |
| 1:b:620:PRO:HD2 | 2:SA:997:DA:H2'' | 0.91                     | 0.87              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:i:619:HIS:HA  | 2:aA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:l:619:HIS:HA  | 2:dA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:r:619:HIS:HA  | 2:kA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:5:619:HIS:HA  | 2:yA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:K:619:HIS:HA  | 2:AA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:e:619:HIS:HA  | 2:WA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:t:619:HIS:HA  | 2:mA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:v:620:PRO:HD2 | 2:oA:997:DA:H2'' | 0.91                     | 0.87              |
| 1:D:619:HIS:HA  | 2:fA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:F:619:HIS:HA  | 2:1A:997:DA:C2'  | 2.05                     | 0.87              |
| 1:J:619:HIS:HA  | 2:9:997:DA:C2'   | 2.05                     | 0.87              |
| 1:2:619:HIS:HA  | 2:vA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:I:619:HIS:HA  | 2:5A:997:DA:C2'  | 2.05                     | 0.87              |
| 1:Y:619:HIS:HA  | 2:PA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:7:619:HIS:HA  | 2:0A:997:DA:C2'  | 2.05                     | 0.87              |
| 1:c:619:HIS:HA  | 2:TA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:d:619:HIS:HA  | 2:VA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:g:619:HIS:HA  | 2:YA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:q:619:HIS:HA  | 2:jA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:E:619:HIS:HA  | 2:qA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:V:619:HIS:HA  | 2:MA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:Z:619:HIS:HA  | 2:QA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:b:619:HIS:HA  | 2:SA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:k:619:HIS:HA  | 2:cA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:m:619:HIS:HA  | 2:eA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:u:619:HIS:HA  | 2:nA:997:DA:C2'  | 2.05                     | 0.87              |
| 1:G:619:HIS:HA  | 2:3A:997:DA:C2'  | 2.05                     | 0.86              |
| 1:L:619:HIS:HA  | 2:BA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:M:619:HIS:HA  | 2:CA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:O:619:HIS:HA  | 2:EA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:f:619:HIS:HA  | 2:XA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:6:619:HIS:HA  | 2:zA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:B:619:HIS:HA  | 2:JA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:a:619:HIS:HA  | 2:RA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:x:619:HIS:HA  | 2:rA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:4:619:HIS:HA  | 2:xA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:U:619:HIS:HA  | 2:LA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:y:619:HIS:HA  | 2:sA:997:DA:C2'  | 2.05                     | 0.86              |
| 1:8:619:HIS:HA  | 2:2A:997:DA:C2'  | 2.05                     | 0.86              |
| 1:M:620:PRO:HD2 | 2:CA:997:DA:H2'' | 0.91                     | 0.86              |
| 1:3:619:HIS:HA  | 2:wA:997:DA:C2'  | 2.05                     | 0.86              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:R:619:HIS:HA | 2:HA:997:DA:C2' | 2.05                     | 0.86              |
| 1:1:619:HIS:HA | 2:uA:997:DA:C2' | 2.05                     | 0.86              |
| 1:C:619:HIS:HA | 2:UA:997:DA:C2' | 2.05                     | 0.86              |
| 1:w:619:HIS:HA | 2:pA:997:DA:C2' | 2.05                     | 0.86              |
| 1:P:619:HIS:HA | 2:FA:997:DA:C2' | 2.05                     | 0.86              |
| 1:S:619:HIS:HA | 2:IA:997:DA:C2' | 2.05                     | 0.86              |
| 1:n:619:HIS:HA | 2:gA:997:DA:C2' | 2.05                     | 0.86              |
| 1:z:619:HIS:HA | 2:tA:997:DA:C2' | 2.05                     | 0.86              |
| 1:N:619:HIS:HA | 2:DA:997:DA:C2' | 2.05                     | 0.86              |
| 1:Q:619:HIS:HA | 2:GA:997:DA:C2' | 2.05                     | 0.86              |
| 1:h:619:HIS:HA | 2:ZA:997:DA:C2' | 2.05                     | 0.86              |
| 1:v:619:HIS:HA | 2:oA:997:DA:C2' | 2.05                     | 0.86              |
| 1:X:619:HIS:HA | 2:OA:997:DA:C2' | 2.05                     | 0.85              |
| 1:j:619:HIS:HA | 2:bA:997:DA:C2' | 2.05                     | 0.85              |
| 1:T:619:HIS:HA | 2:KA:997:DA:C2' | 2.05                     | 0.85              |
| 1:s:619:HIS:HA | 2:lA:997:DA:C2' | 2.05                     | 0.85              |
| 1:p:619:HIS:HA | 2:iA:997:DA:C2' | 2.05                     | 0.85              |
| 1:W:619:HIS:HA | 2:NA:997:DA:C2' | 2.05                     | 0.85              |
| 1:H:619:HIS:HA | 2:4A:997:DA:C2' | 2.05                     | 0.85              |
| 1:o:619:HIS:HA | 2:hA:997:DA:C2' | 2.05                     | 0.85              |
| 1:y:619:HIS:HA | 2:sA:997:DA:O3' | 1.83                     | 0.79              |
| 1:N:619:HIS:HA | 2:DA:997:DA:O3' | 1.83                     | 0.79              |
| 1:P:619:HIS:HA | 2:FA:997:DA:O3' | 1.83                     | 0.79              |
| 1:S:619:HIS:HA | 2:IA:997:DA:O3' | 1.83                     | 0.79              |
| 1:w:619:HIS:HA | 2:pA:997:DA:O3' | 1.83                     | 0.79              |
| 1:8:619:HIS:HA | 2:2A:997:DA:O3' | 1.83                     | 0.79              |
| 1:B:619:HIS:HA | 2:JA:997:DA:O3' | 1.83                     | 0.79              |
| 1:R:619:HIS:HA | 2:HA:997:DA:O3' | 1.83                     | 0.79              |
| 1:V:619:HIS:HA | 2:MA:997:DA:O3' | 1.83                     | 0.79              |
| 1:q:619:HIS:HA | 2:jA:997:DA:O3' | 1.83                     | 0.79              |
| 1:H:619:HIS:HA | 2:4A:997:DA:O3' | 1.83                     | 0.79              |
| 1:o:619:HIS:HA | 2:hA:997:DA:O3' | 1.83                     | 0.79              |
| 1:r:619:HIS:HA | 2:kA:997:DA:O3' | 1.83                     | 0.79              |
| 1:s:619:HIS:HA | 2:lA:997:DA:O3' | 1.83                     | 0.79              |
| 1:z:619:HIS:HA | 2:tA:997:DA:O3' | 1.83                     | 0.79              |
| 1:1:619:HIS:HA | 2:uA:997:DA:O3' | 1.83                     | 0.79              |
| 1:X:619:HIS:HA | 2:OA:997:DA:O3' | 1.83                     | 0.79              |
| 1:e:619:HIS:HA | 2:WA:997:DA:O3' | 1.83                     | 0.79              |
| 1:7:619:HIS:HA | 2:0A:997:DA:O3' | 1.83                     | 0.79              |
| 1:C:619:HIS:HA | 2:UA:997:DA:O3' | 1.83                     | 0.79              |
| 1:T:619:HIS:HA | 2:KA:997:DA:O3' | 1.83                     | 0.79              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:p:619:HIS:HA  | 2:iA:997:DA:O3' | 1.83                     | 0.79              |
| 1:l:619:HIS:HA  | 2:5A:997:DA:O3' | 1.83                     | 0.79              |
| 1:j:619:HIS:HA  | 2:bA:997:DA:O3' | 1.83                     | 0.79              |
| 1:l:619:HIS:HA  | 2:dA:997:DA:O3' | 1.83                     | 0.79              |
| 1:3:619:HIS:HA  | 2:wA:997:DA:O3' | 1.83                     | 0.79              |
| 1:D:619:HIS:HA  | 2:fA:997:DA:O3' | 1.83                     | 0.79              |
| 1:i:619:HIS:HA  | 2:aA:997:DA:O3' | 1.83                     | 0.79              |
| 1:U:619:HIS:HA  | 2:LA:997:DA:O3' | 1.83                     | 0.79              |
| 1:W:619:HIS:HA  | 2:NA:997:DA:O3' | 1.83                     | 0.79              |
| 1:x:619:HIS:HA  | 2:rA:997:DA:O3' | 1.83                     | 0.78              |
| 1:2:619:HIS:HA  | 2:vA:997:DA:O3' | 1.83                     | 0.78              |
| 1:F:619:HIS:HA  | 2:1A:997:DA:O3' | 1.83                     | 0.78              |
| 1:Y:619:HIS:HA  | 2:PA:997:DA:O3' | 1.83                     | 0.78              |
| 1:t:619:HIS:HA  | 2:mA:997:DA:O3' | 1.83                     | 0.78              |
| 1:c:619:HIS:HA  | 2:TA:997:DA:O3' | 1.83                     | 0.78              |
| 1:Z:619:HIS:HA  | 2:QA:997:DA:O3' | 1.83                     | 0.78              |
| 1:b:619:HIS:HA  | 2:SA:997:DA:O3' | 1.83                     | 0.78              |
| 1:m:619:HIS:HA  | 2:eA:997:DA:O3' | 1.83                     | 0.78              |
| 1:A:619:HIS:HA  | 2:O:997:DA:O3'  | 1.83                     | 0.78              |
| 1:E:619:HIS:HA  | 2:qA:997:DA:O3' | 1.83                     | 0.78              |
| 1:J:619:HIS:HA  | 2:9:997:DA:O3'  | 1.83                     | 0.78              |
| 1:O:619:HIS:HA  | 2:EA:997:DA:O3' | 1.83                     | 0.78              |
| 1:Q:619:HIS:HA  | 2:GA:997:DA:O3' | 1.83                     | 0.78              |
| 1:d:619:HIS:HA  | 2:VA:997:DA:O3' | 1.83                     | 0.78              |
| 1:n:619:HIS:HA  | 2:gA:997:DA:O3' | 1.83                     | 0.78              |
| 1:K:619:HIS:HA  | 2:AA:997:DA:O3' | 1.83                     | 0.78              |
| 1:v:619:HIS:HA  | 2:oA:997:DA:O3' | 1.83                     | 0.78              |
| 1:f:619:HIS:HA  | 2:XA:997:DA:O3' | 1.83                     | 0.78              |
| 1:g:619:HIS:HA  | 2:YA:997:DA:O3' | 1.83                     | 0.78              |
| 1:u:619:HIS:HA  | 2:nA:997:DA:O3' | 1.83                     | 0.78              |
| 1:h:619:HIS:HA  | 2:ZA:997:DA:O3' | 1.83                     | 0.78              |
| 1:k:619:HIS:HA  | 2:cA:997:DA:O3' | 1.83                     | 0.78              |
| 1:4:619:HIS:HA  | 2:xA:997:DA:O3' | 1.83                     | 0.78              |
| 1:5:619:HIS:HA  | 2:yA:997:DA:O3' | 1.83                     | 0.78              |
| 1:G:619:HIS:HA  | 2:3A:997:DA:O3' | 1.83                     | 0.77              |
| 1:M:619:HIS:HA  | 2:CA:997:DA:O3' | 1.83                     | 0.77              |
| 1:6:619:HIS:HA  | 2:zA:997:DA:O3' | 1.83                     | 0.77              |
| 1:a:619:HIS:HA  | 2:RA:997:DA:O3' | 1.83                     | 0.77              |
| 1:L:619:HIS:HA  | 2:BA:997:DA:O3' | 1.83                     | 0.77              |
| 1:J:410:GLU:HG3 | 2:9:996:DA:N1   | 2.00                     | 0.77              |
| 1:M:410:GLU:HG3 | 2:CA:996:DA:N1  | 2.00                     | 0.77              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:c:410:GLU:HG3 | 2:TA:996:DA:N1  | 2.00                     | 0.77              |
| 1:4:410:GLU:HG3 | 2:xA:996:DA:N1  | 2.00                     | 0.77              |
| 1:A:410:GLU:HG3 | 2:0:996:DA:N1   | 2.00                     | 0.77              |
| 1:G:410:GLU:HG3 | 2:3A:996:DA:N1  | 2.00                     | 0.77              |
| 1:K:410:GLU:HG3 | 2:AA:996:DA:N1  | 2.00                     | 0.77              |
| 1:Y:410:GLU:HG3 | 2:PA:996:DA:N1  | 2.00                     | 0.77              |
| 1:x:410:GLU:HG3 | 2:rA:996:DA:N1  | 2.00                     | 0.77              |
| 1:6:410:GLU:HG3 | 2:zA:996:DA:N1  | 2.00                     | 0.77              |
| 1:H:410:GLU:HG3 | 2:4A:996:DA:N1  | 2.00                     | 0.77              |
| 1:U:410:GLU:HG3 | 2:LA:996:DA:N1  | 2.00                     | 0.77              |
| 1:o:410:GLU:HG3 | 2:hA:996:DA:N1  | 2.00                     | 0.77              |
| 1:y:410:GLU:HG3 | 2:sA:996:DA:N1  | 2.00                     | 0.77              |
| 1:R:410:GLU:HG3 | 2:HA:996:DA:N1  | 2.00                     | 0.77              |
| 1:W:410:GLU:HG3 | 2:NA:996:DA:N1  | 2.00                     | 0.77              |
| 1:Z:410:GLU:HG3 | 2:QA:996:DA:N1  | 2.00                     | 0.77              |
| 1:b:410:GLU:HG3 | 2:SA:996:DA:N1  | 2.00                     | 0.77              |
| 1:k:410:GLU:HG3 | 2:cA:996:DA:N1  | 2.00                     | 0.77              |
| 1:5:410:GLU:HG3 | 2:yA:996:DA:N1  | 2.00                     | 0.77              |
| 1:D:410:GLU:HG3 | 2:fA:996:DA:N1  | 2.00                     | 0.76              |
| 1:d:410:GLU:HG3 | 2:VA:996:DA:N1  | 2.00                     | 0.76              |
| 1:n:410:GLU:HG3 | 2:gA:996:DA:N1  | 2.00                     | 0.76              |
| 1:p:410:GLU:HG3 | 2:iA:996:DA:N1  | 2.00                     | 0.76              |
| 1:2:410:GLU:HG3 | 2:vA:996:DA:N1  | 2.00                     | 0.76              |
| 1:f:410:GLU:HG3 | 2:XA:996:DA:N1  | 2.00                     | 0.76              |
| 1:h:410:GLU:HG3 | 2:ZA:996:DA:N1  | 2.00                     | 0.76              |
| 1:t:410:GLU:HG3 | 2:mA:996:DA:N1  | 2.00                     | 0.76              |
| 1:F:410:GLU:HG3 | 2:1A:996:DA:N1  | 2.00                     | 0.76              |
| 1:i:410:GLU:HG3 | 2:aA:996:DA:N1  | 2.00                     | 0.76              |
| 1:m:410:GLU:HG3 | 2:eA:996:DA:N1  | 2.00                     | 0.76              |
| 1:R:476:ASN:HB3 | 1:R:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:W:476:ASN:HB3 | 1:W:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:X:410:GLU:HG3 | 2:OA:996:DA:N1  | 2.00                     | 0.76              |
| 1:s:410:GLU:HG3 | 2:lA:996:DA:N1  | 2.00                     | 0.76              |
| 1:y:476:ASN:HB3 | 1:y:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:8:410:GLU:HG3 | 2:2A:996:DA:N1  | 2.00                     | 0.76              |
| 1:B:410:GLU:HG3 | 2:JA:996:DA:N1  | 2.00                     | 0.76              |
| 1:h:476:ASN:HB3 | 1:h:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:l:410:GLU:HG3 | 2:dA:996:DA:N1  | 2.00                     | 0.76              |
| 1:n:476:ASN:HB3 | 1:n:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:p:476:ASN:HB3 | 1:p:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:q:476:ASN:HB3 | 1:q:480:GLY:HA3 | 1.68                     | 0.76              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:V:476:ASN:HB3 | 1:V:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:q:410:GLU:HG3 | 2:jA:996:DA:N1  | 2.00                     | 0.76              |
| 1:C:410:GLU:HG3 | 2:UA:996:DA:N1  | 2.00                     | 0.76              |
| 1:c:476:ASN:HB3 | 1:c:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:w:410:GLU:HG3 | 2:pA:996:DA:N1  | 2.00                     | 0.76              |
| 1:x:476:ASN:HB3 | 1:x:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:z:410:GLU:HG3 | 2:tA:996:DA:N1  | 2.00                     | 0.76              |
| 1:I:476:ASN:HB3 | 1:I:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:N:410:GLU:HG3 | 2:DA:996:DA:N1  | 2.00                     | 0.76              |
| 1:P:410:GLU:HG3 | 2:FA:996:DA:N1  | 2.00                     | 0.76              |
| 1:S:410:GLU:HG3 | 2:IA:996:DA:N1  | 2.00                     | 0.76              |
| 1:U:476:ASN:HB3 | 1:U:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:V:410:GLU:HG3 | 2:MA:996:DA:N1  | 2.00                     | 0.76              |
| 1:X:476:ASN:HB3 | 1:X:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:Y:476:ASN:HB3 | 1:Y:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:s:476:ASN:HB3 | 1:s:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:v:410:GLU:HG3 | 2:oA:996:DA:N1  | 2.00                     | 0.76              |
| 1:3:410:GLU:HG3 | 2:wA:996:DA:N1  | 2.00                     | 0.76              |
| 1:E:410:GLU:HG3 | 2:qA:996:DA:N1  | 2.00                     | 0.76              |
| 1:Q:410:GLU:HG3 | 2:GA:996:DA:N1  | 2.00                     | 0.76              |
| 1:u:410:GLU:HG3 | 2:nA:996:DA:N1  | 2.00                     | 0.76              |
| 1:1:410:GLU:HG3 | 2:uA:996:DA:N1  | 2.00                     | 0.76              |
| 1:7:476:ASN:HB3 | 1:7:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:8:476:ASN:HB3 | 1:8:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:I:410:GLU:HG3 | 2:5A:996:DA:N1  | 2.00                     | 0.76              |
| 1:T:410:GLU:HG3 | 2:KA:996:DA:N1  | 2.00                     | 0.76              |
| 1:a:476:ASN:HB3 | 1:a:480:GLY:HA3 | 1.68                     | 0.76              |
| 1:B:476:ASN:HB3 | 1:B:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:j:410:GLU:HG3 | 2:bA:996:DA:N1  | 2.00                     | 0.75              |
| 1:t:476:ASN:HB3 | 1:t:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:1:476:ASN:HB3 | 1:1:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:7:410:GLU:HG3 | 2:0A:996:DA:N1  | 2.00                     | 0.75              |
| 1:L:410:GLU:HG3 | 2:BA:996:DA:N1  | 2.00                     | 0.75              |
| 1:L:476:ASN:HB3 | 1:L:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:P:476:ASN:HB3 | 1:P:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:i:476:ASN:HB3 | 1:i:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:A:476:ASN:HB3 | 1:A:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:F:476:ASN:HB3 | 1:F:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:T:476:ASN:HB3 | 1:T:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:a:410:GLU:HG3 | 2:RA:996:DA:N1  | 2.00                     | 0.75              |
| 1:j:476:ASN:HB3 | 1:j:480:GLY:HA3 | 1.68                     | 0.75              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:l:476:ASN:HB3 | 1:l:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:5:476:ASN:HB3 | 1:5:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:O:410:GLU:HG3 | 2:EA:996:DA:N1  | 2.00                     | 0.75              |
| 1:g:410:GLU:HG3 | 2:YA:996:DA:N1  | 2.00                     | 0.75              |
| 1:E:476:ASN:HB3 | 1:E:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:e:410:GLU:HG3 | 2:WA:996:DA:N1  | 2.00                     | 0.75              |
| 1:r:410:GLU:HG3 | 2:kA:996:DA:N1  | 2.00                     | 0.75              |
| 1:u:476:ASN:HB3 | 1:u:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:H:476:ASN:HB3 | 1:H:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:o:476:ASN:HB3 | 1:o:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:Z:476:ASN:HB3 | 1:Z:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:4:476:ASN:HB3 | 1:4:480:GLY:HA3 | 1.68                     | 0.75              |
| 1:b:476:ASN:HB3 | 1:b:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:Q:476:ASN:HB3 | 1:Q:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:M:476:ASN:HB3 | 1:M:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:k:476:ASN:HB3 | 1:k:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:J:476:ASN:HB3 | 1:J:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:v:476:ASN:HB3 | 1:v:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:2:476:ASN:HB3 | 1:2:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:d:476:ASN:HB3 | 1:d:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:C:476:ASN:HB3 | 1:C:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:e:476:ASN:HB3 | 1:e:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:m:476:ASN:HB3 | 1:m:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:D:476:ASN:HB3 | 1:D:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:K:476:ASN:HB3 | 1:K:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:S:476:ASN:HB3 | 1:S:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:r:476:ASN:HB3 | 1:r:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:f:476:ASN:HB3 | 1:f:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:w:476:ASN:HB3 | 1:w:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:3:476:ASN:HB3 | 1:3:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:z:476:ASN:HB3 | 1:z:480:GLY:HA3 | 1.68                     | 0.74              |
| 1:G:476:ASN:HB3 | 1:G:480:GLY:HA3 | 1.68                     | 0.73              |
| 1:N:476:ASN:HB3 | 1:N:480:GLY:HA3 | 1.68                     | 0.73              |
| 1:6:476:ASN:HB3 | 1:6:480:GLY:HA3 | 1.68                     | 0.73              |
| 1:O:476:ASN:HB3 | 1:O:480:GLY:HA3 | 1.68                     | 0.72              |
| 1:g:476:ASN:HB3 | 1:g:480:GLY:HA3 | 1.68                     | 0.72              |
| 1:B:228:ARG:NH1 | 1:B:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:8:228:ARG:NH1 | 1:8:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:R:228:ARG:NH1 | 1:R:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:p:228:ARG:NH1 | 1:p:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:y:228:ARG:NH1 | 1:y:672:GLU:OE2 | 2.23                     | 0.72              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:W:228:ARG:NH1 | 1:W:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:e:228:ARG:NH1 | 1:e:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:n:228:ARG:NH1 | 1:n:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:r:228:ARG:NH1 | 1:r:672:GLU:OE2 | 2.23                     | 0.72              |
| 1:C:228:ARG:NH1 | 1:C:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:h:228:ARG:NH1 | 1:h:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:A:228:ARG:NH1 | 1:A:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:o:228:ARG:NH1 | 1:o:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:t:228:ARG:NH1 | 1:t:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:3:228:ARG:NH1 | 1:3:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:F:228:ARG:NH1 | 1:F:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:H:228:ARG:NH1 | 1:H:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:Q:228:ARG:NH1 | 1:Q:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:f:228:ARG:NH1 | 1:f:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:v:228:ARG:NH1 | 1:v:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:5:228:ARG:NH1 | 1:5:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:N:228:ARG:NH1 | 1:N:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:m:228:ARG:NH1 | 1:m:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:z:228:ARG:NH1 | 1:z:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:Y:228:ARG:NH1 | 1:Y:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:l:228:ARG:NH1 | 1:l:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:o:620:PRO:N   | 2:hA:997:DA:H2' | 2.06                     | 0.71              |
| 1:H:620:PRO:N   | 2:4A:997:DA:H2' | 2.06                     | 0.71              |
| 1:K:228:ARG:NH1 | 1:K:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:T:228:ARG:NH1 | 1:T:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:b:620:PRO:N   | 2:SA:997:DA:H2' | 2.06                     | 0.71              |
| 1:c:228:ARG:NH1 | 1:c:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:A:620:PRO:N   | 2:O:997:DA:H2'  | 2.06                     | 0.71              |
| 1:J:228:ARG:NH1 | 1:J:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:Z:228:ARG:NH1 | 1:Z:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:Z:620:PRO:N   | 2:QA:997:DA:H2' | 2.06                     | 0.71              |
| 1:b:228:ARG:NH1 | 1:b:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:x:228:ARG:NH1 | 1:x:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:5:620:PRO:N   | 2:yA:997:DA:H2' | 2.06                     | 0.71              |
| 1:U:228:ARG:NH1 | 1:U:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:j:228:ARG:NH1 | 1:j:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:E:228:ARG:NH1 | 1:E:672:GLU:OE2 | 2.23                     | 0.71              |
| 1:L:620:PRO:N   | 2:BA:997:DA:H2' | 2.06                     | 0.71              |
| 1:a:620:PRO:N   | 2:RA:997:DA:H2' | 2.06                     | 0.71              |
| 1:k:620:PRO:N   | 2:cA:997:DA:H2' | 2.06                     | 0.71              |
| 1:P:228:ARG:NH1 | 1:P:672:GLU:OE2 | 2.23                     | 0.70              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:d:620:PRO:N   | 2:VA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:m:620:PRO:N   | 2:eA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:q:620:PRO:N   | 2:jA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:u:228:ARG:NH1 | 1:u:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:1:228:ARG:NH1 | 1:1:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:S:620:PRO:N   | 2:IA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:V:620:PRO:N   | 2:MA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:f:620:PRO:N   | 2:XA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:w:620:PRO:N   | 2:pA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:6:228:ARG:NH1 | 1:6:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:G:228:ARG:NH1 | 1:G:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:I:620:PRO:N   | 2:5A:997:DA:H2'  | 2.06                     | 0.70              |
| 1:R:678:GLU:HG3 | 1:R:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:D:620:PRO:N   | 2:fA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:D:678:GLU:HG3 | 1:D:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:R:620:PRO:N   | 2:HA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:i:620:PRO:N   | 2:aA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:l:620:PRO:N   | 2:dA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:t:678:GLU:HG3 | 1:t:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:2:620:PRO:N   | 2:vA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:4:228:ARG:NH1 | 1:4:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:7:620:PRO:N   | 2:0A:997:DA:H2'  | 2.06                     | 0.70              |
| 1:E:678:GLU:HG3 | 1:E:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:F:678:GLU:HG3 | 1:F:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:u:678:GLU:HG3 | 1:u:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:y:620:PRO:N   | 2:sA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:2:678:GLU:HG3 | 1:2:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:E:620:PRO:N   | 2:qA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:M:228:ARG:NH1 | 1:M:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:X:678:GLU:HG3 | 1:X:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:g:228:ARG:NH1 | 1:g:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:j:678:GLU:HG3 | 1:j:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:n:620:PRO:N   | 2:gA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:w:228:ARG:NH1 | 1:w:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:y:678:GLU:HG3 | 1:y:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:C:678:GLU:HG3 | 1:C:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:I:678:GLU:HG3 | 1:I:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:O:620:PRO:N   | 2:EA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:e:620:PRO:N   | 2:WA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:s:678:GLU:HG3 | 1:s:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:u:620:PRO:N   | 2:nA:997:DA:H2'  | 2.06                     | 0.70              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:1:678:GLU:HG3 | 1:1:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:3:678:GLU:HG3 | 1:3:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:7:678:GLU:HG3 | 1:7:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:L:678:GLU:HG3 | 1:L:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:O:228:ARG:NH1 | 1:O:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:P:678:GLU:HG3 | 1:P:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:S:228:ARG:NH1 | 1:S:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:T:678:GLU:HG3 | 1:T:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:b:678:GLU:HG3 | 1:b:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:g:620:PRO:N   | 2:YA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:k:228:ARG:NH1 | 1:k:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:r:620:PRO:N   | 2:kA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:4:620:PRO:N   | 2:xA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:B:678:GLU:HG3 | 1:B:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:C:620:PRO:N   | 2:UA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:G:620:PRO:N   | 2:3A:997:DA:H2'  | 2.06                     | 0.70              |
| 1:M:620:PRO:N   | 2:CA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:N:620:PRO:N   | 2:DA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:Z:678:GLU:HG3 | 1:Z:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:h:620:PRO:N   | 2:ZA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:x:620:PRO:N   | 2:rA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:7:228:ARG:NH1 | 1:7:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:8:678:GLU:HG3 | 1:8:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:G:678:GLU:HG3 | 1:G:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:U:678:GLU:HG3 | 1:U:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:a:678:GLU:HG3 | 1:a:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:d:228:ARG:NH1 | 1:d:672:GLU:OE2  | 2.23                     | 0.70              |
| 1:e:678:GLU:HG3 | 1:e:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:r:678:GLU:HG3 | 1:r:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:3:620:PRO:N   | 2:wA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:5:678:GLU:HG3 | 1:5:720:LEU:HD13 | 1.74                     | 0.70              |
| 1:6:620:PRO:N   | 2:zA:997:DA:H2'  | 2.06                     | 0.70              |
| 1:I:228:ARG:NH1 | 1:I:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:U:620:PRO:N   | 2:LA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:x:678:GLU:HG3 | 1:x:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:z:620:PRO:N   | 2:tA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:1:620:PRO:N   | 2:uA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:2:228:ARG:NH1 | 1:2:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:A:678:GLU:HG3 | 1:A:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:B:620:PRO:N   | 2:JA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:D:228:ARG:NH1 | 1:D:672:GLU:OE2  | 2.23                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:620:PRO:N    | 2:1A:997:DA:H2'  | 2.06                     | 0.69              |
| 1:i:228:ARG:NH1  | 1:i:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:s:228:ARG:NH1  | 1:s:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:6:678:GLU:HG3  | 1:6:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:Q:620:PRO:N    | 2:GA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:Q:678:GLU:HG3  | 1:Q:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:W:678:GLU:HG3  | 1:W:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:X:228:ARG:NH1  | 1:X:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:h:678:GLU:HG3  | 1:h:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:p:678:GLU:HG3  | 1:p:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:t:620:PRO:N    | 2:mA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:8:620:PRO:N    | 2:2A:997:DA:H2'  | 2.06                     | 0.69              |
| 1:N:678:GLU:HG3  | 1:N:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:P:620:PRO:N    | 2:FA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:j:620:PRO:N    | 2:bA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:v:620:PRO:N    | 2:oA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:v:678:GLU:HG3  | 1:v:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:z:678:GLU:HG3  | 1:z:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:J:620:PRO:N    | 2:9:997:DA:H2'   | 2.06                     | 0.69              |
| 1:T:620:PRO:N    | 2:KA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:X:620:PRO:N    | 2:OA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:n:678:GLU:HG3  | 1:n:720:LEU:HD13 | 1.74                     | 0.69              |
| 2:PA:996:DA:H2'' | 2:PA:997:DA:H5'  | 1.75                     | 0.69              |
| 1:K:620:PRO:N    | 2:AA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:O:678:GLU:HG3  | 1:O:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:a:228:ARG:NH1  | 1:a:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:g:678:GLU:HG3  | 1:g:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:L:228:ARG:NH1  | 1:L:672:GLU:OE2  | 2.23                     | 0.69              |
| 2:IA:996:DA:H2'' | 2:IA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:TA:996:DA:H2'' | 2:TA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:iA:996:DA:H2'' | 2:iA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:pA:996:DA:H2'' | 2:pA:997:DA:H5'  | 1.75                     | 0.69              |
| 1:H:678:GLU:HG3  | 1:H:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:c:620:PRO:N    | 2:TA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:p:620:PRO:N    | 2:iA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:q:228:ARG:NH1  | 1:q:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:s:620:PRO:N    | 2:lA:997:DA:H2'  | 2.06                     | 0.69              |
| 2:DA:996:DA:H2'' | 2:DA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:NA:996:DA:H2'' | 2:NA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:ZA:996:DA:H2'' | 2:ZA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:gA:996:DA:H2'' | 2:gA:997:DA:H5'  | 1.75                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:tA:996:DA:H2'' | 2:tA:997:DA:H5'  | 1.75                     | 0.69              |
| 1:S:678:GLU:HG3  | 1:S:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:V:228:ARG:NH1  | 1:V:672:GLU:OE2  | 2.23                     | 0.69              |
| 1:W:620:PRO:N    | 2:NA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:Y:620:PRO:N    | 2:PA:997:DA:H2'  | 2.06                     | 0.69              |
| 1:c:678:GLU:HG3  | 1:c:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:o:678:GLU:HG3  | 1:o:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:w:678:GLU:HG3  | 1:w:720:LEU:HD13 | 1.74                     | 0.69              |
| 2:qA:996:DA:H2'' | 2:qA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:5A:996:DA:H2'' | 2:5A:997:DA:H5'  | 1.75                     | 0.69              |
| 2:OA:996:DA:H2'' | 2:OA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:XA:996:DA:H2'' | 2:XA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:0A:996:DA:H2'' | 2:0A:997:DA:H5'  | 1.75                     | 0.69              |
| 1:V:678:GLU:HG3  | 1:V:720:LEU:HD13 | 1.74                     | 0.69              |
| 1:q:678:GLU:HG3  | 1:q:720:LEU:HD13 | 1.74                     | 0.69              |
| 2:1A:996:DA:H2'' | 2:1A:997:DA:H5'  | 1.75                     | 0.69              |
| 2:eA:996:DA:H2'' | 2:eA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:lA:996:DA:H2'' | 2:lA:997:DA:H5'  | 1.75                     | 0.69              |
| 2:nA:996:DA:H2'' | 2:nA:997:DA:H5'  | 1.75                     | 0.69              |
| 1:Y:678:GLU:HG3  | 1:Y:720:LEU:HD13 | 1.74                     | 0.68              |
| 1:k:678:GLU:HG3  | 1:k:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:4A:996:DA:H2'' | 2:4A:997:DA:H5'  | 1.75                     | 0.68              |
| 2:VA:996:DA:H2'' | 2:VA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:mA:996:DA:H2'' | 2:mA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:d:678:GLU:HG3  | 1:d:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:cA:996:DA:H2'' | 2:cA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:hA:996:DA:H2'' | 2:hA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:i:678:GLU:HG3  | 1:i:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:UA:996:DA:H2'' | 2:UA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:KA:996:DA:H2'' | 2:KA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:LA:996:DA:H2'' | 2:LA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:l:678:GLU:HG3  | 1:l:720:LEU:HD13 | 1.74                     | 0.68              |
| 1:4:678:GLU:HG3  | 1:4:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:HA:996:DA:H2'' | 2:HA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:MA:996:DA:H2'' | 2:MA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:QA:996:DA:H2'' | 2:QA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:SA:996:DA:H2'' | 2:SA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:bA:996:DA:H2'' | 2:bA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:rA:996:DA:H2'' | 2:rA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:K:678:GLU:HG3  | 1:K:720:LEU:HD13 | 1.74                     | 0.68              |
| 1:M:678:GLU:HG3  | 1:M:720:LEU:HD13 | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:BA:996:DA:H2'' | 2:BA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:aA:996:DA:H2'' | 2:aA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:jA:996:DA:H2'' | 2:jA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:wA:996:DA:H2'' | 2:wA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:J:678:GLU:HG3  | 1:J:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:RA:996:DA:H2'' | 2:RA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:dA:996:DA:H2'' | 2:dA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:sA:996:DA:H2'' | 2:sA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:0:996:DA:H2''  | 2:0:997:DA:H5'   | 1.75                     | 0.68              |
| 2:fA:996:DA:H2'' | 2:fA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:vA:996:DA:H2'' | 2:vA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:f:678:GLU:HG3  | 1:f:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:yA:996:DA:H2'' | 2:yA:997:DA:H5'  | 1.75                     | 0.68              |
| 1:m:678:GLU:HG3  | 1:m:720:LEU:HD13 | 1.74                     | 0.68              |
| 2:2A:996:DA:H2'' | 2:2A:997:DA:H5'  | 1.75                     | 0.68              |
| 2:JA:996:DA:H2'' | 2:JA:997:DA:H5'  | 1.75                     | 0.68              |
| 2:FA:996:DA:H2'' | 2:FA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:CA:996:DA:H2'' | 2:CA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:uA:996:DA:H2'' | 2:uA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:xA:996:DA:H2'' | 2:xA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:GA:996:DA:H2'' | 2:GA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:oA:996:DA:H2'' | 2:oA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:WA:996:DA:H2'' | 2:WA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:EA:996:DA:H2'' | 2:EA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:YA:996:DA:H2'' | 2:YA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:kA:996:DA:H2'' | 2:kA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:9:996:DA:H2''  | 2:9:997:DA:H5'   | 1.75                     | 0.67              |
| 2:AA:996:DA:H2'' | 2:AA:997:DA:H5'  | 1.75                     | 0.67              |
| 2:3A:996:DA:H2'' | 2:3A:997:DA:H5'  | 1.75                     | 0.67              |
| 2:zA:996:DA:H2'' | 2:zA:997:DA:H5'  | 1.75                     | 0.67              |
| 1:4:272:TYR:HB3  | 1:4:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:M:272:TYR:HB3  | 1:M:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:f:272:TYR:HB3  | 1:f:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:h:272:TYR:HB3  | 1:h:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:m:272:TYR:HB3  | 1:m:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:n:272:TYR:HB3  | 1:n:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:B:272:TYR:HB3  | 1:B:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:D:272:TYR:HB3  | 1:D:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:F:272:TYR:HB3  | 1:F:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:J:272:TYR:HB3  | 1:J:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:p:272:TYR:HB3  | 1:p:637:LEU:HD23 | 1.78                     | 0.66              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:t:272:TYR:HB3 | 1:t:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:x:272:TYR:HB3 | 1:x:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:8:272:TYR:HB3 | 1:8:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:H:420:SER:HB2 | 1:H:721:THR:HG22 | 1.78                     | 0.66              |
| 1:K:272:TYR:HB3 | 1:K:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:U:272:TYR:HB3 | 1:U:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:W:272:TYR:HB3 | 1:W:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:2:272:TYR:HB3 | 1:2:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:J:420:SER:HB2 | 1:J:721:THR:HG22 | 1.78                     | 0.66              |
| 1:K:420:SER:HB2 | 1:K:721:THR:HG22 | 1.78                     | 0.66              |
| 1:N:272:TYR:HB3 | 1:N:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:X:420:SER:HB2 | 1:X:721:THR:HG22 | 1.78                     | 0.66              |
| 1:e:420:SER:HB2 | 1:e:721:THR:HG22 | 1.78                     | 0.66              |
| 1:o:420:SER:HB2 | 1:o:721:THR:HG22 | 1.78                     | 0.66              |
| 1:q:420:SER:HB2 | 1:q:721:THR:HG22 | 1.78                     | 0.66              |
| 1:r:420:SER:HB2 | 1:r:721:THR:HG22 | 1.78                     | 0.66              |
| 1:T:420:SER:HB2 | 1:T:721:THR:HG22 | 1.78                     | 0.66              |
| 1:V:420:SER:HB2 | 1:V:721:THR:HG22 | 1.78                     | 0.66              |
| 1:Y:272:TYR:HB3 | 1:Y:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:h:475:TRP:HB2 | 1:h:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:j:420:SER:HB2 | 1:j:721:THR:HG22 | 1.78                     | 0.66              |
| 1:n:475:TRP:HB2 | 1:n:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:s:420:SER:HB2 | 1:s:721:THR:HG22 | 1.78                     | 0.66              |
| 1:z:272:TYR:HB3 | 1:z:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:8:475:TRP:HB2 | 1:8:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:A:272:TYR:HB3 | 1:A:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:B:475:TRP:HB2 | 1:B:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:L:272:TYR:HB3 | 1:L:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:V:475:TRP:HB2 | 1:V:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:c:272:TYR:HB3 | 1:c:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:c:373:ARG:NH2 | 1:s:695:ASP:OD1  | 2.29                     | 0.66              |
| 1:q:475:TRP:HB2 | 1:q:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:N:475:TRP:HB2 | 1:N:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:W:475:TRP:HB2 | 1:W:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:Z:272:TYR:HB3 | 1:Z:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:Z:475:TRP:HB2 | 1:Z:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:b:272:TYR:HB3 | 1:b:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:b:420:SER:HB2 | 1:b:721:THR:HG22 | 1.78                     | 0.66              |
| 1:b:475:TRP:HB2 | 1:b:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:c:420:SER:HB2 | 1:c:721:THR:HG22 | 1.78                     | 0.66              |
| 1:2:475:TRP:HB2 | 1:2:523:LEU:HD23 | 1.78                     | 0.66              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:5:272:TYR:HB3 | 1:5:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:A:475:TRP:HB2 | 1:A:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:D:475:TRP:HB2 | 1:D:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:H:272:TYR:HB3 | 1:H:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:Y:420:SER:HB2 | 1:Y:721:THR:HG22 | 1.78                     | 0.66              |
| 1:Z:420:SER:HB2 | 1:Z:721:THR:HG22 | 1.78                     | 0.66              |
| 1:a:272:TYR:HB3 | 1:a:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:p:475:TRP:HB2 | 1:p:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:y:420:SER:HB2 | 1:y:721:THR:HG22 | 1.78                     | 0.66              |
| 1:R:420:SER:HB2 | 1:R:721:THR:HG22 | 1.78                     | 0.66              |
| 1:i:272:TYR:HB3 | 1:i:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:l:272:TYR:HB3 | 1:l:637:LEU:HD23 | 1.78                     | 0.66              |
| 1:p:420:SER:HB2 | 1:p:721:THR:HG22 | 1.78                     | 0.66              |
| 1:w:420:SER:HB2 | 1:w:721:THR:HG22 | 1.78                     | 0.66              |
| 1:5:475:TRP:HB2 | 1:5:523:LEU:HD23 | 1.78                     | 0.66              |
| 1:E:272:TYR:HB3 | 1:E:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:W:420:SER:HB2 | 1:W:721:THR:HG22 | 1.78                     | 0.65              |
| 1:k:475:TRP:HB2 | 1:k:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:o:272:TYR:HB3 | 1:o:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:z:475:TRP:HB2 | 1:z:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:S:420:SER:HB2 | 1:S:721:THR:HG22 | 1.78                     | 0.65              |
| 1:d:475:TRP:HB2 | 1:d:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:q:272:TYR:HB3 | 1:q:637:LEU:HD23 | 1.77                     | 0.65              |
| 1:G:420:SER:HB2 | 1:G:721:THR:HG22 | 1.78                     | 0.65              |
| 1:u:272:TYR:HB3 | 1:u:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:v:475:TRP:HB2 | 1:v:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:6:420:SER:HB2 | 1:6:721:THR:HG22 | 1.78                     | 0.65              |
| 1:K:475:TRP:HB2 | 1:K:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:Q:475:TRP:HB2 | 1:Q:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:e:272:TYR:HB3 | 1:e:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:r:272:TYR:HB3 | 1:r:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:B:420:SER:HB2 | 1:B:721:THR:HG22 | 1.78                     | 0.65              |
| 1:I:272:TYR:HB3 | 1:I:637:LEU:HD23 | 1.77                     | 0.65              |
| 1:J:475:TRP:HB2 | 1:J:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:V:272:TYR:HB3 | 1:V:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:u:420:SER:HB2 | 1:u:721:THR:HG22 | 1.78                     | 0.65              |
| 1:E:420:SER:HB2 | 1:E:721:THR:HG22 | 1.78                     | 0.65              |
| 1:H:475:TRP:HB2 | 1:H:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:Q:272:TYR:HB3 | 1:Q:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:3:475:TRP:HB2 | 1:3:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:8:420:SER:HB2 | 1:8:721:THR:HG22 | 1.78                     | 0.65              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:475:TRP:HB2 | 1:C:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:I:475:TRP:HB2 | 1:I:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:R:475:TRP:HB2 | 1:R:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:T:272:TYR:HB3 | 1:T:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:a:420:SER:HB2 | 1:a:721:THR:HG22 | 1.78                     | 0.65              |
| 1:f:475:TRP:HB2 | 1:f:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:n:420:SER:HB2 | 1:n:721:THR:HG22 | 1.78                     | 0.65              |
| 1:o:475:TRP:HB2 | 1:o:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:v:272:TYR:HB3 | 1:v:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:6:272:TYR:HB3 | 1:6:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:7:272:TYR:HB3 | 1:7:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:C:272:TYR:HB3 | 1:C:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:G:272:TYR:HB3 | 1:G:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:O:475:TRP:HB2 | 1:O:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:U:420:SER:HB2 | 1:U:721:THR:HG22 | 1.78                     | 0.65              |
| 1:Y:475:TRP:HB2 | 1:Y:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:d:272:TYR:HB3 | 1:d:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:j:272:TYR:HB3 | 1:j:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:k:272:TYR:HB3 | 1:k:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:u:475:TRP:HB2 | 1:u:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:y:475:TRP:HB2 | 1:y:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:7:475:TRP:HB2 | 1:7:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:L:420:SER:HB2 | 1:L:721:THR:HG22 | 1.78                     | 0.65              |
| 1:c:475:TRP:HB2 | 1:c:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:g:475:TRP:HB2 | 1:g:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:h:420:SER:HB2 | 1:h:721:THR:HG22 | 1.78                     | 0.65              |
| 1:m:475:TRP:HB2 | 1:m:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:m:695:ASP:OD1 | 1:s:373:ARG:NH2  | 2.30                     | 0.65              |
| 1:x:420:SER:HB2 | 1:x:721:THR:HG22 | 1.78                     | 0.65              |
| 1:1:272:TYR:HB3 | 1:1:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:1:475:TRP:HB2 | 1:1:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:E:475:TRP:HB2 | 1:E:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:L:475:TRP:HB2 | 1:L:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:a:475:TRP:HB2 | 1:a:523:LEU:HD23 | 1.78                     | 0.65              |
| 1:f:420:SER:HB2 | 1:f:721:THR:HG22 | 1.78                     | 0.65              |
| 1:s:272:TYR:HB3 | 1:s:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:3:272:TYR:HB3 | 1:3:637:LEU:HD23 | 1.78                     | 0.65              |
| 1:P:272:TYR:HB3 | 1:P:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:P:475:TRP:HB2 | 1:P:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:X:272:TYR:HB3 | 1:X:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:i:475:TRP:HB2 | 1:i:523:LEU:HD23 | 1.78                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:m:420:SER:HB2 | 1:m:721:THR:HG22 | 1.78                     | 0.64              |
| 1:l:420:SER:HB2 | 1:l:721:THR:HG22 | 1.78                     | 0.64              |
| 1:O:695:ASP:OD1 | 1:P:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:U:475:TRP:HB2 | 1:U:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:X:475:TRP:HB2 | 1:X:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:x:475:TRP:HB2 | 1:x:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:4:420:SER:HB2 | 1:4:721:THR:HG22 | 1.78                     | 0.64              |
| 1:6:475:TRP:HB2 | 1:6:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:D:373:ARG:NH2 | 1:E:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:G:475:TRP:HB2 | 1:G:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:J:695:ASP:OD1 | 1:a:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:K:695:ASP:OD1 | 1:L:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:M:420:SER:HB2 | 1:M:721:THR:HG22 | 1.78                     | 0.64              |
| 1:O:420:SER:HB2 | 1:O:721:THR:HG22 | 1.78                     | 0.64              |
| 1:T:475:TRP:HB2 | 1:T:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:X:373:ARG:NH2 | 1:f:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:g:373:ARG:NH2 | 1:k:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:g:695:ASP:OD1 | 1:l:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:l:475:TRP:HB2 | 1:l:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:u:695:ASP:OD1 | 1:2:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:w:475:TRP:HB2 | 1:w:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:y:272:TYR:HB3 | 1:y:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:A:420:SER:HB2 | 1:A:721:THR:HG22 | 1.78                     | 0.64              |
| 1:C:420:SER:HB2 | 1:C:721:THR:HG22 | 1.78                     | 0.64              |
| 1:D:420:SER:HB2 | 1:D:721:THR:HG22 | 1.78                     | 0.64              |
| 1:M:373:ARG:NH2 | 1:c:695:ASP:OD1  | 2.30                     | 0.64              |
| 1:O:373:ARG:NH2 | 1:d:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:R:373:ARG:NH2 | 1:V:695:ASP:OD1  | 2.30                     | 0.64              |
| 1:S:475:TRP:HB2 | 1:S:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:X:695:ASP:OD1 | 1:Y:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:Y:695:ASP:OD1 | 1:4:373:ARG:NH2  | 2.30                     | 0.64              |
| 1:l:420:SER:HB2 | 1:l:721:THR:HG22 | 1.78                     | 0.64              |
| 1:r:475:TRP:HB2 | 1:r:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:s:475:TRP:HB2 | 1:s:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:t:420:SER:HB2 | 1:t:721:THR:HG22 | 1.78                     | 0.64              |
| 1:3:420:SER:HB2 | 1:3:721:THR:HG22 | 1.78                     | 0.64              |
| 1:7:420:SER:HB2 | 1:7:721:THR:HG22 | 1.78                     | 0.64              |
| 1:E:351:GLY:HA3 | 1:E:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:H:695:ASP:OD1 | 1:I:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:I:695:ASP:OD1 | 1:J:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:K:373:ARG:NH2 | 1:7:695:ASP:OD1  | 2.31                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:R:272:TYR:HB3 | 1:R:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:e:351:GLY:HA3 | 1:e:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:g:420:SER:HB2 | 1:g:721:THR:HG22 | 1.78                     | 0.64              |
| 1:o:695:ASP:OD1 | 1:7:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:q:695:ASP:OD1 | 1:y:373:ARG:NH2  | 2.30                     | 0.64              |
| 1:5:420:SER:HB2 | 1:5:721:THR:HG22 | 1.78                     | 0.64              |
| 1:C:351:GLY:HA3 | 1:C:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:F:351:GLY:HA3 | 1:F:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:F:420:SER:HB2 | 1:F:721:THR:HG22 | 1.78                     | 0.64              |
| 1:L:351:GLY:HA3 | 1:L:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:a:351:GLY:HA3 | 1:a:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:e:475:TRP:HB2 | 1:e:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:i:420:SER:HB2 | 1:i:721:THR:HG22 | 1.78                     | 0.64              |
| 1:j:475:TRP:HB2 | 1:j:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:l:373:ARG:NH2 | 1:n:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:n:373:ARG:NH2 | 1:r:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:u:351:GLY:HA3 | 1:u:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:2:420:SER:HB2 | 1:2:721:THR:HG22 | 1.78                     | 0.64              |
| 1:3:351:GLY:HA3 | 1:3:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:P:420:SER:HB2 | 1:P:721:THR:HG22 | 1.78                     | 0.64              |
| 1:S:272:TYR:HB3 | 1:S:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:h:695:ASP:OD1 | 1:i:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:r:351:GLY:HA3 | 1:r:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:t:351:GLY:HA3 | 1:t:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:5:373:ARG:NH2 | 1:8:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:M:475:TRP:HB2 | 1:M:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:O:351:GLY:HA3 | 1:O:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:g:272:TYR:HB3 | 1:g:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:g:351:GLY:HA3 | 1:g:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:j:695:ASP:OD1 | 1:x:373:ARG:NH2  | 2.30                     | 0.64              |
| 1:k:420:SER:HB2 | 1:k:721:THR:HG22 | 1.78                     | 0.64              |
| 1:z:420:SER:HB2 | 1:z:721:THR:HG22 | 1.78                     | 0.64              |
| 1:1:420:SER:HB2 | 1:1:721:THR:HG22 | 1.78                     | 0.64              |
| 1:2:695:ASP:OD1 | 1:3:373:ARG:NH2  | 2.30                     | 0.64              |
| 1:A:373:ARG:NH2 | 1:B:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:C:373:ARG:NH2 | 1:D:695:ASP:OD1  | 2.30                     | 0.64              |
| 1:G:351:GLY:HA3 | 1:G:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:N:351:GLY:HA3 | 1:N:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:N:420:SER:HB2 | 1:N:721:THR:HG22 | 1.78                     | 0.64              |
| 1:P:351:GLY:HA3 | 1:P:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:S:351:GLY:HA3 | 1:S:364:PRO:HG3  | 1.80                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:T:620:PRO:HG2 | 2:KA:997:DA:C4   | 2.33                     | 0.64              |
| 1:T:695:ASP:OD1 | 1:U:373:ARG:NH2  | 2.30                     | 0.64              |
| 1:e:695:ASP:OD1 | 1:h:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:g:620:PRO:HG2 | 2:YA:997:DA:C4   | 2.33                     | 0.64              |
| 1:p:373:ARG:NH2 | 1:6:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:t:475:TRP:HB2 | 1:t:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:z:351:GLY:HA3 | 1:z:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:6:351:GLY:HA3 | 1:6:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:E:620:PRO:HG2 | 2:qA:997:DA:C4   | 2.33                     | 0.64              |
| 1:F:373:ARG:NH2 | 1:R:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:F:475:TRP:HB2 | 1:F:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:G:695:ASP:OD1 | 1:W:373:ARG:NH2  | 2.31                     | 0.64              |
| 1:O:272:TYR:HB3 | 1:O:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:O:620:PRO:HG2 | 2:EA:997:DA:C4   | 2.33                     | 0.64              |
| 1:Q:420:SER:HB2 | 1:Q:721:THR:HG22 | 1.78                     | 0.64              |
| 1:d:420:SER:HB2 | 1:d:721:THR:HG22 | 1.78                     | 0.64              |
| 1:j:620:PRO:HG2 | 2:bA:997:DA:C4   | 2.33                     | 0.64              |
| 1:t:373:ARG:NH2 | 1:y:695:ASP:OD1  | 2.31                     | 0.64              |
| 1:t:620:PRO:HG2 | 2:mA:997:DA:C4   | 2.33                     | 0.64              |
| 1:u:620:PRO:HG2 | 2:nA:997:DA:C4   | 2.33                     | 0.64              |
| 1:w:272:TYR:HB3 | 1:w:637:LEU:HD23 | 1.78                     | 0.64              |
| 1:w:351:GLY:HA3 | 1:w:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:1:351:GLY:HA3 | 1:1:364:PRO:HG3  | 1.80                     | 0.64              |
| 1:4:475:TRP:HB2 | 1:4:523:LEU:HD23 | 1.78                     | 0.64              |
| 1:F:620:PRO:HG2 | 2:1A:997:DA:C4   | 2.33                     | 0.63              |
| 1:F:695:ASP:OD1 | 1:G:373:ARG:NH2  | 2.31                     | 0.63              |
| 1:Q:695:ASP:OD1 | 1:S:373:ARG:NH2  | 2.30                     | 0.63              |
| 1:v:420:SER:HB2 | 1:v:721:THR:HG22 | 1.78                     | 0.63              |
| 1:v:695:ASP:OD1 | 1:w:373:ARG:NH2  | 2.30                     | 0.63              |
| 1:P:695:ASP:OD1 | 1:Q:373:ARG:NH2  | 2.31                     | 0.63              |
| 1:R:620:PRO:HG2 | 2:HA:997:DA:C4   | 2.34                     | 0.63              |
| 1:T:351:GLY:HA3 | 1:T:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:U:620:PRO:HG2 | 2:LA:997:DA:C4   | 2.33                     | 0.63              |
| 1:V:373:ARG:NH2 | 1:W:695:ASP:OD1  | 2.31                     | 0.63              |
| 1:h:351:GLY:HA3 | 1:h:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:k:351:GLY:HA3 | 1:k:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:m:351:GLY:HA3 | 1:m:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:n:351:GLY:HA3 | 1:n:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:t:695:ASP:OD1 | 1:6:373:ARG:NH2  | 2.31                     | 0.63              |
| 1:v:351:GLY:HA3 | 1:v:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:v:373:ARG:NH2 | 1:1:695:ASP:OD1  | 2.31                     | 0.63              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:x:620:PRO:HG2 | 2:rA:997:DA:C4  | 2.33                     | 0.63              |
| 1:y:620:PRO:HG2 | 2:sA:997:DA:C4  | 2.33                     | 0.63              |
| 1:A:620:PRO:HG2 | 2:0:997:DA:C4   | 2.33                     | 0.63              |
| 1:G:620:PRO:HG2 | 2:3A:997:DA:C4  | 2.33                     | 0.63              |
| 1:H:620:PRO:HG2 | 2:4A:997:DA:C4  | 2.33                     | 0.63              |
| 1:J:620:PRO:HG2 | 2:9:997:DA:C4   | 2.33                     | 0.63              |
| 1:K:620:PRO:HG2 | 2:AA:997:DA:C4  | 2.33                     | 0.63              |
| 1:L:695:ASP:OD1 | 1:b:373:ARG:NH2 | 2.30                     | 0.63              |
| 1:Q:351:GLY:HA3 | 1:Q:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:Y:620:PRO:HG2 | 2:PA:997:DA:C4  | 2.33                     | 0.63              |
| 1:c:620:PRO:HG2 | 2:TA:997:DA:C4  | 2.33                     | 0.63              |
| 1:d:351:GLY:HA3 | 1:d:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:f:351:GLY:HA3 | 1:f:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:o:620:PRO:HG2 | 2:hA:997:DA:C4  | 2.33                     | 0.63              |
| 1:p:695:ASP:OD1 | 1:q:373:ARG:NH2 | 2.31                     | 0.63              |
| 1:7:620:PRO:HG2 | 2:0A:997:DA:C4  | 2.33                     | 0.63              |
| 1:B:373:ARG:NH2 | 1:C:695:ASP:OD1 | 2.31                     | 0.63              |
| 1:I:620:PRO:HG2 | 2:5A:997:DA:C4  | 2.33                     | 0.63              |
| 1:N:695:ASP:OD1 | 1:m:373:ARG:NH2 | 2.31                     | 0.63              |
| 1:V:351:GLY:HA3 | 1:V:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:Z:373:ARG:NH2 | 1:a:695:ASP:OD1 | 2.30                     | 0.63              |
| 1:f:373:ARG:NH2 | 1:z:695:ASP:OD1 | 2.31                     | 0.63              |
| 1:3:695:ASP:OD1 | 1:8:373:ARG:NH2 | 2.31                     | 0.63              |
| 1:5:620:PRO:HG2 | 2:yA:997:DA:C4  | 2.33                     | 0.63              |
| 1:D:351:GLY:HA3 | 1:D:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:D:620:PRO:HG2 | 2:fA:997:DA:C4  | 2.33                     | 0.63              |
| 1:H:373:ARG:NH2 | 1:Z:695:ASP:OD1 | 2.31                     | 0.63              |
| 1:T:373:ARG:NH2 | 1:i:695:ASP:OD1 | 2.31                     | 0.63              |
| 1:j:351:GLY:HA3 | 1:j:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:j:373:ARG:NH2 | 1:l:695:ASP:OD1 | 2.31                     | 0.63              |
| 1:q:351:GLY:HA3 | 1:q:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:6:620:PRO:HG2 | 2:zA:997:DA:C4  | 2.33                     | 0.63              |
| 1:M:695:ASP:OD1 | 1:N:373:ARG:NH2 | 2.31                     | 0.63              |
| 1:U:695:ASP:OD1 | 1:e:373:ARG:NH2 | 2.31                     | 0.63              |
| 1:i:620:PRO:HG2 | 2:aA:997:DA:C4  | 2.33                     | 0.63              |
| 1:2:351:GLY:HA3 | 1:2:364:PRO:HG3 | 1.80                     | 0.63              |
| 1:2:620:PRO:HG2 | 2:vA:997:DA:C4  | 2.33                     | 0.63              |
| 1:B:620:PRO:HG2 | 2:JA:997:DA:C4  | 2.33                     | 0.63              |
| 1:b:695:ASP:OD1 | 1:o:373:ARG:NH2 | 2.31                     | 0.63              |
| 1:f:620:PRO:HG2 | 2:XA:997:DA:C4  | 2.33                     | 0.63              |
| 1:l:620:PRO:HG2 | 2:dA:997:DA:C4  | 2.33                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:620:PRO:HG2  | 2:eA:997:DA:C4   | 2.33                     | 0.63              |
| 1:r:373:ARG:NH2  | 1:x:695:ASP:OD1  | 2.31                     | 0.63              |
| 1:z:373:ARG:NH2  | 1:4:695:ASP:OD1  | 2.31                     | 0.63              |
| 1:A:695:ASP:OD1  | 1:E:373:ARG:NH2  | 2.31                     | 0.63              |
| 1:B:423:LEU:HD12 | 1:B:558:VAL:HG23 | 1.81                     | 0.63              |
| 1:R:351:GLY:HA3  | 1:R:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:W:351:GLY:HA3  | 1:W:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:p:351:GLY:HA3  | 1:p:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:s:351:GLY:HA3  | 1:s:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:u:373:ARG:NH2  | 1:5:695:ASP:OD1  | 2.31                     | 0.63              |
| 1:w:620:PRO:HG2  | 2:pA:997:DA:C4   | 2.33                     | 0.63              |
| 1:y:351:GLY:HA3  | 1:y:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:8:423:LEU:HD12 | 1:8:558:VAL:HG23 | 1.81                     | 0.63              |
| 1:8:620:PRO:HG2  | 2:2A:997:DA:C4   | 2.33                     | 0.63              |
| 1:A:423:LEU:HD12 | 1:A:558:VAL:HG23 | 1.81                     | 0.63              |
| 1:H:351:GLY:HA3  | 1:H:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:S:423:LEU:HD12 | 1:S:558:VAL:HG23 | 1.81                     | 0.63              |
| 1:S:620:PRO:HG2  | 2:IA:997:DA:C4   | 2.34                     | 0.63              |
| 1:U:351:GLY:HA3  | 1:U:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:X:423:LEU:HD12 | 1:X:558:VAL:HG23 | 1.81                     | 0.63              |
| 1:Y:351:GLY:HA3  | 1:Y:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:c:351:GLY:HA3  | 1:c:364:PRO:HG3  | 1.80                     | 0.63              |
| 1:s:423:LEU:HD12 | 1:s:558:VAL:HG23 | 1.81                     | 0.63              |
| 1:L:620:PRO:HG2  | 2:BA:997:DA:C4   | 2.33                     | 0.62              |
| 1:X:351:GLY:HA3  | 1:X:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:X:620:PRO:HG2  | 2:OA:997:DA:C4   | 2.33                     | 0.62              |
| 1:o:351:GLY:HA3  | 1:o:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:w:423:LEU:HD12 | 1:w:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:x:351:GLY:HA3  | 1:x:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:T:423:LEU:HD12 | 1:T:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:U:423:LEU:HD12 | 1:U:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:a:620:PRO:HG2  | 2:RA:997:DA:C4   | 2.33                     | 0.62              |
| 1:j:423:LEU:HD12 | 1:j:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:k:373:ARG:NH2  | 1:w:695:ASP:OD1  | 2.31                     | 0.62              |
| 1:s:620:PRO:HG2  | 2:lA:997:DA:C4   | 2.33                     | 0.62              |
| 1:u:423:LEU:HD12 | 1:u:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:x:423:LEU:HD12 | 1:x:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:5:423:LEU:HD12 | 1:5:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:E:423:LEU:HD12 | 1:E:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:N:620:PRO:HG2  | 2:DA:997:DA:C4   | 2.33                     | 0.62              |
| 1:P:620:PRO:HG2  | 2:FA:997:DA:C4   | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:695:ASP:OD1  | 1:d:373:ARG:NH2  | 2.31                     | 0.62              |
| 1:Z:351:GLY:HA3  | 1:Z:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:b:351:GLY:HA3  | 1:b:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:v:423:LEU:HD12 | 1:v:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:1:620:PRO:HG2  | 2:uA:997:DA:C4   | 2.33                     | 0.62              |
| 1:M:620:PRO:HG2  | 2:CA:997:DA:C4   | 2.33                     | 0.62              |
| 1:Q:423:LEU:HD12 | 1:Q:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:Q:620:PRO:HG2  | 2:GA:997:DA:C4   | 2.33                     | 0.62              |
| 1:d:423:LEU:HD12 | 1:d:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:e:423:LEU:HD12 | 1:e:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:e:620:PRO:HG2  | 2:WA:997:DA:C4   | 2.33                     | 0.62              |
| 1:l:351:GLY:HA3  | 1:l:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:n:423:LEU:HD12 | 1:n:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:r:423:LEU:HD12 | 1:r:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:r:620:PRO:HG2  | 2:kA:997:DA:C4   | 2.33                     | 0.62              |
| 1:v:620:PRO:HG2  | 2:oA:997:DA:C4   | 2.33                     | 0.62              |
| 1:z:620:PRO:HG2  | 2:tA:997:DA:C4   | 2.33                     | 0.62              |
| 1:4:620:PRO:HG2  | 2:xA:997:DA:C4   | 2.33                     | 0.62              |
| 1:6:423:LEU:HD12 | 1:6:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:7:351:GLY:HA3  | 1:7:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:C:423:LEU:HD12 | 1:C:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:G:423:LEU:HD12 | 1:G:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:N:423:LEU:HD12 | 1:N:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:Z:620:PRO:HG2  | 2:QA:997:DA:C4   | 2.33                     | 0.62              |
| 1:i:351:GLY:HA3  | 1:i:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:k:423:LEU:HD12 | 1:k:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:K:351:GLY:HA3  | 1:K:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:b:620:PRO:HG2  | 2:SA:997:DA:C4   | 2.33                     | 0.62              |
| 1:d:620:PRO:HG2  | 2:VA:997:DA:C4   | 2.33                     | 0.62              |
| 1:h:423:LEU:HD12 | 1:h:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:k:620:PRO:HG2  | 2:cA:997:DA:C4   | 2.33                     | 0.62              |
| 1:n:620:PRO:HG2  | 2:gA:997:DA:C4   | 2.33                     | 0.62              |
| 1:z:423:LEU:HD12 | 1:z:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:3:423:LEU:HD12 | 1:3:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:8:351:GLY:HA3  | 1:8:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:B:351:GLY:HA3  | 1:B:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:C:620:PRO:HG2  | 2:UA:997:DA:C4   | 2.34                     | 0.62              |
| 1:I:351:GLY:HA3  | 1:I:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:J:351:GLY:HA3  | 1:J:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:M:351:GLY:HA3  | 1:M:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:h:620:PRO:HG2  | 2:ZA:997:DA:C4   | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:423:LEU:HD12 | 1:t:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:4:351:GLY:HA3  | 1:4:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:5:351:GLY:HA3  | 1:5:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:A:351:GLY:HA3  | 1:A:364:PRO:HG3  | 1.80                     | 0.62              |
| 1:c:423:LEU:HD12 | 1:c:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:3:620:PRO:HG2  | 2:wA:997:DA:C4   | 2.33                     | 0.62              |
| 1:B:628:GLY:O    | 2:JA:997:DA:C2   | 2.53                     | 0.62              |
| 1:F:423:LEU:HD12 | 1:F:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:W:620:PRO:HG2  | 2:NA:997:DA:C4   | 2.33                     | 0.62              |
| 1:Y:423:LEU:HD12 | 1:Y:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:e:628:GLY:O    | 2:WA:997:DA:C2   | 2.53                     | 0.62              |
| 1:f:423:LEU:HD12 | 1:f:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:p:423:LEU:HD12 | 1:p:558:VAL:HG23 | 1.81                     | 0.62              |
| 1:r:628:GLY:O    | 2:kA:997:DA:C2   | 2.53                     | 0.62              |
| 1:p:620:PRO:HG2  | 2:iA:997:DA:C4   | 2.33                     | 0.62              |
| 1:q:620:PRO:HG2  | 2:jA:997:DA:C4   | 2.33                     | 0.62              |
| 1:t:628:GLY:O    | 2:mA:997:DA:C2   | 2.53                     | 0.62              |
| 1:D:423:LEU:HD12 | 1:D:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:F:628:GLY:O    | 2:1A:997:DA:C2   | 2.53                     | 0.61              |
| 1:V:620:PRO:HG2  | 2:MA:997:DA:C4   | 2.33                     | 0.61              |
| 1:W:423:LEU:HD12 | 1:W:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:l:423:LEU:HD12 | 1:l:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:m:310:GLN:HG2  | 1:s:328:THR:HG22 | 1.82                     | 0.61              |
| 1:m:423:LEU:HD12 | 1:m:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:2:423:LEU:HD12 | 1:2:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:i:423:LEU:HD12 | 1:i:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:j:628:GLY:O    | 2:bA:997:DA:C2   | 2.53                     | 0.61              |
| 1:q:628:GLY:O    | 2:jA:997:DA:C2   | 2.53                     | 0.61              |
| 1:3:628:GLY:O    | 2:wA:997:DA:C2   | 2.53                     | 0.61              |
| 1:C:628:GLY:O    | 2:UA:997:DA:C2   | 2.53                     | 0.61              |
| 1:T:628:GLY:O    | 2:KA:997:DA:C2   | 2.53                     | 0.61              |
| 1:V:628:GLY:O    | 2:MA:997:DA:C2   | 2.53                     | 0.61              |
| 1:f:628:GLY:O    | 2:XA:997:DA:C2   | 2.53                     | 0.61              |
| 1:m:628:GLY:O    | 2:eA:997:DA:C2   | 2.53                     | 0.61              |
| 1:P:423:LEU:HD12 | 1:P:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:I:423:LEU:HD12 | 1:I:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:N:558:VAL:HG11 | 1:N:597:MET:HG3  | 1.83                     | 0.61              |
| 1:O:423:LEU:HD12 | 1:O:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:f:558:VAL:HG11 | 1:f:597:MET:HG3  | 1.83                     | 0.61              |
| 1:m:558:VAL:HG11 | 1:m:597:MET:HG3  | 1.83                     | 0.61              |
| 1:1:423:LEU:HD12 | 1:1:558:VAL:HG23 | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:7:423:LEU:HD12 | 1:7:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:G:558:VAL:HG11 | 1:G:597:MET:HG3  | 1.83                     | 0.61              |
| 1:J:423:LEU:HD12 | 1:J:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:K:423:LEU:HD12 | 1:K:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:R:423:LEU:HD12 | 1:R:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:S:558:VAL:HG11 | 1:S:597:MET:HG3  | 1.83                     | 0.61              |
| 1:g:423:LEU:HD12 | 1:g:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:o:423:LEU:HD12 | 1:o:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:z:558:VAL:HG11 | 1:z:597:MET:HG3  | 1.83                     | 0.61              |
| 1:6:558:VAL:HG11 | 1:6:597:MET:HG3  | 1.83                     | 0.61              |
| 1:H:423:LEU:HD12 | 1:H:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:Q:558:VAL:HG11 | 1:Q:597:MET:HG3  | 1.83                     | 0.61              |
| 1:Z:423:LEU:HD12 | 1:Z:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:v:558:VAL:HG11 | 1:v:597:MET:HG3  | 1.83                     | 0.61              |
| 1:w:558:VAL:HG11 | 1:w:597:MET:HG3  | 1.83                     | 0.61              |
| 1:y:423:LEU:HD12 | 1:y:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:V:423:LEU:HD12 | 1:V:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:p:558:VAL:HG11 | 1:p:597:MET:HG3  | 1.83                     | 0.61              |
| 1:q:423:LEU:HD12 | 1:q:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:I:558:VAL:HG11 | 1:I:597:MET:HG3  | 1.83                     | 0.61              |
| 1:J:558:VAL:HG11 | 1:J:597:MET:HG3  | 1.83                     | 0.61              |
| 1:K:558:VAL:HG11 | 1:K:597:MET:HG3  | 1.83                     | 0.61              |
| 1:U:628:GLY:O    | 2:LA:997:DA:C2   | 2.53                     | 0.61              |
| 1:W:558:VAL:HG11 | 1:W:597:MET:HG3  | 1.83                     | 0.61              |
| 1:b:423:LEU:HD12 | 1:b:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:b:558:VAL:HG11 | 1:b:597:MET:HG3  | 1.83                     | 0.61              |
| 1:i:628:GLY:O    | 2:aA:997:DA:C2   | 2.53                     | 0.61              |
| 1:7:558:VAL:HG11 | 1:7:597:MET:HG3  | 1.83                     | 0.61              |
| 1:M:423:LEU:HD12 | 1:M:558:VAL:HG23 | 1.81                     | 0.61              |
| 1:Z:558:VAL:HG11 | 1:Z:597:MET:HG3  | 1.83                     | 0.61              |
| 1:d:558:VAL:HG11 | 1:d:597:MET:HG3  | 1.83                     | 0.61              |
| 1:j:310:GLN:HG2  | 1:x:328:THR:HG22 | 1.83                     | 0.61              |
| 1:l:628:GLY:O    | 2:dA:997:DA:C2   | 2.53                     | 0.61              |
| 1:x:628:GLY:O    | 2:rA:997:DA:C2   | 2.53                     | 0.61              |
| 1:1:558:VAL:HG11 | 1:1:597:MET:HG3  | 1.83                     | 0.61              |
| 1:A:558:VAL:HG11 | 1:A:597:MET:HG3  | 1.83                     | 0.60              |
| 1:H:558:VAL:HG11 | 1:H:597:MET:HG3  | 1.83                     | 0.60              |
| 1:P:558:VAL:HG11 | 1:P:597:MET:HG3  | 1.83                     | 0.60              |
| 1:T:310:GLN:HG2  | 1:U:328:THR:HG22 | 1.83                     | 0.60              |
| 1:Z:628:GLY:O    | 2:QA:997:DA:C2   | 2.53                     | 0.60              |
| 1:g:558:VAL:HG11 | 1:g:597:MET:HG3  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:558:VAL:HG11 | 1:k:597:MET:HG3  | 1.83                     | 0.60              |
| 1:o:558:VAL:HG11 | 1:o:597:MET:HG3  | 1.83                     | 0.60              |
| 1:3:558:VAL:HG11 | 1:3:597:MET:HG3  | 1.83                     | 0.60              |
| 1:4:423:LEU:HD12 | 1:4:558:VAL:HG23 | 1.81                     | 0.60              |
| 1:5:558:VAL:HG11 | 1:5:597:MET:HG3  | 1.83                     | 0.60              |
| 1:O:558:VAL:HG11 | 1:O:597:MET:HG3  | 1.83                     | 0.60              |
| 1:b:628:GLY:O    | 2:SA:997:DA:C2   | 2.53                     | 0.60              |
| 1:s:558:VAL:HG11 | 1:s:597:MET:HG3  | 1.83                     | 0.60              |
| 1:w:628:GLY:O    | 2:pA:997:DA:C2   | 2.53                     | 0.60              |
| 1:C:558:VAL:HG11 | 1:C:597:MET:HG3  | 1.83                     | 0.60              |
| 1:S:628:GLY:O    | 2:IA:997:DA:C2   | 2.53                     | 0.60              |
| 1:V:328:THR:HG22 | 1:W:310:GLN:HG2  | 1.83                     | 0.60              |
| 1:Z:328:THR:HG22 | 1:a:310:GLN:HG2  | 1.83                     | 0.60              |
| 1:c:381:GLU:OE2  | 1:s:693:TYR:HB2  | 2.02                     | 0.60              |
| 1:t:310:GLN:HG2  | 1:6:328:THR:HG22 | 1.84                     | 0.60              |
| 1:F:310:GLN:HG2  | 1:G:328:THR:HG22 | 1.84                     | 0.60              |
| 1:G:310:GLN:HG2  | 1:W:328:THR:HG22 | 1.84                     | 0.60              |
| 1:J:310:GLN:HG2  | 1:a:328:THR:HG22 | 1.84                     | 0.60              |
| 1:J:628:GLY:O    | 2:9:997:DA:C2    | 2.53                     | 0.60              |
| 1:K:310:GLN:HG2  | 1:L:328:THR:HG22 | 1.84                     | 0.60              |
| 1:K:628:GLY:O    | 2:AA:997:DA:C2   | 2.53                     | 0.60              |
| 1:L:310:GLN:HG2  | 1:b:328:THR:HG22 | 1.83                     | 0.60              |
| 1:T:328:THR:HG22 | 1:i:310:GLN:HG2  | 1.83                     | 0.60              |
| 1:X:328:THR:HG22 | 1:f:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:X:558:VAL:HG11 | 1:X:597:MET:HG3  | 1.83                     | 0.60              |
| 1:a:423:LEU:HD12 | 1:a:558:VAL:HG23 | 1.81                     | 0.60              |
| 1:p:310:GLN:HG2  | 1:q:328:THR:HG22 | 1.83                     | 0.60              |
| 1:L:423:LEU:HD12 | 1:L:558:VAL:HG23 | 1.81                     | 0.60              |
| 1:M:310:GLN:HG2  | 1:N:328:THR:HG22 | 1.84                     | 0.60              |
| 1:2:558:VAL:HG11 | 1:2:597:MET:HG3  | 1.83                     | 0.60              |
| 1:D:558:VAL:HG11 | 1:D:597:MET:HG3  | 1.83                     | 0.60              |
| 1:L:558:VAL:HG11 | 1:L:597:MET:HG3  | 1.83                     | 0.60              |
| 1:N:310:GLN:HG2  | 1:m:328:THR:HG22 | 1.84                     | 0.60              |
| 1:j:328:THR:HG22 | 1:l:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:p:328:THR:HG22 | 1:6:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:z:328:THR:HG22 | 1:4:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:R:628:GLY:O    | 2:HA:997:DA:C2   | 2.53                     | 0.60              |
| 1:a:558:VAL:HG11 | 1:a:597:MET:HG3  | 1.83                     | 0.60              |
| 1:t:328:THR:HG22 | 1:y:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:F:328:THR:HG22 | 1:R:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:O:310:GLN:HG2  | 1:P:328:THR:HG22 | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:328:THR:HG22 | 1:z:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:t:558:VAL:HG11 | 1:t:597:MET:HG3  | 1.83                     | 0.60              |
| 1:u:558:VAL:HG11 | 1:u:597:MET:HG3  | 1.83                     | 0.60              |
| 1:y:628:GLY:O    | 2:sA:997:DA:C2   | 2.53                     | 0.60              |
| 1:z:628:GLY:O    | 2:tA:997:DA:C2   | 2.53                     | 0.60              |
| 1:H:628:GLY:O    | 2:4A:997:DA:C2   | 2.53                     | 0.60              |
| 1:L:628:GLY:O    | 2:BA:997:DA:C2   | 2.53                     | 0.60              |
| 1:g:310:GLN:HG2  | 1:l:328:THR:HG22 | 1.83                     | 0.60              |
| 1:o:628:GLY:O    | 2:hA:997:DA:C2   | 2.53                     | 0.60              |
| 1:2:310:GLN:HG2  | 1:3:328:THR:HG22 | 1.84                     | 0.60              |
| 1:7:628:GLY:O    | 2:0A:997:DA:C2   | 2.53                     | 0.60              |
| 1:8:558:VAL:HG11 | 1:8:597:MET:HG3  | 1.83                     | 0.60              |
| 1:B:558:VAL:HG11 | 1:B:597:MET:HG3  | 1.83                     | 0.60              |
| 1:C:328:THR:HG22 | 1:D:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:E:558:VAL:HG11 | 1:E:597:MET:HG3  | 1.83                     | 0.60              |
| 1:F:558:VAL:HG11 | 1:F:597:MET:HG3  | 1.83                     | 0.60              |
| 1:N:628:GLY:O    | 2:DA:997:DA:C2   | 2.53                     | 0.60              |
| 1:a:628:GLY:O    | 2:RA:997:DA:C2   | 2.53                     | 0.60              |
| 1:e:310:GLN:HG2  | 1:h:328:THR:HG22 | 1.84                     | 0.60              |
| 1:n:328:THR:HG22 | 1:r:310:GLN:HG2  | 1.84                     | 0.60              |
| 1:C:530:ASN:HB2  | 1:M:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:D:381:GLU:OE2  | 1:E:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:H:328:THR:HG22 | 1:Z:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:I:628:GLY:O    | 2:5A:997:DA:C2   | 2.53                     | 0.59              |
| 1:m:693:TYR:HB2  | 1:s:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:o:310:GLN:HG2  | 1:7:328:THR:HG22 | 1.84                     | 0.59              |
| 1:u:693:TYR:HB2  | 1:2:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:U:558:VAL:HG11 | 1:U:597:MET:HG3  | 1.83                     | 0.59              |
| 1:b:310:GLN:HG2  | 1:o:328:THR:HG22 | 1.84                     | 0.59              |
| 1:j:558:VAL:HG11 | 1:j:597:MET:HG3  | 1.83                     | 0.59              |
| 1:u:381:GLU:OE2  | 1:5:693:TYR:HB2  | 2.03                     | 0.59              |
| 1:3:530:ASN:HB2  | 1:4:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:A:310:GLN:HG2  | 1:E:328:THR:HG22 | 1.83                     | 0.59              |
| 1:H:310:GLN:HG2  | 1:I:328:THR:HG22 | 1.84                     | 0.59              |
| 1:M:628:GLY:O    | 2:CA:997:DA:C2   | 2.53                     | 0.59              |
| 1:R:381:GLU:OE2  | 1:V:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:T:558:VAL:HG11 | 1:T:597:MET:HG3  | 1.83                     | 0.59              |
| 1:Y:693:TYR:HB2  | 1:4:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:2:693:TYR:HB2  | 1:3:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:4:628:GLY:O    | 2:xA:997:DA:C2   | 2.53                     | 0.59              |
| 1:C:381:GLU:OE2  | 1:D:693:TYR:HB2  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:530:ASN:HB2  | 1:Q:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:M:381:GLU:OE2  | 1:c:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:T:381:GLU:OE2  | 1:i:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:c:328:THR:HG22 | 1:s:310:GLN:HG2  | 1.83                     | 0.59              |
| 1:e:558:VAL:HG11 | 1:e:597:MET:HG3  | 1.83                     | 0.59              |
| 1:g:693:TYR:HB2  | 1:l:381:GLU:OE2  | 2.03                     | 0.59              |
| 1:q:693:TYR:HB2  | 1:y:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:r:558:VAL:HG11 | 1:r:597:MET:HG3  | 1.83                     | 0.59              |
| 1:u:310:GLN:HG2  | 1:2:328:THR:HG22 | 1.84                     | 0.59              |
| 1:x:558:VAL:HG11 | 1:x:597:MET:HG3  | 1.83                     | 0.59              |
| 1:4:558:VAL:HG11 | 1:4:597:MET:HG3  | 1.83                     | 0.59              |
| 1:5:530:ASN:HB2  | 1:7:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:O:381:GLU:OE2  | 1:d:693:TYR:HB2  | 2.03                     | 0.59              |
| 1:O:693:TYR:HB2  | 1:P:381:GLU:OE2  | 2.03                     | 0.59              |
| 1:S:310:GLN:HG2  | 1:d:328:THR:HG22 | 1.84                     | 0.59              |
| 1:X:310:GLN:HG2  | 1:Y:328:THR:HG22 | 1.83                     | 0.59              |
| 1:X:693:TYR:HB2  | 1:Y:381:GLU:OE2  | 2.03                     | 0.59              |
| 1:g:328:THR:HG22 | 1:k:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:h:628:GLY:O    | 2:ZA:997:DA:C2   | 2.53                     | 0.59              |
| 1:i:436:TYR:CE2  | 1:j:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:j:381:GLU:OE2  | 1:l:693:TYR:HB2  | 2.03                     | 0.59              |
| 1:n:381:GLU:OE2  | 1:r:693:TYR:HB2  | 2.03                     | 0.59              |
| 1:p:381:GLU:OE2  | 1:6:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:t:530:ASN:HB2  | 1:v:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:6:628:GLY:O    | 2:zA:997:DA:C2   | 2.53                     | 0.59              |
| 1:A:530:ASN:HB2  | 1:I:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:D:328:THR:HG22 | 1:E:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:G:693:TYR:HB2  | 1:W:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:M:558:VAL:HG11 | 1:M:597:MET:HG3  | 1.83                     | 0.59              |
| 1:O:328:THR:HG22 | 1:d:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:S:436:TYR:CE2  | 1:U:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:T:530:ASN:HB2  | 1:l:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:X:530:ASN:HB2  | 1:e:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:Y:310:GLN:HG2  | 1:4:328:THR:HG22 | 1.84                     | 0.59              |
| 1:Y:628:GLY:O    | 2:PA:997:DA:C2   | 2.53                     | 0.59              |
| 1:e:693:TYR:HB2  | 1:h:381:GLU:OE2  | 2.03                     | 0.59              |
| 1:g:373:ARG:O    | 1:g:376:THR:OG1  | 2.19                     | 0.59              |
| 1:g:381:GLU:OE2  | 1:k:693:TYR:HB2  | 2.03                     | 0.59              |
| 1:w:436:TYR:CE2  | 1:x:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:A:693:TYR:HB2  | 1:E:381:GLU:OE2  | 2.03                     | 0.59              |
| 1:D:530:ASN:HB2  | 1:P:436:TYR:CE2  | 2.38                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:628:GLY:O    | 2:3A:997:DA:C2   | 2.53                     | 0.59              |
| 1:M:328:THR:HG22 | 1:c:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:O:373:ARG:O    | 1:O:376:THR:OG1  | 2.19                     | 0.59              |
| 1:Z:530:ASN:HB2  | 1:3:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:c:628:GLY:O    | 2:TA:997:DA:C2   | 2.53                     | 0.59              |
| 1:d:436:TYR:CE2  | 1:l:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:e:373:ARG:O    | 1:e:376:THR:OG1  | 2.19                     | 0.59              |
| 1:g:530:ASN:HB2  | 1:h:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:h:558:VAL:HG11 | 1:h:597:MET:HG3  | 1.83                     | 0.59              |
| 1:k:328:THR:HG22 | 1:w:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:n:558:VAL:HG11 | 1:n:597:MET:HG3  | 1.83                     | 0.59              |
| 1:u:328:THR:HG22 | 1:5:310:GLN:HG2  | 1.83                     | 0.59              |
| 1:1:436:TYR:CE2  | 1:2:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:5:436:TYR:CE2  | 1:6:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:B:530:ASN:HB2  | 1:L:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:C:436:TYR:CE2  | 1:b:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:G:373:ARG:O    | 1:G:376:THR:OG1  | 2.19                     | 0.59              |
| 1:I:310:GLN:HG2  | 1:J:328:THR:HG22 | 1.84                     | 0.59              |
| 1:V:436:TYR:CE2  | 1:e:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:X:381:GLU:OE2  | 1:f:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:a:436:TYR:CE2  | 1:8:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:c:558:VAL:HG11 | 1:c:597:MET:HG3  | 1.83                     | 0.59              |
| 1:g:628:GLY:O    | 2:YA:997:DA:C2   | 2.53                     | 0.59              |
| 1:i:530:ASN:HB2  | 1:k:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:n:628:GLY:O    | 2:gA:997:DA:C2   | 2.53                     | 0.59              |
| 1:q:436:TYR:CE2  | 1:r:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:v:381:GLU:OE2  | 1:1:693:TYR:HB2  | 2.02                     | 0.59              |
| 1:y:558:VAL:HG11 | 1:y:597:MET:HG3  | 1.83                     | 0.59              |
| 1:K:328:THR:HG22 | 1:7:310:GLN:HG2  | 1.84                     | 0.59              |
| 1:O:436:TYR:CE2  | 1:m:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:O:530:ASN:HB2  | 1:n:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:P:693:TYR:HB2  | 1:Q:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:R:436:TYR:CE2  | 1:S:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:R:558:VAL:HG11 | 1:R:597:MET:HG3  | 1.83                     | 0.59              |
| 1:Z:436:TYR:CE2  | 1:4:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:f:530:ASN:HB2  | 1:g:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:i:558:VAL:HG11 | 1:i:597:MET:HG3  | 1.83                     | 0.59              |
| 1:l:558:VAL:HG11 | 1:l:597:MET:HG3  | 1.83                     | 0.59              |
| 1:r:373:ARG:O    | 1:r:376:THR:OG1  | 2.19                     | 0.59              |
| 1:w:530:ASN:HB2  | 1:y:436:TYR:CE2  | 2.37                     | 0.59              |
| 1:5:628:GLY:O    | 2:yA:997:DA:C2   | 2.53                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6:373:ARG:O    | 1:6:376:THR:OG1  | 2.19                     | 0.59              |
| 1:M:530:ASN:HB2  | 1:b:436:TYR:CE2  | 2.38                     | 0.59              |
| 1:O:628:GLY:O    | 2:EA:997:DA:C2   | 2.53                     | 0.59              |
| 1:V:558:VAL:HG11 | 1:V:597:MET:HG3  | 1.83                     | 0.59              |
| 1:X:628:GLY:O    | 2:OA:997:DA:C2   | 2.53                     | 0.59              |
| 1:Y:558:VAL:HG11 | 1:Y:597:MET:HG3  | 1.83                     | 0.59              |
| 1:r:436:TYR:CE2  | 1:s:530:ASN:HB2  | 2.38                     | 0.59              |
| 1:v:310:GLN:HG2  | 1:w:328:THR:HG22 | 1.84                     | 0.59              |
| 1:v:693:TYR:HB2  | 1:w:381:GLU:OE2  | 2.02                     | 0.59              |
| 1:E:530:ASN:HB2  | 1:F:436:TYR:CE2  | 2.38                     | 0.58              |
| 1:H:381:GLU:OE2  | 1:Z:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:N:436:TYR:CE2  | 1:P:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:Q:310:GLN:HG2  | 1:S:328:THR:HG22 | 1.84                     | 0.58              |
| 1:Q:373:ARG:O    | 1:Q:376:THR:OG1  | 2.19                     | 0.58              |
| 1:f:436:TYR:CE2  | 1:h:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:h:693:TYR:HB2  | 1:i:381:GLU:OE2  | 2.02                     | 0.58              |
| 1:s:628:GLY:O    | 2:lA:997:DA:C2   | 2.53                     | 0.58              |
| 1:z:436:TYR:CE2  | 1:l:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:l:628:GLY:O    | 2:uA:997:DA:C2   | 2.53                     | 0.58              |
| 1:A:628:GLY:O    | 2:0:997:DA:C2    | 2.53                     | 0.58              |
| 1:D:436:TYR:CE2  | 1:N:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:E:436:TYR:CE2  | 1:Q:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:F:693:TYR:HB2  | 1:G:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:N:693:TYR:HB2  | 1:m:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:Q:693:TYR:HB2  | 1:S:381:GLU:OE2  | 2.02                     | 0.58              |
| 1:R:328:THR:HG22 | 1:V:310:GLN:HG2  | 1.84                     | 0.58              |
| 1:U:693:TYR:HB2  | 1:e:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:b:693:TYR:HB2  | 1:o:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:h:310:GLN:HG2  | 1:i:328:THR:HG22 | 1.84                     | 0.58              |
| 1:k:628:GLY:O    | 2:cA:997:DA:C2   | 2.53                     | 0.58              |
| 1:m:436:TYR:CE2  | 1:n:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:q:558:VAL:HG11 | 1:q:597:MET:HG3  | 1.83                     | 0.58              |
| 1:t:436:TYR:CE2  | 1:u:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:t:693:TYR:HB2  | 1:6:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:u:436:TYR:CE2  | 1:v:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:z:530:ASN:HB2  | 1:2:436:TYR:CE2  | 2.38                     | 0.58              |
| 1:5:328:THR:HG22 | 1:8:310:GLN:HG2  | 1.84                     | 0.58              |
| 1:B:328:THR:HG22 | 1:C:310:GLN:HG2  | 1.84                     | 0.58              |
| 1:F:381:GLU:OE2  | 1:R:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:J:436:TYR:CE2  | 1:L:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:K:381:GLU:OE2  | 1:7:693:TYR:HB2  | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:436:TYR:CE2  | 1:Y:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:W:628:GLY:O    | 2:NA:997:DA:C2   | 2.53                     | 0.58              |
| 1:c:530:ASN:HB2  | 1:p:436:TYR:CE2  | 2.38                     | 0.58              |
| 1:l:381:GLU:OE2  | 1:n:693:TYR:HB2  | 2.02                     | 0.58              |
| 1:o:693:TYR:HB2  | 1:7:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:q:310:GLN:HG2  | 1:y:328:THR:HG22 | 1.84                     | 0.58              |
| 1:r:381:GLU:OE2  | 1:x:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:t:381:GLU:OE2  | 1:y:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:v:328:THR:HG22 | 1:l:310:GLN:HG2  | 1.84                     | 0.58              |
| 1:P:628:GLY:O    | 2:FA:997:DA:C2   | 2.53                     | 0.58              |
| 1:d:628:GLY:O    | 2:VA:997:DA:C2   | 2.53                     | 0.58              |
| 1:j:373:ARG:O    | 1:j:376:THR:OG1  | 2.19                     | 0.58              |
| 1:o:436:TYR:CE2  | 1:p:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:p:693:TYR:HB2  | 1:q:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:H:693:TYR:HB2  | 1:I:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:I:693:TYR:HB2  | 1:J:381:GLU:OE2  | 2.02                     | 0.58              |
| 1:K:436:TYR:CE2  | 1:a:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:V:381:GLU:OE2  | 1:W:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:V:530:ASN:HB2  | 1:X:436:TYR:CE2  | 2.38                     | 0.58              |
| 1:Z:381:GLU:OE2  | 1:a:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:j:436:TYR:CE2  | 1:k:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:l:328:THR:HG22 | 1:n:310:GLN:HG2  | 1.84                     | 0.58              |
| 1:p:628:GLY:O    | 2:iA:997:DA:C2   | 2.53                     | 0.58              |
| 1:r:328:THR:HG22 | 1:x:310:GLN:HG2  | 1.84                     | 0.58              |
| 1:v:628:GLY:O    | 2:oA:997:DA:C2   | 2.53                     | 0.58              |
| 1:3:310:GLN:HG2  | 1:8:328:THR:HG22 | 1.84                     | 0.58              |
| 1:G:436:TYR:CE2  | 1:I:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:H:436:TYR:CE2  | 1:W:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:H:530:ASN:HB2  | 1:Y:436:TYR:CE2  | 2.38                     | 0.58              |
| 1:K:693:TYR:HB2  | 1:L:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:L:693:TYR:HB2  | 1:b:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:P:310:GLN:HG2  | 1:Q:328:THR:HG22 | 1.84                     | 0.58              |
| 1:T:373:ARG:O    | 1:T:376:THR:OG1  | 2.19                     | 0.58              |
| 1:U:310:GLN:HG2  | 1:e:328:THR:HG22 | 1.84                     | 0.58              |
| 1:f:381:GLU:OE2  | 1:z:693:TYR:HB2  | 2.03                     | 0.58              |
| 1:6:436:TYR:CE2  | 1:7:530:ASN:HB2  | 2.38                     | 0.58              |
| 1:Q:628:GLY:O    | 2:GA:997:DA:C2   | 2.53                     | 0.58              |
| 1:S:693:TYR:HB2  | 1:d:381:GLU:OE2  | 2.03                     | 0.58              |
| 1:q:530:ASN:HB2  | 1:s:436:TYR:CE2  | 2.38                     | 0.58              |
| 1:u:628:GLY:O    | 2:nA:997:DA:C2   | 2.53                     | 0.58              |
| 1:5:381:GLU:OE2  | 1:8:693:TYR:HB2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:328:THR:HG22 | 1:B:310:GLN:HG2 | 1.84                     | 0.58              |
| 1:A:436:TYR:CE2  | 1:G:530:ASN:HB2 | 2.39                     | 0.58              |
| 1:J:693:TYR:HB2  | 1:a:381:GLU:OE2 | 2.03                     | 0.58              |
| 1:T:436:TYR:CE2  | 1:d:530:ASN:HB2 | 2.38                     | 0.58              |
| 1:c:436:TYR:CE2  | 1:o:530:ASN:HB2 | 2.38                     | 0.58              |
| 1:K:530:ASN:HB2  | 1:8:436:TYR:CE2 | 2.38                     | 0.58              |
| 1:T:693:TYR:HB2  | 1:U:381:GLU:OE2 | 2.03                     | 0.58              |
| 1:k:381:GLU:OE2  | 1:w:693:TYR:HB2 | 2.03                     | 0.58              |
| 1:2:628:GLY:O    | 2:vA:997:DA:C2  | 2.53                     | 0.58              |
| 1:E:628:GLY:O    | 2:qA:997:DA:C2  | 2.53                     | 0.58              |
| 1:x:436:TYR:CE2  | 1:y:530:ASN:HB2 | 2.38                     | 0.58              |
| 1:3:693:TYR:HB2  | 1:8:381:GLU:OE2 | 2.03                     | 0.58              |
| 1:B:436:TYR:CE2  | 1:J:530:ASN:HB2 | 2.38                     | 0.57              |
| 1:R:530:ASN:HB2  | 1:U:436:TYR:CE2 | 2.38                     | 0.57              |
| 1:j:693:TYR:HB2  | 1:x:381:GLU:OE2 | 2.03                     | 0.57              |
| 1:B:381:GLU:OE2  | 1:C:693:TYR:HB2 | 2.03                     | 0.57              |
| 1:D:628:GLY:O    | 2:fA:997:DA:C2  | 2.53                     | 0.57              |
| 1:k:373:ARG:O    | 1:k:376:THR:OG1 | 2.19                     | 0.57              |
| 1:p:373:ARG:O    | 1:p:376:THR:OG1 | 2.19                     | 0.57              |
| 1:d:373:ARG:O    | 1:d:376:THR:OG1 | 2.19                     | 0.57              |
| 1:M:693:TYR:HB2  | 1:N:381:GLU:OE2 | 2.03                     | 0.57              |
| 1:z:373:ARG:O    | 1:z:376:THR:OG1 | 2.19                     | 0.57              |
| 1:z:381:GLU:OE2  | 1:4:693:TYR:HB2 | 2.03                     | 0.57              |
| 1:N:373:ARG:O    | 1:N:376:THR:OG1 | 2.19                     | 0.57              |
| 1:W:330:THR:HG21 | 1:W:395:MET:HB3 | 1.87                     | 0.57              |
| 1:p:330:THR:HG21 | 1:p:395:MET:HB3 | 1.87                     | 0.57              |
| 1:M:330:THR:HG21 | 1:M:395:MET:HB3 | 1.87                     | 0.57              |
| 1:r:330:THR:HG21 | 1:r:395:MET:HB3 | 1.87                     | 0.57              |
| 1:4:330:THR:HG21 | 1:4:395:MET:HB3 | 1.87                     | 0.57              |
| 1:C:330:THR:HG21 | 1:C:395:MET:HB3 | 1.87                     | 0.57              |
| 1:C:373:ARG:O    | 1:C:376:THR:OG1 | 2.19                     | 0.57              |
| 1:V:330:THR:HG21 | 1:V:395:MET:HB3 | 1.87                     | 0.57              |
| 1:e:330:THR:HG21 | 1:e:395:MET:HB3 | 1.87                     | 0.57              |
| 1:3:330:THR:HG21 | 1:3:395:MET:HB3 | 1.87                     | 0.57              |
| 1:E:373:ARG:O    | 1:E:376:THR:OG1 | 2.19                     | 0.57              |
| 1:o:330:THR:HG21 | 1:o:395:MET:HB3 | 1.87                     | 0.57              |
| 1:q:330:THR:HG21 | 1:q:395:MET:HB3 | 1.87                     | 0.57              |
| 1:u:373:ARG:O    | 1:u:376:THR:OG1 | 2.19                     | 0.57              |
| 1:A:381:GLU:OE2  | 1:B:693:TYR:HB2 | 2.04                     | 0.57              |
| 1:L:330:THR:HG21 | 1:L:395:MET:HB3 | 1.87                     | 0.57              |
| 1:6:469:MET:SD   | 1:6:566:GLY:HA3 | 2.45                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:469:MET:SD   | 1:G:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:H:330:THR:HG21 | 1:H:395:MET:HB3  | 1.87                     | 0.56              |
| 1:V:489:PHE:O    | 1:V:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:Y:373:ARG:O    | 1:Y:376:THR:OG1  | 2.19                     | 0.56              |
| 1:a:330:THR:HG21 | 1:a:395:MET:HB3  | 1.87                     | 0.56              |
| 1:k:489:PHE:O    | 1:k:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:3:373:ARG:O    | 1:3:376:THR:OG1  | 2.19                     | 0.56              |
| 1:Q:469:MET:SD   | 1:Q:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:R:330:THR:HG21 | 1:R:395:MET:HB3  | 1.87                     | 0.56              |
| 1:X:619:HIS:HA   | 2:OA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:c:373:ARG:O    | 1:c:376:THR:OG1  | 2.19                     | 0.56              |
| 1:e:469:MET:SD   | 1:e:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:l:373:ARG:O    | 1:l:376:THR:OG1  | 2.19                     | 0.56              |
| 1:p:469:MET:SD   | 1:p:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:r:469:MET:SD   | 1:r:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:t:373:ARG:O    | 1:t:376:THR:OG1  | 2.19                     | 0.56              |
| 1:y:330:THR:HG21 | 1:y:395:MET:HB3  | 1.87                     | 0.56              |
| 1:z:330:THR:HG21 | 1:z:395:MET:HB3  | 1.87                     | 0.56              |
| 1:z:469:MET:SD   | 1:z:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:8:628:GLY:O    | 2:2A:997:DA:C2   | 2.53                     | 0.56              |
| 1:B:469:MET:SD   | 1:B:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:C:469:MET:SD   | 1:C:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:E:330:THR:HG21 | 1:E:395:MET:HB3  | 1.87                     | 0.56              |
| 1:N:456:ARG:O    | 1:N:460:THR:HG23 | 2.06                     | 0.56              |
| 1:N:469:MET:SD   | 1:N:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:O:330:THR:HG21 | 1:O:395:MET:HB3  | 1.87                     | 0.56              |
| 1:R:469:MET:SD   | 1:R:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:U:469:MET:SD   | 1:U:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:W:456:ARG:O    | 1:W:460:THR:HG23 | 2.06                     | 0.56              |
| 1:W:469:MET:SD   | 1:W:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:f:469:MET:SD   | 1:f:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:g:330:THR:HG21 | 1:g:395:MET:HB3  | 1.87                     | 0.56              |
| 1:h:330:THR:HG21 | 1:h:395:MET:HB3  | 1.87                     | 0.56              |
| 1:h:619:HIS:HA   | 2:ZA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:i:330:THR:HG21 | 1:i:395:MET:HB3  | 1.87                     | 0.56              |
| 1:j:469:MET:SD   | 1:j:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:l:330:THR:HG21 | 1:l:395:MET:HB3  | 1.87                     | 0.56              |
| 1:m:469:MET:SD   | 1:m:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:p:456:ARG:O    | 1:p:460:THR:HG23 | 2.06                     | 0.56              |
| 1:q:489:PHE:O    | 1:q:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:s:330:THR:HG21 | 1:s:395:MET:HB3  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:330:THR:HG21 | 1:u:395:MET:HB3  | 1.87                     | 0.56              |
| 1:v:469:MET:SD   | 1:v:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:w:373:ARG:O    | 1:w:376:THR:OG1  | 2.19                     | 0.56              |
| 1:x:330:THR:HG21 | 1:x:395:MET:HB3  | 1.87                     | 0.56              |
| 1:x:469:MET:SD   | 1:x:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:y:469:MET:SD   | 1:y:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:z:456:ARG:O    | 1:z:460:THR:HG23 | 2.06                     | 0.56              |
| 1:3:469:MET:SD   | 1:3:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:3:489:PHE:O    | 1:3:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:6:330:THR:HG21 | 1:6:395:MET:HB3  | 1.87                     | 0.56              |
| 1:7:456:ARG:O    | 1:7:460:THR:HG23 | 2.06                     | 0.56              |
| 1:8:469:MET:SD   | 1:8:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:G:330:THR:HG21 | 1:G:395:MET:HB3  | 1.87                     | 0.56              |
| 1:G:456:ARG:O    | 1:G:460:THR:HG23 | 2.06                     | 0.56              |
| 1:I:456:ARG:O    | 1:I:460:THR:HG23 | 2.06                     | 0.56              |
| 1:N:330:THR:HG21 | 1:N:395:MET:HB3  | 1.87                     | 0.56              |
| 1:T:469:MET:SD   | 1:T:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:U:330:THR:HG21 | 1:U:395:MET:HB3  | 1.87                     | 0.56              |
| 1:V:456:ARG:O    | 1:V:460:THR:HG23 | 2.06                     | 0.56              |
| 1:X:330:THR:HG21 | 1:X:395:MET:HB3  | 1.87                     | 0.56              |
| 1:Z:456:ARG:O    | 1:Z:460:THR:HG23 | 2.06                     | 0.56              |
| 1:b:456:ARG:O    | 1:b:460:THR:HG23 | 2.06                     | 0.56              |
| 1:n:330:THR:HG21 | 1:n:395:MET:HB3  | 1.87                     | 0.56              |
| 1:q:456:ARG:O    | 1:q:460:THR:HG23 | 2.06                     | 0.56              |
| 1:s:619:HIS:HA   | 2:lA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:v:456:ARG:O    | 1:v:460:THR:HG23 | 2.06                     | 0.56              |
| 1:6:456:ARG:O    | 1:6:460:THR:HG23 | 2.06                     | 0.56              |
| 1:D:469:MET:SD   | 1:D:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:Q:456:ARG:O    | 1:Q:460:THR:HG23 | 2.06                     | 0.56              |
| 1:U:373:ARG:O    | 1:U:376:THR:OG1  | 2.19                     | 0.56              |
| 1:Z:489:PHE:O    | 1:Z:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:h:456:ARG:O    | 1:h:460:THR:HG23 | 2.06                     | 0.56              |
| 1:i:373:ARG:O    | 1:i:376:THR:OG1  | 2.19                     | 0.56              |
| 1:i:489:PHE:O    | 1:i:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:l:469:MET:SD   | 1:l:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:2:469:MET:SD   | 1:2:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:C:472:THR:HG22 | 1:C:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:H:469:MET:SD   | 1:H:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:I:469:MET:SD   | 1:I:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:T:330:THR:HG21 | 1:T:395:MET:HB3  | 1.87                     | 0.56              |
| 1:c:456:ARG:O    | 1:c:460:THR:HG23 | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:456:ARG:O    | 1:n:460:THR:HG23 | 2.06                     | 0.56              |
| 1:3:472:THR:HG22 | 1:3:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:4:619:HIS:HA   | 2:xA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:A:336:ASP:O    | 1:A:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:A:469:MET:SD   | 1:A:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:G:472:THR:HG22 | 1:G:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:J:469:MET:SD   | 1:J:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:J:472:THR:HG22 | 1:J:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:K:330:THR:HG21 | 1:K:395:MET:HB3  | 1.87                     | 0.56              |
| 1:K:469:MET:SD   | 1:K:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:K:472:THR:HG22 | 1:K:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:L:472:THR:HG22 | 1:L:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:O:456:ARG:O    | 1:O:460:THR:HG23 | 2.06                     | 0.56              |
| 1:Q:472:THR:HG22 | 1:Q:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:R:336:ASP:O    | 1:R:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:R:456:ARG:O    | 1:R:460:THR:HG23 | 2.06                     | 0.56              |
| 1:T:619:HIS:HA   | 2:KA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:Y:330:THR:HG21 | 1:Y:395:MET:HB3  | 1.87                     | 0.56              |
| 1:Y:456:ARG:O    | 1:Y:460:THR:HG23 | 2.06                     | 0.56              |
| 1:Z:469:MET:SD   | 1:Z:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:b:469:MET:SD   | 1:b:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:c:469:MET:SD   | 1:c:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:f:330:THR:HG21 | 1:f:395:MET:HB3  | 1.87                     | 0.56              |
| 1:g:456:ARG:O    | 1:g:460:THR:HG23 | 2.06                     | 0.56              |
| 1:i:469:MET:SD   | 1:i:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:j:330:THR:HG21 | 1:j:395:MET:HB3  | 1.87                     | 0.56              |
| 1:l:489:PHE:O    | 1:l:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:n:469:MET:SD   | 1:n:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:o:469:MET:SD   | 1:o:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:u:472:THR:HG22 | 1:u:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:v:472:THR:HG22 | 1:v:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:y:336:ASP:O    | 1:y:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:5:336:ASP:O    | 1:5:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:5:469:MET:SD   | 1:5:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:6:472:THR:HG22 | 1:6:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:7:469:MET:SD   | 1:7:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:7:489:PHE:O    | 1:7:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:B:456:ARG:O    | 1:B:460:THR:HG23 | 2.06                     | 0.56              |
| 1:C:336:ASP:O    | 1:C:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:E:472:THR:HG22 | 1:E:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:F:469:MET:SD   | 1:F:566:GLY:HA3  | 2.45                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:489:PHE:O    | 1:I:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:J:330:THR:HG21 | 1:J:395:MET:HB3  | 1.87                     | 0.56              |
| 1:Y:472:THR:HG22 | 1:Y:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:a:472:THR:HG22 | 1:a:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:b:489:PHE:O    | 1:b:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:c:330:THR:HG21 | 1:c:395:MET:HB3  | 1.87                     | 0.56              |
| 1:c:472:THR:HG22 | 1:c:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:j:336:ASP:O    | 1:j:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:j:619:HIS:HA   | 2:bA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:m:330:THR:HG21 | 1:m:395:MET:HB3  | 1.87                     | 0.56              |
| 1:r:619:HIS:HA   | 2:kA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:t:456:ARG:O    | 1:t:460:THR:HG23 | 2.06                     | 0.56              |
| 1:t:469:MET:SD   | 1:t:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:x:373:ARG:O    | 1:x:376:THR:OG1  | 2.19                     | 0.56              |
| 1:y:456:ARG:O    | 1:y:460:THR:HG23 | 2.06                     | 0.56              |
| 1:2:336:ASP:O    | 1:2:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:3:336:ASP:O    | 1:3:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:4:469:MET:SD   | 1:4:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:4:472:THR:HG22 | 1:4:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:5:330:THR:HG21 | 1:5:395:MET:HB3  | 1.87                     | 0.56              |
| 1:D:336:ASP:O    | 1:D:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:F:456:ARG:O    | 1:F:460:THR:HG23 | 2.06                     | 0.56              |
| 1:I:336:ASP:O    | 1:I:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:L:469:MET:SD   | 1:L:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:M:456:ARG:O    | 1:M:460:THR:HG23 | 2.06                     | 0.56              |
| 1:M:469:MET:SD   | 1:M:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:M:472:THR:HG22 | 1:M:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:T:336:ASP:O    | 1:T:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:T:472:THR:HG22 | 1:T:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:U:472:THR:HG22 | 1:U:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:e:619:HIS:HA   | 2:WA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:h:469:MET:SD   | 1:h:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:v:336:ASP:O    | 1:v:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:w:330:THR:HG21 | 1:w:395:MET:HB3  | 1.87                     | 0.56              |
| 1:x:489:PHE:O    | 1:x:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:z:472:THR:HG22 | 1:z:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:2:330:THR:HG21 | 1:2:395:MET:HB3  | 1.87                     | 0.56              |
| 1:7:336:ASP:O    | 1:7:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:8:330:THR:HG21 | 1:8:395:MET:HB3  | 1.87                     | 0.56              |
| 1:8:456:ARG:O    | 1:8:460:THR:HG23 | 2.06                     | 0.56              |
| 1:B:489:PHE:O    | 1:B:494:ARG:NH1  | 2.37                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:330:THR:HG21 | 1:D:395:MET:HB3  | 1.87                     | 0.56              |
| 1:N:472:THR:HG22 | 1:N:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:P:330:THR:HG21 | 1:P:395:MET:HB3  | 1.87                     | 0.56              |
| 1:Q:336:ASP:O    | 1:Q:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:R:472:THR:HG22 | 1:R:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:R:619:HIS:HA   | 2:HA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:S:330:THR:HG21 | 1:S:395:MET:HB3  | 1.87                     | 0.56              |
| 1:U:489:PHE:O    | 1:U:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:Y:469:MET:SD   | 1:Y:566:GLY:HA3  | 2.45                     | 0.56              |
| 1:Z:472:THR:HG22 | 1:Z:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:a:469:MET:SD   | 1:a:566:GLY:HA3  | 2.46                     | 0.56              |
| 1:d:456:ARG:O    | 1:d:460:THR:HG23 | 2.06                     | 0.56              |
| 1:e:456:ARG:O    | 1:e:460:THR:HG23 | 2.06                     | 0.56              |
| 1:h:336:ASP:O    | 1:h:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:j:456:ARG:O    | 1:j:460:THR:HG23 | 2.06                     | 0.56              |
| 1:j:472:THR:HG22 | 1:j:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:l:619:HIS:HA   | 2:dA:997:DA:H2'  | 1.88                     | 0.56              |
| 1:o:489:PHE:O    | 1:o:494:ARG:NH1  | 2.37                     | 0.56              |
| 1:t:330:THR:HG21 | 1:t:395:MET:HB3  | 1.87                     | 0.56              |
| 1:x:336:ASP:O    | 1:x:634:PRO:HB3  | 2.06                     | 0.56              |
| 1:x:472:THR:HG22 | 1:x:562:ALA:HB1  | 1.88                     | 0.56              |
| 1:4:456:ARG:O    | 1:4:460:THR:HG23 | 2.06                     | 0.56              |
| 1:B:330:THR:HG21 | 1:B:395:MET:HB3  | 1.87                     | 0.55              |
| 1:B:336:ASP:O    | 1:B:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:C:456:ARG:O    | 1:C:460:THR:HG23 | 2.06                     | 0.55              |
| 1:L:456:ARG:O    | 1:L:460:THR:HG23 | 2.06                     | 0.55              |
| 1:T:456:ARG:O    | 1:T:460:THR:HG23 | 2.06                     | 0.55              |
| 1:a:336:ASP:O    | 1:a:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:b:472:THR:HG22 | 1:b:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:h:472:THR:HG22 | 1:h:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:h:513:ASN:ND2  | 1:h:526:THR:HG22 | 2.10                     | 0.55              |
| 1:i:619:HIS:HA   | 2:aA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:k:456:ARG:O    | 1:k:460:THR:HG23 | 2.06                     | 0.55              |
| 1:n:336:ASP:O    | 1:n:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:q:469:MET:SD   | 1:q:566:GLY:HA3  | 2.45                     | 0.55              |
| 1:r:456:ARG:O    | 1:r:460:THR:HG23 | 2.06                     | 0.55              |
| 1:s:469:MET:SD   | 1:s:566:GLY:HA3  | 2.45                     | 0.55              |
| 1:8:336:ASP:O    | 1:8:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:8:489:PHE:O    | 1:8:494:ARG:NH1  | 2.37                     | 0.55              |
| 1:A:330:THR:HG21 | 1:A:395:MET:HB3  | 1.87                     | 0.55              |
| 1:A:472:THR:HG22 | 1:A:562:ALA:HB1  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:456:ARG:O    | 1:D:460:THR:HG23 | 2.06                     | 0.55              |
| 1:G:336:ASP:O    | 1:G:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:H:489:PHE:O    | 1:H:494:ARG:NH1  | 2.37                     | 0.55              |
| 1:L:336:ASP:O    | 1:L:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:O:469:MET:SD   | 1:O:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:U:336:ASP:O    | 1:U:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:X:469:MET:SD   | 1:X:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:d:330:THR:HG21 | 1:d:395:MET:HB3  | 1.87                     | 0.55              |
| 1:g:469:MET:SD   | 1:g:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:n:472:THR:HG22 | 1:n:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:u:456:ARG:O    | 1:u:460:THR:HG23 | 2.06                     | 0.55              |
| 1:y:472:THR:HG22 | 1:y:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:y:619:HIS:HA   | 2:sA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:1:469:MET:SD   | 1:1:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:2:456:ARG:O    | 1:2:460:THR:HG23 | 2.06                     | 0.55              |
| 1:6:336:ASP:O    | 1:6:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:E:469:MET:SD   | 1:E:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:F:330:THR:HG21 | 1:F:395:MET:HB3  | 1.87                     | 0.55              |
| 1:S:469:MET:SD   | 1:S:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:W:472:THR:HG22 | 1:W:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:a:373:ARG:O    | 1:a:376:THR:OG1  | 2.19                     | 0.55              |
| 1:a:456:ARG:O    | 1:a:460:THR:HG23 | 2.06                     | 0.55              |
| 1:f:472:THR:HG22 | 1:f:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:o:373:ARG:O    | 1:o:376:THR:OG1  | 2.19                     | 0.55              |
| 1:p:472:THR:HG22 | 1:p:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:1:330:THR:HG21 | 1:1:395:MET:HB3  | 1.87                     | 0.55              |
| 1:3:456:ARG:O    | 1:3:460:THR:HG23 | 2.06                     | 0.55              |
| 1:5:472:THR:HG22 | 1:5:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:7:330:THR:HG21 | 1:7:395:MET:HB3  | 1.87                     | 0.55              |
| 1:8:472:THR:HG22 | 1:8:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:E:456:ARG:O    | 1:E:460:THR:HG23 | 2.06                     | 0.55              |
| 1:H:373:ARG:O    | 1:H:376:THR:OG1  | 2.19                     | 0.55              |
| 1:I:330:THR:HG21 | 1:I:395:MET:HB3  | 1.87                     | 0.55              |
| 1:J:336:ASP:O    | 1:J:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:N:513:ASN:ND2  | 1:N:526:THR:HG22 | 2.10                     | 0.55              |
| 1:O:472:THR:HG22 | 1:O:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:R:247:TYR:O    | 1:V:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:c:247:TYR:O    | 1:s:707:GLY:HA2  | 2.06                     | 0.55              |
| 1:g:336:ASP:O    | 1:g:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:i:456:ARG:O    | 1:i:460:THR:HG23 | 2.06                     | 0.55              |
| 1:k:330:THR:HG21 | 1:k:395:MET:HB3  | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:373:ARG:O    | 1:m:376:THR:OG1  | 2.19                     | 0.55              |
| 1:m:456:ARG:O    | 1:m:460:THR:HG23 | 2.06                     | 0.55              |
| 1:m:707:GLY:HA2  | 1:s:247:TYR:O    | 2.06                     | 0.55              |
| 1:q:707:GLY:HA2  | 1:y:247:TYR:O    | 2.07                     | 0.55              |
| 1:r:336:ASP:O    | 1:r:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:u:336:ASP:O    | 1:u:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:w:469:MET:SD   | 1:w:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:4:336:ASP:O    | 1:4:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:B:472:THR:HG22 | 1:B:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:E:336:ASP:O    | 1:E:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:I:530:ASN:ND2  | 1:I:532:GLN:O    | 2.40                     | 0.55              |
| 1:J:707:GLY:HA2  | 1:a:247:TYR:O    | 2.07                     | 0.55              |
| 1:K:336:ASP:O    | 1:K:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:M:336:ASP:O    | 1:M:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:O:336:ASP:O    | 1:O:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:O:530:ASN:ND2  | 1:O:532:GLN:O    | 2.40                     | 0.55              |
| 1:P:336:ASP:O    | 1:P:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:S:472:THR:HG22 | 1:S:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:V:469:MET:SD   | 1:V:566:GLY:HA3  | 2.45                     | 0.55              |
| 1:e:336:ASP:O    | 1:e:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:f:456:ARG:O    | 1:f:460:THR:HG23 | 2.06                     | 0.55              |
| 1:f:619:HIS:HA   | 2:XA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:g:472:THR:HG22 | 1:g:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:i:472:THR:HG22 | 1:i:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:l:456:ARG:O    | 1:l:460:THR:HG23 | 2.06                     | 0.55              |
| 1:m:472:THR:HG22 | 1:m:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:u:469:MET:SD   | 1:u:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:5:456:ARG:O    | 1:5:460:THR:HG23 | 2.06                     | 0.55              |
| 1:7:530:ASN:ND2  | 1:7:532:GLN:O    | 2.40                     | 0.55              |
| 1:A:456:ARG:O    | 1:A:460:THR:HG23 | 2.06                     | 0.55              |
| 1:B:432:ASP:HA   | 1:B:454:ALA:H    | 1.72                     | 0.55              |
| 1:C:530:ASN:ND2  | 1:C:532:GLN:O    | 2.40                     | 0.55              |
| 1:H:530:ASN:ND2  | 1:H:532:GLN:O    | 2.40                     | 0.55              |
| 1:K:707:GLY:HA2  | 1:L:247:TYR:O    | 2.07                     | 0.55              |
| 1:L:373:ARG:O    | 1:L:376:THR:OG1  | 2.19                     | 0.55              |
| 1:M:530:ASN:ND2  | 1:M:532:GLN:O    | 2.40                     | 0.55              |
| 1:P:469:MET:SD   | 1:P:566:GLY:HA3  | 2.46                     | 0.55              |
| 1:P:472:THR:HG22 | 1:P:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:R:530:ASN:ND2  | 1:R:532:GLN:O    | 2.40                     | 0.55              |
| 1:U:456:ARG:O    | 1:U:460:THR:HG23 | 2.06                     | 0.55              |
| 1:g:530:ASN:ND2  | 1:g:532:GLN:O    | 2.40                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:469:MET:SD   | 1:k:566:GLY:HA3  | 2.45                     | 0.55              |
| 1:l:472:THR:HG22 | 1:l:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:n:247:TYR:O    | 1:r:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:n:530:ASN:ND2  | 1:n:532:GLN:O    | 2.40                     | 0.55              |
| 1:o:530:ASN:ND2  | 1:o:532:GLN:O    | 2.40                     | 0.55              |
| 1:q:472:THR:HG22 | 1:q:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:q:530:ASN:ND2  | 1:q:532:GLN:O    | 2.40                     | 0.55              |
| 1:w:336:ASP:O    | 1:w:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:w:456:ARG:O    | 1:w:460:THR:HG23 | 2.06                     | 0.55              |
| 1:w:472:THR:HG22 | 1:w:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:x:456:ARG:O    | 1:x:460:THR:HG23 | 2.06                     | 0.55              |
| 1:y:530:ASN:ND2  | 1:y:532:GLN:O    | 2.40                     | 0.55              |
| 1:1:336:ASP:O    | 1:1:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:1:456:ARG:O    | 1:1:460:THR:HG23 | 2.06                     | 0.55              |
| 1:3:530:ASN:ND2  | 1:3:532:GLN:O    | 2.40                     | 0.55              |
| 1:4:530:ASN:ND2  | 1:4:532:GLN:O    | 2.40                     | 0.55              |
| 1:8:432:ASP:HA   | 1:8:454:ALA:H    | 1.72                     | 0.55              |
| 1:J:456:ARG:O    | 1:J:460:THR:HG23 | 2.06                     | 0.55              |
| 1:K:456:ARG:O    | 1:K:460:THR:HG23 | 2.06                     | 0.55              |
| 1:S:336:ASP:O    | 1:S:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:V:472:THR:HG22 | 1:V:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:V:530:ASN:ND2  | 1:V:532:GLN:O    | 2.40                     | 0.55              |
| 1:d:469:MET:SD   | 1:d:566:GLY:HA3  | 2.45                     | 0.55              |
| 1:e:707:GLY:HA2  | 1:h:247:TYR:O    | 2.07                     | 0.55              |
| 1:f:373:ARG:O    | 1:f:376:THR:OG1  | 2.19                     | 0.55              |
| 1:h:530:ASN:ND2  | 1:h:532:GLN:O    | 2.40                     | 0.55              |
| 1:m:619:HIS:HA   | 2:eA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:o:456:ARG:O    | 1:o:460:THR:HG23 | 2.06                     | 0.55              |
| 1:p:530:ASN:ND2  | 1:p:532:GLN:O    | 2.40                     | 0.55              |
| 1:q:336:ASP:O    | 1:q:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:t:336:ASP:O    | 1:t:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:z:513:ASN:ND2  | 1:z:526:THR:HG22 | 2.10                     | 0.55              |
| 1:1:472:THR:HG22 | 1:1:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:2:619:HIS:HA   | 2:vA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:D:619:HIS:HA   | 2:fA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:F:336:ASP:O    | 1:F:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:F:432:ASP:HA   | 1:F:454:ALA:H    | 1.72                     | 0.55              |
| 1:F:707:GLY:HA2  | 1:G:247:TYR:O    | 2.07                     | 0.55              |
| 1:M:247:TYR:O    | 1:c:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:N:432:ASP:HA   | 1:N:454:ALA:H    | 1.72                     | 0.55              |
| 1:O:247:TYR:O    | 1:d:707:GLY:HA2  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:456:ARG:O    | 1:P:460:THR:HG23 | 2.06                     | 0.55              |
| 1:S:456:ARG:O    | 1:S:460:THR:HG23 | 2.06                     | 0.55              |
| 1:V:336:ASP:O    | 1:V:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:W:530:ASN:ND2  | 1:W:532:GLN:O    | 2.40                     | 0.55              |
| 1:Z:330:THR:HG21 | 1:Z:395:MET:HB3  | 1.87                     | 0.55              |
| 1:g:247:TYR:O    | 1:k:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:r:472:THR:HG22 | 1:r:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:t:432:ASP:HA   | 1:t:454:ALA:H    | 1.72                     | 0.55              |
| 1:t:707:GLY:HA2  | 1:6:247:TYR:O    | 2.07                     | 0.55              |
| 1:u:247:TYR:O    | 1:5:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:w:619:HIS:HA   | 2:pA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:8:530:ASN:ND2  | 1:8:532:GLN:O    | 2.40                     | 0.55              |
| 1:B:530:ASN:ND2  | 1:B:532:GLN:O    | 2.40                     | 0.55              |
| 1:D:432:ASP:HA   | 1:D:454:ALA:H    | 1.72                     | 0.55              |
| 1:H:456:ARG:O    | 1:H:460:THR:HG23 | 2.06                     | 0.55              |
| 1:I:472:THR:HG22 | 1:I:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:J:530:ASN:ND2  | 1:J:532:GLN:O    | 2.40                     | 0.55              |
| 1:K:530:ASN:ND2  | 1:K:532:GLN:O    | 2.40                     | 0.55              |
| 1:N:336:ASP:O    | 1:N:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:N:707:GLY:HA2  | 1:m:247:TYR:O    | 2.07                     | 0.55              |
| 1:X:707:GLY:HA2  | 1:Y:247:TYR:O    | 2.07                     | 0.55              |
| 1:Y:336:ASP:O    | 1:Y:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:Z:610:LYS:HB2  | 1:Z:632:PRO:HG3  | 1.89                     | 0.55              |
| 1:b:610:LYS:HB2  | 1:b:632:PRO:HG3  | 1.89                     | 0.55              |
| 1:c:336:ASP:O    | 1:c:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:i:530:ASN:ND2  | 1:i:532:GLN:O    | 2.40                     | 0.55              |
| 1:k:530:ASN:ND2  | 1:k:532:GLN:O    | 2.40                     | 0.55              |
| 1:l:247:TYR:O    | 1:n:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:l:530:ASN:ND2  | 1:l:532:GLN:O    | 2.40                     | 0.55              |
| 1:s:472:THR:HG22 | 1:s:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:z:336:ASP:O    | 1:z:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:z:530:ASN:ND2  | 1:z:532:GLN:O    | 2.40                     | 0.55              |
| 1:2:432:ASP:HA   | 1:2:454:ALA:H    | 1.72                     | 0.55              |
| 1:7:472:THR:HG22 | 1:7:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:B:247:TYR:O    | 1:C:707:GLY:HA2  | 2.08                     | 0.55              |
| 1:C:247:TYR:O    | 1:D:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:G:707:GLY:HA2  | 1:W:247:TYR:O    | 2.07                     | 0.55              |
| 1:H:472:THR:HG22 | 1:H:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:I:707:GLY:HA2  | 1:J:247:TYR:O    | 2.07                     | 0.55              |
| 1:N:530:ASN:ND2  | 1:N:532:GLN:O    | 2.40                     | 0.55              |
| 1:S:619:HIS:HA   | 2:IA:997:DA:H2'  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:513:ASN:ND2  | 1:V:526:THR:HG22 | 2.10                     | 0.55              |
| 1:V:619:HIS:HA   | 2:MA:997:DA:H2'  | 1.88                     | 0.55              |
| 1:X:336:ASP:O    | 1:X:634:PRO:HB3  | 2.06                     | 0.55              |
| 1:Y:707:GLY:HA2  | 1:4:247:TYR:O    | 2.07                     | 0.55              |
| 1:b:330:THR:HG21 | 1:b:395:MET:HB3  | 1.87                     | 0.55              |
| 1:d:530:ASN:ND2  | 1:d:532:GLN:O    | 2.40                     | 0.55              |
| 1:e:472:THR:HG22 | 1:e:562:ALA:HB1  | 1.88                     | 0.55              |
| 1:f:247:TYR:O    | 1:z:707:GLY:HA2  | 2.07                     | 0.55              |
| 1:h:707:GLY:HA2  | 1:i:247:TYR:O    | 2.07                     | 0.55              |
| 1:s:456:ARG:O    | 1:s:460:THR:HG23 | 2.06                     | 0.55              |
| 1:z:432:ASP:HA   | 1:z:454:ALA:H    | 1.72                     | 0.55              |
| 1:2:707:GLY:HA2  | 1:3:247:TYR:O    | 2.07                     | 0.55              |
| 1:3:707:GLY:HA2  | 1:8:247:TYR:O    | 2.08                     | 0.55              |
| 1:6:530:ASN:ND2  | 1:6:532:GLN:O    | 2.40                     | 0.55              |
| 1:A:373:ARG:O    | 1:A:376:THR:OG1  | 2.19                     | 0.54              |
| 1:G:530:ASN:ND2  | 1:G:532:GLN:O    | 2.40                     | 0.54              |
| 1:H:619:HIS:HA   | 2:4A:997:DA:H2'  | 1.88                     | 0.54              |
| 1:L:707:GLY:HA2  | 1:b:247:TYR:O    | 2.07                     | 0.54              |
| 1:P:373:ARG:O    | 1:P:376:THR:OG1  | 2.19                     | 0.54              |
| 1:X:472:THR:HG22 | 1:X:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:Z:247:TYR:O    | 1:a:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:Z:530:ASN:ND2  | 1:Z:532:GLN:O    | 2.40                     | 0.54              |
| 1:a:432:ASP:HA   | 1:a:454:ALA:H    | 1.72                     | 0.54              |
| 1:i:432:ASP:HA   | 1:i:454:ALA:H    | 1.72                     | 0.54              |
| 1:l:432:ASP:HA   | 1:l:454:ALA:H    | 1.72                     | 0.54              |
| 1:p:247:TYR:O    | 1:6:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:v:247:TYR:O    | 1:1:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:w:432:ASP:HA   | 1:w:454:ALA:H    | 1.72                     | 0.54              |
| 1:w:530:ASN:ND2  | 1:w:532:GLN:O    | 2.40                     | 0.54              |
| 1:y:432:ASP:HA   | 1:y:454:ALA:H    | 1.72                     | 0.54              |
| 1:y:489:PHE:O    | 1:y:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:1:610:LYS:HB2  | 1:1:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:4:432:ASP:HA   | 1:4:454:ALA:H    | 1.72                     | 0.54              |
| 1:5:373:ARG:O    | 1:5:376:THR:OG1  | 2.19                     | 0.54              |
| 1:F:530:ASN:ND2  | 1:F:532:GLN:O    | 2.40                     | 0.54              |
| 1:K:247:TYR:O    | 1:7:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:L:432:ASP:HA   | 1:L:454:ALA:H    | 1.72                     | 0.54              |
| 1:M:432:ASP:HA   | 1:M:454:ALA:H    | 1.72                     | 0.54              |
| 1:P:530:ASN:ND2  | 1:P:532:GLN:O    | 2.40                     | 0.54              |
| 1:P:610:LYS:HB2  | 1:P:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:P:707:GLY:HA2  | 1:Q:247:TYR:O    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:373:ARG:O    | 1:R:376:THR:OG1  | 2.19                     | 0.54              |
| 1:R:432:ASP:HA   | 1:R:454:ALA:H    | 1.72                     | 0.54              |
| 1:R:489:PHE:O    | 1:R:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:S:530:ASN:ND2  | 1:S:532:GLN:O    | 2.40                     | 0.54              |
| 1:W:336:ASP:O    | 1:W:634:PRO:HB3  | 2.06                     | 0.54              |
| 1:b:336:ASP:O    | 1:b:634:PRO:HB3  | 2.06                     | 0.54              |
| 1:b:530:ASN:ND2  | 1:b:532:GLN:O    | 2.40                     | 0.54              |
| 1:e:432:ASP:HA   | 1:e:454:ALA:H    | 1.72                     | 0.54              |
| 1:j:247:TYR:O    | 1:l:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:j:489:PHE:O    | 1:j:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:m:336:ASP:O    | 1:m:634:PRO:HB3  | 2.06                     | 0.54              |
| 1:o:472:THR:HG22 | 1:o:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:p:336:ASP:O    | 1:p:634:PRO:HB3  | 2.06                     | 0.54              |
| 1:p:610:LYS:HB2  | 1:p:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:q:619:HIS:HA   | 2:jA:997:DA:H2'  | 1.88                     | 0.54              |
| 1:r:432:ASP:HA   | 1:r:454:ALA:H    | 1.72                     | 0.54              |
| 1:u:530:ASN:ND2  | 1:u:532:GLN:O    | 2.40                     | 0.54              |
| 1:z:247:TYR:O    | 1:4:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:1:373:ARG:O    | 1:1:376:THR:OG1  | 2.19                     | 0.54              |
| 1:1:530:ASN:ND2  | 1:1:532:GLN:O    | 2.40                     | 0.54              |
| 1:2:472:THR:HG22 | 1:2:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:D:472:THR:HG22 | 1:D:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:D:530:ASN:ND2  | 1:D:532:GLN:O    | 2.40                     | 0.54              |
| 1:E:530:ASN:ND2  | 1:E:532:GLN:O    | 2.40                     | 0.54              |
| 1:M:707:GLY:HA2  | 1:N:247:TYR:O    | 2.08                     | 0.54              |
| 1:O:707:GLY:HA2  | 1:P:247:TYR:O    | 2.07                     | 0.54              |
| 1:Q:330:THR:HG21 | 1:Q:395:MET:HB3  | 1.87                     | 0.54              |
| 1:Q:596:TRP:NE1  | 1:Q:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:S:432:ASP:HA   | 1:S:454:ALA:H    | 1.72                     | 0.54              |
| 1:T:247:TYR:O    | 1:i:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:T:707:GLY:HA2  | 1:U:247:TYR:O    | 2.07                     | 0.54              |
| 1:W:610:LYS:HB2  | 1:W:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:X:456:ARG:O    | 1:X:460:THR:HG23 | 2.06                     | 0.54              |
| 1:Y:432:ASP:HA   | 1:Y:454:ALA:H    | 1.72                     | 0.54              |
| 1:Z:596:TRP:NE1  | 1:Z:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:b:596:TRP:NE1  | 1:b:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:c:432:ASP:HA   | 1:c:454:ALA:H    | 1.72                     | 0.54              |
| 1:d:610:LYS:HB2  | 1:d:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:f:610:LYS:HB2  | 1:f:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:g:707:GLY:HA2  | 1:1:247:TYR:O    | 2.07                     | 0.54              |
| 1:k:610:LYS:HB2  | 1:k:632:PRO:HG3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:l:336:ASP:O    | 1:l:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:o:619:HIS:HA   | 2:hA:997:DA:H2' | 1.88                     | 0.54              |
| 1:q:432:ASP:HA   | 1:q:454:ALA:H   | 1.72                     | 0.54              |
| 1:s:336:ASP:O    | 1:s:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:v:330:THR:HG21 | 1:v:395:MET:HB3 | 1.87                     | 0.54              |
| 1:v:596:TRP:NE1  | 1:v:598:GLU:OE2 | 2.41                     | 0.54              |
| 1:z:610:LYS:HB2  | 1:z:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:E:596:TRP:NE1  | 1:E:598:GLU:OE2 | 2.41                     | 0.54              |
| 1:H:336:ASP:O    | 1:H:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:M:610:LYS:HB2  | 1:M:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:N:610:LYS:HB2  | 1:N:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:T:489:PHE:O    | 1:T:494:ARG:NH1 | 2.37                     | 0.54              |
| 1:V:432:ASP:HA   | 1:V:454:ALA:H   | 1.72                     | 0.54              |
| 1:V:596:TRP:NE1  | 1:V:598:GLU:OE2 | 2.41                     | 0.54              |
| 1:X:247:TYR:O    | 1:f:707:GLY:HA2 | 2.07                     | 0.54              |
| 1:Z:336:ASP:O    | 1:Z:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:b:432:ASP:HA   | 1:b:454:ALA:H   | 1.72                     | 0.54              |
| 1:d:432:ASP:HA   | 1:d:454:ALA:H   | 1.72                     | 0.54              |
| 1:f:336:ASP:O    | 1:f:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:g:610:LYS:HB2  | 1:g:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:h:432:ASP:HA   | 1:h:454:ALA:H   | 1.72                     | 0.54              |
| 1:i:336:ASP:O    | 1:i:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:j:707:GLY:HA2  | 1:x:247:TYR:O   | 2.07                     | 0.54              |
| 1:k:336:ASP:O    | 1:k:634:PRO:HB3 | 2.06                     | 0.54              |
| 1:m:610:LYS:HB2  | 1:m:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:n:432:ASP:HA   | 1:n:454:ALA:H   | 1.72                     | 0.54              |
| 1:o:610:LYS:HB2  | 1:o:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:p:432:ASP:HA   | 1:p:454:ALA:H   | 1.72                     | 0.54              |
| 1:q:610:LYS:HB2  | 1:q:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:t:530:ASN:ND2  | 1:t:532:GLN:O   | 2.40                     | 0.54              |
| 1:u:596:TRP:NE1  | 1:u:598:GLU:OE2 | 2.41                     | 0.54              |
| 1:y:373:ARG:O    | 1:y:376:THR:OG1 | 2.19                     | 0.54              |
| 1:2:530:ASN:ND2  | 1:2:532:GLN:O   | 2.40                     | 0.54              |
| 1:5:247:TYR:O    | 1:8:707:GLY:HA2 | 2.07                     | 0.54              |
| 1:D:247:TYR:O    | 1:E:707:GLY:HA2 | 2.07                     | 0.54              |
| 1:H:610:LYS:HB2  | 1:H:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:O:610:LYS:HB2  | 1:O:632:PRO:HG3 | 1.89                     | 0.54              |
| 1:O:681:LYS:HG3  | 1:m:391:PHE:CZ  | 2.43                     | 0.54              |
| 1:T:530:ASN:ND2  | 1:T:532:GLN:O   | 2.40                     | 0.54              |
| 1:U:530:ASN:ND2  | 1:U:532:GLN:O   | 2.40                     | 0.54              |
| 1:U:707:GLY:HA2  | 1:e:247:TYR:O   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:610:LYS:HB2  | 1:V:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:W:432:ASP:HA   | 1:W:454:ALA:H    | 1.72                     | 0.54              |
| 1:c:530:ASN:ND2  | 1:c:532:GLN:O    | 2.40                     | 0.54              |
| 1:d:336:ASP:O    | 1:d:634:PRO:HB3  | 2.06                     | 0.54              |
| 1:j:432:ASP:HA   | 1:j:454:ALA:H    | 1.72                     | 0.54              |
| 1:j:530:ASN:ND2  | 1:j:532:GLN:O    | 2.40                     | 0.54              |
| 1:m:432:ASP:HA   | 1:m:454:ALA:H    | 1.72                     | 0.54              |
| 1:n:610:LYS:HB2  | 1:n:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:q:596:TRP:NE1  | 1:q:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:r:247:TYR:O    | 1:x:707:GLY:HA2  | 2.08                     | 0.54              |
| 1:s:373:ARG:O    | 1:s:376:THR:OG1  | 2.19                     | 0.54              |
| 1:t:472:THR:HG22 | 1:t:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:u:432:ASP:HA   | 1:u:454:ALA:H    | 1.72                     | 0.54              |
| 1:z:489:PHE:O    | 1:z:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:7:596:TRP:NE1  | 1:7:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:8:513:ASN:ND2  | 1:8:526:THR:HG22 | 2.10                     | 0.54              |
| 1:B:610:LYS:HB2  | 1:B:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:D:373:ARG:O    | 1:D:376:THR:OG1  | 2.19                     | 0.54              |
| 1:F:247:TYR:O    | 1:R:707:GLY:HA2  | 2.08                     | 0.54              |
| 1:F:472:THR:HG22 | 1:F:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:I:596:TRP:NE1  | 1:I:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:N:596:TRP:NE1  | 1:N:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:O:432:ASP:HA   | 1:O:454:ALA:H    | 1.72                     | 0.54              |
| 1:Q:489:PHE:O    | 1:Q:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:V:247:TYR:O    | 1:W:707:GLY:HA2  | 2.07                     | 0.54              |
| 1:Y:530:ASN:ND2  | 1:Y:532:GLN:O    | 2.40                     | 0.54              |
| 1:Z:432:ASP:HA   | 1:Z:454:ALA:H    | 1.72                     | 0.54              |
| 1:f:432:ASP:HA   | 1:f:454:ALA:H    | 1.72                     | 0.54              |
| 1:i:596:TRP:NE1  | 1:i:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:k:432:ASP:HA   | 1:k:454:ALA:H    | 1.72                     | 0.54              |
| 1:m:530:ASN:ND2  | 1:m:532:GLN:O    | 2.40                     | 0.54              |
| 1:o:336:ASP:O    | 1:o:634:PRO:HB3  | 2.06                     | 0.54              |
| 1:o:707:GLY:HA2  | 1:7:247:TYR:O    | 2.07                     | 0.54              |
| 1:r:610:LYS:HB2  | 1:r:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:x:530:ASN:ND2  | 1:x:532:GLN:O    | 2.40                     | 0.54              |
| 1:4:610:LYS:HB2  | 1:4:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:8:610:LYS:HB2  | 1:8:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:A:432:ASP:HA   | 1:A:454:ALA:H    | 1.72                     | 0.54              |
| 1:A:707:GLY:HA2  | 1:E:247:TYR:O    | 2.08                     | 0.54              |
| 1:E:432:ASP:HA   | 1:E:454:ALA:H    | 1.72                     | 0.54              |
| 1:H:707:GLY:HA2  | 1:I:247:TYR:O    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:610:LYS:HB2  | 1:J:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:K:432:ASP:HA   | 1:K:454:ALA:H    | 1.72                     | 0.54              |
| 1:K:610:LYS:HB2  | 1:K:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:L:530:ASN:ND2  | 1:L:532:GLN:O    | 2.40                     | 0.54              |
| 1:M:596:TRP:NE1  | 1:M:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:N:489:PHE:O    | 1:N:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:Q:432:ASP:HA   | 1:Q:454:ALA:H    | 1.72                     | 0.54              |
| 1:T:432:ASP:HA   | 1:T:454:ALA:H    | 1.72                     | 0.54              |
| 1:U:610:LYS:HB2  | 1:U:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:f:391:PHE:CZ   | 1:g:681:LYS:HG3  | 2.43                     | 0.54              |
| 1:f:530:ASN:ND2  | 1:f:532:GLN:O    | 2.40                     | 0.54              |
| 1:g:432:ASP:HA   | 1:g:454:ALA:H    | 1.72                     | 0.54              |
| 1:h:610:LYS:HB2  | 1:h:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:l:596:TRP:NE1  | 1:l:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:m:681:LYS:HG3  | 1:n:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:p:513:ASN:ND2  | 1:p:526:THR:HG22 | 2.10                     | 0.54              |
| 1:t:247:TYR:O    | 1:y:707:GLY:HA2  | 2.08                     | 0.54              |
| 1:u:707:GLY:HA2  | 1:2:247:TYR:O    | 2.07                     | 0.54              |
| 1:x:610:LYS:HB2  | 1:x:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:z:596:TRP:NE1  | 1:z:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:6:432:ASP:HA   | 1:6:454:ALA:H    | 1.72                     | 0.54              |
| 1:F:596:TRP:NE1  | 1:F:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:G:432:ASP:HA   | 1:G:454:ALA:H    | 1.72                     | 0.54              |
| 1:J:432:ASP:HA   | 1:J:454:ALA:H    | 1.72                     | 0.54              |
| 1:Q:610:LYS:HB2  | 1:Q:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:W:681:LYS:HG3  | 1:Y:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:a:530:ASN:ND2  | 1:a:532:GLN:O    | 2.40                     | 0.54              |
| 1:c:391:PHE:CZ   | 1:p:681:LYS:HG3  | 2.43                     | 0.54              |
| 1:c:610:LYS:HB2  | 1:c:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:d:472:THR:HG22 | 1:d:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:e:610:LYS:HB2  | 1:e:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:f:681:LYS:HG3  | 1:h:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:i:610:LYS:HB2  | 1:i:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:t:489:PHE:O    | 1:t:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:v:530:ASN:ND2  | 1:v:532:GLN:O    | 2.40                     | 0.54              |
| 1:1:489:PHE:O    | 1:1:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:2:373:ARG:O    | 1:2:376:THR:OG1  | 2.19                     | 0.54              |
| 1:4:596:TRP:NE1  | 1:4:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:C:619:HIS:HA   | 2:UA:997:DA:H2'  | 1.88                     | 0.54              |
| 1:D:610:LYS:HB2  | 1:D:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:H:247:TYR:O    | 1:Z:707:GLY:HA2  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:681:LYS:HG3  | 1:L:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:K:681:LYS:HG3  | 1:a:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:Q:530:ASN:ND2  | 1:Q:532:GLN:O    | 2.40                     | 0.54              |
| 1:S:707:GLY:HA2  | 1:d:247:TYR:O    | 2.08                     | 0.54              |
| 1:X:373:ARG:O    | 1:X:376:THR:OG1  | 2.19                     | 0.54              |
| 1:e:530:ASN:ND2  | 1:e:532:GLN:O    | 2.40                     | 0.54              |
| 1:i:681:LYS:HG3  | 1:j:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:k:247:TYR:O    | 1:w:707:GLY:HA2  | 2.08                     | 0.54              |
| 1:k:472:THR:HG22 | 1:k:562:ALA:HB1  | 1.88                     | 0.54              |
| 1:p:707:GLY:HA2  | 1:q:247:TYR:O    | 2.07                     | 0.54              |
| 1:t:596:TRP:NE1  | 1:t:598:GLU:OE2  | 2.41                     | 0.54              |
| 1:t:619:HIS:HA   | 2:mA:997:DA:H2'  | 1.88                     | 0.54              |
| 1:v:432:ASP:HA   | 1:v:454:ALA:H    | 1.72                     | 0.54              |
| 1:v:489:PHE:O    | 1:v:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:3:619:HIS:HA   | 2:wA:997:DA:H2'  | 1.88                     | 0.54              |
| 1:5:432:ASP:HA   | 1:5:454:ALA:H    | 1.72                     | 0.54              |
| 1:5:530:ASN:ND2  | 1:5:532:GLN:O    | 2.40                     | 0.54              |
| 1:A:530:ASN:ND2  | 1:A:532:GLN:O    | 2.40                     | 0.54              |
| 1:B:513:ASN:ND2  | 1:B:526:THR:HG22 | 2.10                     | 0.54              |
| 1:E:610:LYS:HB2  | 1:E:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:F:619:HIS:HA   | 2:1A:997:DA:H2'  | 1.88                     | 0.54              |
| 1:I:619:HIS:HA   | 2:5A:997:DA:H2'  | 1.88                     | 0.54              |
| 1:L:610:LYS:HB2  | 1:L:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:P:489:PHE:O    | 1:P:494:ARG:NH1  | 2.37                     | 0.54              |
| 1:T:391:PHE:CZ   | 1:l:681:LYS:HG3  | 2.43                     | 0.54              |
| 1:U:619:HIS:HA   | 2:LA:997:DA:H2'  | 1.88                     | 0.54              |
| 1:W:513:ASN:ND2  | 1:W:526:THR:HG22 | 2.10                     | 0.54              |
| 1:X:610:LYS:HB2  | 1:X:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:Y:610:LYS:HB2  | 1:Y:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:b:707:GLY:HA2  | 1:o:247:TYR:O    | 2.07                     | 0.54              |
| 1:l:610:LYS:HB2  | 1:l:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:r:530:ASN:ND2  | 1:r:532:GLN:O    | 2.40                     | 0.54              |
| 1:r:681:LYS:HG3  | 1:s:391:PHE:CZ   | 2.43                     | 0.54              |
| 1:s:610:LYS:HB2  | 1:s:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:u:610:LYS:HB2  | 1:u:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:w:610:LYS:HB2  | 1:w:632:PRO:HG3  | 1.89                     | 0.54              |
| 1:x:619:HIS:HA   | 2:rA:997:DA:H2'  | 1.88                     | 0.54              |
| 1:5:391:PHE:CZ   | 1:7:681:LYS:HG3  | 2.43                     | 0.54              |
| 1:F:489:PHE:O    | 1:F:494:ARG:NH1  | 2.37                     | 0.53              |
| 1:L:619:HIS:HA   | 2:BA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:S:610:LYS:HB2  | 1:S:632:PRO:HG3  | 1.89                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:X:432:ASP:HA  | 1:X:454:ALA:H    | 1.72                     | 0.53              |
| 1:X:530:ASN:ND2 | 1:X:532:GLN:O    | 2.40                     | 0.53              |
| 1:a:610:LYS:HB2 | 1:a:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:a:619:HIS:HA  | 2:RA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:c:596:TRP:NE1 | 1:c:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:c:619:HIS:HA  | 2:TA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:d:619:HIS:HA  | 2:VA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:h:596:TRP:NE1 | 1:h:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:j:610:LYS:HB2 | 1:j:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:k:619:HIS:HA  | 2:cA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:m:489:PHE:O   | 1:m:494:ARG:NH1  | 2.37                     | 0.53              |
| 1:m:513:ASN:ND2 | 1:m:526:THR:HG22 | 2.10                     | 0.53              |
| 1:s:530:ASN:ND2 | 1:s:532:GLN:O    | 2.40                     | 0.53              |
| 1:s:596:TRP:NE1 | 1:s:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:v:610:LYS:HB2 | 1:v:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:v:707:GLY:HA2 | 1:w:247:TYR:O    | 2.07                     | 0.53              |
| 1:3:596:TRP:NE1 | 1:3:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:6:610:LYS:HB2 | 1:6:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:7:432:ASP:HA  | 1:7:454:ALA:H    | 1.72                     | 0.53              |
| 1:A:247:TYR:O   | 1:B:707:GLY:HA2  | 2.08                     | 0.53              |
| 1:C:596:TRP:NE1 | 1:C:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:D:596:TRP:NE1 | 1:D:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:G:610:LYS:HB2 | 1:G:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:X:391:PHE:CZ  | 1:e:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:Y:619:HIS:HA  | 2:PA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:a:596:TRP:NE1 | 1:a:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:c:328:THR:CG2 | 1:s:310:GLN:HG2  | 2.38                     | 0.53              |
| 1:n:596:TRP:NE1 | 1:n:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:o:681:LYS:HG3 | 1:p:391:PHE:CZ   | 2.43                     | 0.53              |
| 1:q:342:PRO:HB3 | 1:s:421:GLN:NE2  | 2.23                     | 0.53              |
| 1:s:432:ASP:HA  | 1:s:454:ALA:H    | 1.72                     | 0.53              |
| 1:w:391:PHE:CZ  | 1:y:681:LYS:HG3  | 2.43                     | 0.53              |
| 1:2:610:LYS:HB2 | 1:2:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:3:610:LYS:HB2 | 1:3:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:C:610:LYS:HB2 | 1:C:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:C:681:LYS:HG3 | 1:b:391:PHE:CZ   | 2.43                     | 0.53              |
| 1:H:681:LYS:HG3 | 1:W:391:PHE:CZ   | 2.44                     | 0.53              |
| 1:I:432:ASP:HA  | 1:I:454:ALA:H    | 1.72                     | 0.53              |
| 1:L:596:TRP:NE1 | 1:L:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:O:489:PHE:O   | 1:O:494:ARG:NH1  | 2.37                     | 0.53              |
| 1:Q:707:GLY:HA2 | 1:S:247:TYR:O    | 2.07                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:R:681:LYS:HG3 | 1:S:391:PHE:CZ   | 2.44                     | 0.53              |
| 1:T:610:LYS:HB2 | 1:T:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:X:596:TRP:NE1 | 1:X:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:Y:596:TRP:NE1 | 1:Y:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:f:489:PHE:O   | 1:f:494:ARG:NH1  | 2.37                     | 0.53              |
| 1:o:432:ASP:HA  | 1:o:454:ALA:H    | 1.72                     | 0.53              |
| 1:2:596:TRP:NE1 | 1:2:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:5:610:LYS:HB2 | 1:5:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:7:619:HIS:HA  | 2:0A:997:DA:H2'  | 1.88                     | 0.53              |
| 1:A:391:PHE:CZ  | 1:I:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:A:610:LYS:HB2 | 1:A:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:B:619:HIS:HA  | 2:JA:997:DA:H2'  | 1.88                     | 0.53              |
| 1:C:432:ASP:HA  | 1:C:454:ALA:H    | 1.72                     | 0.53              |
| 1:H:391:PHE:CZ  | 1:Y:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:R:391:PHE:CZ  | 1:U:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:Z:391:PHE:CZ  | 1:3:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:c:681:LYS:HG3 | 1:o:391:PHE:CZ   | 2.44                     | 0.53              |
| 1:g:489:PHE:O   | 1:g:494:ARG:NH1  | 2.37                     | 0.53              |
| 1:x:681:LYS:HG3 | 1:y:391:PHE:CZ   | 2.44                     | 0.53              |
| 1:C:391:PHE:CZ  | 1:M:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:E:391:PHE:CZ  | 1:F:681:LYS:HG3  | 2.43                     | 0.53              |
| 1:F:391:PHE:CZ  | 1:Q:681:LYS:HG3  | 2.43                     | 0.53              |
| 1:H:432:ASP:HA  | 1:H:454:ALA:H    | 1.72                     | 0.53              |
| 1:U:596:TRP:NE1 | 1:U:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:V:391:PHE:CZ  | 1:X:681:LYS:HG3  | 2.43                     | 0.53              |
| 1:f:513:ASN:ND2 | 1:f:526:THR:HG22 | 2.10                     | 0.53              |
| 1:j:681:LYS:HG3 | 1:k:391:PHE:CZ   | 2.43                     | 0.53              |
| 1:q:681:LYS:HG3 | 1:r:391:PHE:CZ   | 2.44                     | 0.53              |
| 1:r:596:TRP:NE1 | 1:r:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:s:489:PHE:O   | 1:s:494:ARG:NH1  | 2.37                     | 0.53              |
| 1:t:391:PHE:CZ  | 1:v:681:LYS:HG3  | 2.43                     | 0.53              |
| 1:t:681:LYS:HG3 | 1:u:391:PHE:CZ   | 2.43                     | 0.53              |
| 1:x:596:TRP:NE1 | 1:x:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:3:391:PHE:CZ  | 1:4:681:LYS:HG3  | 2.44                     | 0.53              |
| 1:3:432:ASP:HA  | 1:3:454:ALA:H    | 1.72                     | 0.53              |
| 1:5:681:LYS:HG3 | 1:6:391:PHE:CZ   | 2.43                     | 0.53              |
| 1:B:596:TRP:NE1 | 1:B:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:E:681:LYS:HG3 | 1:Q:391:PHE:CZ   | 2.44                     | 0.53              |
| 1:I:610:LYS:HB2 | 1:I:632:PRO:HG3  | 1.89                     | 0.53              |
| 1:K:596:TRP:NE1 | 1:K:598:GLU:OE2  | 2.41                     | 0.53              |
| 1:T:681:LYS:HG3 | 1:d:391:PHE:CZ   | 2.44                     | 0.53              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:X:489:PHE:O   | 1:X:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:e:596:TRP:NE1 | 1:e:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:t:610:LYS:HB2 | 1:t:632:PRO:HG3 | 1.89                     | 0.53              |
| 1:1:432:ASP:HA  | 1:1:454:ALA:H   | 1.72                     | 0.53              |
| 1:8:596:TRP:NE1 | 1:8:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:8:619:HIS:HA  | 2:2A:997:DA:H2' | 1.88                     | 0.53              |
| 1:P:432:ASP:HA  | 1:P:454:ALA:H   | 1.72                     | 0.53              |
| 1:V:681:LYS:HG3 | 1:e:391:PHE:CZ  | 2.44                     | 0.53              |
| 1:a:681:LYS:HG3 | 1:8:391:PHE:CZ  | 2.44                     | 0.53              |
| 1:k:596:TRP:NE1 | 1:k:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:u:681:LYS:HG3 | 1:v:391:PHE:CZ  | 2.44                     | 0.53              |
| 1:7:610:LYS:HB2 | 1:7:632:PRO:HG3 | 1.89                     | 0.53              |
| 1:A:619:HIS:HA  | 2:0:997:DA:H2'  | 1.88                     | 0.53              |
| 1:B:391:PHE:CZ  | 1:L:681:LYS:HG3 | 2.44                     | 0.53              |
| 1:F:610:LYS:HB2 | 1:F:632:PRO:HG3 | 1.89                     | 0.53              |
| 1:J:596:TRP:NE1 | 1:J:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:K:619:HIS:HA  | 2:AA:997:DA:H2' | 1.88                     | 0.53              |
| 1:R:596:TRP:NE1 | 1:R:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:R:610:LYS:HB2 | 1:R:632:PRO:HG3 | 1.89                     | 0.53              |
| 1:T:596:TRP:NE1 | 1:T:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:W:596:TRP:NE1 | 1:W:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:a:489:PHE:O   | 1:a:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:j:596:TRP:NE1 | 1:j:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:p:596:TRP:NE1 | 1:p:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:J:619:HIS:HA  | 2:9:997:DA:H2'  | 1.88                     | 0.53              |
| 1:L:489:PHE:O   | 1:L:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:M:391:PHE:CZ  | 1:b:681:LYS:HG3 | 2.44                     | 0.53              |
| 1:N:681:LYS:HG3 | 1:P:391:PHE:CZ  | 2.43                     | 0.53              |
| 1:O:421:GLN:NE2 | 1:m:342:PRO:HB3 | 2.24                     | 0.53              |
| 1:O:619:HIS:HA  | 2:EA:997:DA:H2' | 1.88                     | 0.53              |
| 1:P:596:TRP:NE1 | 1:P:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:b:373:ARG:O   | 1:b:376:THR:OG1 | 2.19                     | 0.53              |
| 1:d:596:TRP:NE1 | 1:d:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:f:342:PRO:HB3 | 1:g:421:GLN:NE2 | 2.24                     | 0.53              |
| 1:q:421:GLN:NE2 | 1:r:342:PRO:HB3 | 2.24                     | 0.53              |
| 1:x:432:ASP:HA  | 1:x:454:ALA:H   | 1.72                     | 0.53              |
| 1:y:610:LYS:HB2 | 1:y:632:PRO:HG3 | 1.89                     | 0.53              |
| 1:1:596:TRP:NE1 | 1:1:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:D:489:PHE:O   | 1:D:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:E:489:PHE:O   | 1:E:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:J:373:ARG:O   | 1:J:376:THR:OG1 | 2.19                     | 0.53              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:U:432:ASP:HA  | 1:U:454:ALA:H   | 1.72                     | 0.53              |
| 1:V:421:GLN:NE2 | 1:e:342:PRO:HB3 | 2.24                     | 0.53              |
| 1:h:373:ARG:O   | 1:h:376:THR:OG1 | 2.19                     | 0.53              |
| 1:h:489:PHE:O   | 1:h:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:m:310:GLN:HG2 | 1:s:328:THR:CG2 | 2.39                     | 0.53              |
| 1:n:373:ARG:O   | 1:n:376:THR:OG1 | 2.19                     | 0.53              |
| 1:y:596:TRP:NE1 | 1:y:598:GLU:OE2 | 2.41                     | 0.53              |
| 1:2:489:PHE:O   | 1:2:494:ARG:NH1 | 2.37                     | 0.53              |
| 1:G:681:LYS:HG3 | 1:I:391:PHE:CZ  | 2.43                     | 0.52              |
| 1:S:489:PHE:O   | 1:S:494:ARG:NH1 | 2.37                     | 0.52              |
| 1:Z:681:LYS:HG3 | 1:4:391:PHE:CZ  | 2.44                     | 0.52              |
| 1:g:619:HIS:HA  | 2:YA:997:DA:H2' | 1.88                     | 0.52              |
| 1:n:489:PHE:O   | 1:n:494:ARG:NH1 | 2.37                     | 0.52              |
| 1:M:328:THR:CG2 | 1:c:310:GLN:HG2 | 2.40                     | 0.52              |
| 1:X:310:GLN:HG2 | 1:Y:328:THR:CG2 | 2.39                     | 0.52              |
| 1:z:681:LYS:HG3 | 1:1:391:PHE:CZ  | 2.44                     | 0.52              |
| 1:1:681:LYS:HG3 | 1:2:391:PHE:CZ  | 2.44                     | 0.52              |
| 1:A:681:LYS:HG3 | 1:G:391:PHE:CZ  | 2.44                     | 0.52              |
| 1:B:421:GLN:NE2 | 1:J:342:PRO:HB3 | 2.24                     | 0.52              |
| 1:C:328:THR:CG2 | 1:D:310:GLN:HG2 | 2.40                     | 0.52              |
| 1:D:391:PHE:CZ  | 1:P:681:LYS:HG3 | 2.44                     | 0.52              |
| 1:K:342:PRO:HB3 | 1:8:421:GLN:NE2 | 2.24                     | 0.52              |
| 1:N:421:GLN:NE2 | 1:P:342:PRO:HB3 | 2.24                     | 0.52              |
| 1:O:391:PHE:CZ  | 1:n:681:LYS:HG3 | 2.43                     | 0.52              |
| 1:Z:342:PRO:HB3 | 1:3:421:GLN:NE2 | 2.25                     | 0.52              |
| 1:g:342:PRO:HB3 | 1:h:421:GLN:NE2 | 2.24                     | 0.52              |
| 1:g:391:PHE:CZ  | 1:h:681:LYS:HG3 | 2.43                     | 0.52              |
| 1:1:421:GLN:NE2 | 1:2:342:PRO:HB3 | 2.24                     | 0.52              |
| 1:2:310:GLN:HG2 | 1:3:328:THR:CG2 | 2.40                     | 0.52              |
| 1:5:342:PRO:HB3 | 1:7:421:GLN:NE2 | 2.24                     | 0.52              |
| 1:6:619:HIS:HA  | 2:zA:997:DA:H2' | 1.88                     | 0.52              |
| 1:6:681:LYS:HG3 | 1:7:391:PHE:CZ  | 2.43                     | 0.52              |
| 1:C:421:GLN:NE2 | 1:b:342:PRO:HB3 | 2.25                     | 0.52              |
| 1:D:342:PRO:HB3 | 1:P:421:GLN:NE2 | 2.24                     | 0.52              |
| 1:E:476:ASN:ND2 | 1:E:520:THR:OG1 | 2.43                     | 0.52              |
| 1:K:373:ARG:O   | 1:K:376:THR:OG1 | 2.19                     | 0.52              |
| 1:O:342:PRO:HB3 | 1:n:421:GLN:NE2 | 2.24                     | 0.52              |
| 1:R:342:PRO:HB3 | 1:U:421:GLN:NE2 | 2.25                     | 0.52              |
| 1:S:681:LYS:HG3 | 1:U:391:PHE:CZ  | 2.43                     | 0.52              |
| 1:W:421:GLN:NE2 | 1:Y:342:PRO:HB3 | 2.25                     | 0.52              |
| 1:Z:373:ARG:O   | 1:Z:376:THR:OG1 | 2.19                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:c:342:PRO:HB3 | 1:p:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:i:421:GLN:NE2 | 1:j:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:n:328:THR:CG2 | 1:r:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:u:489:PHE:O   | 1:u:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:v:373:ARG:O   | 1:v:376:THR:OG1  | 2.19                     | 0.52              |
| 1:w:421:GLN:NE2 | 1:x:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:x:421:GLN:NE2 | 1:y:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:z:391:PHE:CZ  | 1:2:681:LYS:HG3  | 2.43                     | 0.52              |
| 1:z:421:GLN:NE2 | 1:1:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:3:310:GLN:HG2 | 1:8:328:THR:CG2  | 2.40                     | 0.52              |
| 1:6:421:GLN:NE2 | 1:7:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:B:328:THR:CG2 | 1:C:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:B:476:ASN:ND2 | 1:B:520:THR:OG1  | 2.43                     | 0.52              |
| 1:C:476:ASN:ND2 | 1:C:520:THR:OG1  | 2.43                     | 0.52              |
| 1:F:342:PRO:HB3 | 1:Q:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:G:421:GLN:NE2 | 1:I:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:K:391:PHE:CZ  | 1:8:681:LYS:HG3  | 2.44                     | 0.52              |
| 1:M:476:ASN:ND2 | 1:M:520:THR:OG1  | 2.43                     | 0.52              |
| 1:O:476:ASN:ND2 | 1:O:520:THR:OG1  | 2.43                     | 0.52              |
| 1:O:596:TRP:NE1 | 1:O:598:GLU:OE2  | 2.41                     | 0.52              |
| 1:S:421:GLN:NE2 | 1:U:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:T:342:PRO:HB3 | 1:l:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:V:328:THR:CG2 | 1:W:310:GLN:HG2  | 2.39                     | 0.52              |
| 1:V:342:PRO:HB3 | 1:X:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:Z:476:ASN:ND2 | 1:Z:520:THR:OG1  | 2.43                     | 0.52              |
| 1:e:310:GLN:HG2 | 1:h:328:THR:CG2  | 2.40                     | 0.52              |
| 1:g:476:ASN:ND2 | 1:g:520:THR:OG1  | 2.43                     | 0.52              |
| 1:t:310:GLN:HG2 | 1:6:328:THR:CG2  | 2.40                     | 0.52              |
| 1:t:342:PRO:HB3 | 1:v:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:u:476:ASN:ND2 | 1:u:520:THR:OG1  | 2.43                     | 0.52              |
| 1:v:619:HIS:HA  | 2:oA:997:DA:H2'  | 1.88                     | 0.52              |
| 1:w:489:PHE:O   | 1:w:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:w:681:LYS:HG3 | 1:x:391:PHE:CZ   | 2.43                     | 0.52              |
| 1:y:513:ASN:ND2 | 1:y:526:THR:HG22 | 2.10                     | 0.52              |
| 1:3:476:ASN:ND2 | 1:3:520:THR:OG1  | 2.43                     | 0.52              |
| 1:4:476:ASN:ND2 | 1:4:520:THR:OG1  | 2.43                     | 0.52              |
| 1:5:328:THR:CG2 | 1:8:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:F:310:GLN:HG2 | 1:G:328:THR:CG2  | 2.40                     | 0.52              |
| 1:F:513:ASN:ND2 | 1:F:526:THR:HG22 | 2.10                     | 0.52              |
| 1:G:476:ASN:ND2 | 1:G:520:THR:OG1  | 2.43                     | 0.52              |
| 1:G:489:PHE:O   | 1:G:494:ARG:NH1  | 2.37                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:619:HIS:HA  | 2:3A:997:DA:H2'  | 1.88                     | 0.52              |
| 1:H:596:TRP:NE1 | 1:H:598:GLU:OE2  | 2.41                     | 0.52              |
| 1:J:489:PHE:O   | 1:J:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:P:476:ASN:ND2 | 1:P:520:THR:OG1  | 2.43                     | 0.52              |
| 1:P:619:HIS:HA  | 2:FA:997:DA:H2'  | 1.88                     | 0.52              |
| 1:T:476:ASN:ND2 | 1:T:520:THR:OG1  | 2.43                     | 0.52              |
| 1:X:476:ASN:ND2 | 1:X:520:THR:OG1  | 2.43                     | 0.52              |
| 1:b:476:ASN:ND2 | 1:b:520:THR:OG1  | 2.43                     | 0.52              |
| 1:j:476:ASN:ND2 | 1:j:520:THR:OG1  | 2.43                     | 0.52              |
| 1:p:310:GLN:HG2 | 1:q:328:THR:CG2  | 2.39                     | 0.52              |
| 1:p:476:ASN:ND2 | 1:p:520:THR:OG1  | 2.43                     | 0.52              |
| 1:s:476:ASN:ND2 | 1:s:520:THR:OG1  | 2.43                     | 0.52              |
| 1:t:513:ASN:ND2 | 1:t:526:THR:HG22 | 2.10                     | 0.52              |
| 1:4:373:ARG:O   | 1:4:376:THR:OG1  | 2.19                     | 0.52              |
| 1:5:421:GLN:NE2 | 1:6:342:PRO:HB3  | 2.24                     | 0.52              |
| 1:6:476:ASN:ND2 | 1:6:520:THR:OG1  | 2.43                     | 0.52              |
| 1:8:476:ASN:ND2 | 1:8:520:THR:OG1  | 2.43                     | 0.52              |
| 1:B:681:LYS:HG3 | 1:J:391:PHE:CZ   | 2.44                     | 0.52              |
| 1:D:681:LYS:HG3 | 1:N:391:PHE:CZ   | 2.43                     | 0.52              |
| 1:G:596:TRP:NE1 | 1:G:598:GLU:OE2  | 2.41                     | 0.52              |
| 1:J:476:ASN:ND2 | 1:J:520:THR:OG1  | 2.43                     | 0.52              |
| 1:K:476:ASN:ND2 | 1:K:520:THR:OG1  | 2.43                     | 0.52              |
| 1:L:476:ASN:ND2 | 1:L:520:THR:OG1  | 2.43                     | 0.52              |
| 1:Q:310:GLN:HG2 | 1:S:328:THR:CG2  | 2.40                     | 0.52              |
| 1:Q:619:HIS:HA  | 2:GA:997:DA:H2'  | 1.88                     | 0.52              |
| 1:R:513:ASN:ND2 | 1:R:526:THR:HG22 | 2.10                     | 0.52              |
| 1:a:421:GLN:NE2 | 1:8:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:d:421:GLN:NE2 | 1:l:342:PRO:HB3  | 2.24                     | 0.52              |
| 1:g:596:TRP:NE1 | 1:g:598:GLU:OE2  | 2.41                     | 0.52              |
| 1:q:486:VAL:HB  | 1:s:441:THR:HG22 | 1.92                     | 0.52              |
| 1:u:310:GLN:HG2 | 1:2:328:THR:CG2  | 2.40                     | 0.52              |
| 1:u:328:THR:CG2 | 1:5:310:GLN:HG2  | 2.39                     | 0.52              |
| 1:y:476:ASN:ND2 | 1:y:520:THR:OG1  | 2.43                     | 0.52              |
| 1:1:619:HIS:HA  | 2:uA:997:DA:H2'  | 1.88                     | 0.52              |
| 1:6:596:TRP:NE1 | 1:6:598:GLU:OE2  | 2.41                     | 0.52              |
| 1:A:310:GLN:HG2 | 1:E:328:THR:CG2  | 2.39                     | 0.52              |
| 1:B:342:PRO:HB3 | 1:L:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:C:488:ALA:HB3 | 1:M:439:VAL:O    | 2.10                     | 0.52              |
| 1:E:421:GLN:NE2 | 1:Q:342:PRO:HB3  | 2.24                     | 0.52              |
| 1:K:489:PHE:O   | 1:K:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:Q:476:ASN:ND2 | 1:Q:520:THR:OG1  | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:476:ASN:ND2  | 1:R:520:THR:OG1  | 2.43                     | 0.52              |
| 1:W:439:VAL:O    | 1:Y:488:ALA:HB3  | 2.10                     | 0.52              |
| 1:W:476:ASN:ND2  | 1:W:520:THR:OG1  | 2.43                     | 0.52              |
| 1:Z:328:THR:CG2  | 1:a:310:GLN:HG2  | 2.39                     | 0.52              |
| 1:a:476:ASN:ND2  | 1:a:520:THR:OG1  | 2.43                     | 0.52              |
| 1:c:488:ALA:HB3  | 1:p:439:VAL:O    | 2.10                     | 0.52              |
| 1:j:421:GLN:NE2  | 1:k:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:o:596:TRP:NE1  | 1:o:598:GLU:OE2  | 2.41                     | 0.52              |
| 1:p:328:THR:CG2  | 1:6:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:v:310:GLN:HG2  | 1:w:328:THR:CG2  | 2.40                     | 0.52              |
| 1:v:476:ASN:ND2  | 1:v:520:THR:OG1  | 2.43                     | 0.52              |
| 1:1:476:ASN:ND2  | 1:1:520:THR:OG1  | 2.43                     | 0.52              |
| 1:3:488:ALA:HB3  | 1:4:439:VAL:O    | 2.10                     | 0.52              |
| 1:5:486:VAL:HB   | 1:7:441:THR:HG22 | 1.92                     | 0.52              |
| 1:D:328:THR:CG2  | 1:E:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:G:310:GLN:HG2  | 1:W:328:THR:CG2  | 2.40                     | 0.52              |
| 1:H:476:ASN:ND2  | 1:H:520:THR:OG1  | 2.43                     | 0.52              |
| 1:J:439:VAL:O    | 1:L:488:ALA:HB3  | 2.10                     | 0.52              |
| 1:L:310:GLN:HG2  | 1:b:328:THR:CG2  | 2.40                     | 0.52              |
| 1:O:328:THR:CG2  | 1:d:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:T:310:GLN:HG2  | 1:U:328:THR:CG2  | 2.40                     | 0.52              |
| 1:T:421:GLN:NE2  | 1:d:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:T:441:THR:HG22 | 1:d:486:VAL:HB   | 1.92                     | 0.52              |
| 1:V:488:ALA:HB3  | 1:X:439:VAL:O    | 2.10                     | 0.52              |
| 1:Y:476:ASN:ND2  | 1:Y:520:THR:OG1  | 2.43                     | 0.52              |
| 1:c:489:PHE:O    | 1:c:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:d:681:LYS:HG3  | 1:l:391:PHE:CZ   | 2.44                     | 0.52              |
| 1:i:342:PRO:HB3  | 1:k:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:i:391:PHE:CZ   | 1:k:681:LYS:HG3  | 2.44                     | 0.52              |
| 1:j:441:THR:HG22 | 1:k:486:VAL:HB   | 1.92                     | 0.52              |
| 1:q:310:GLN:HG2  | 1:y:328:THR:CG2  | 2.40                     | 0.52              |
| 1:q:391:PHE:CZ   | 1:s:681:LYS:HG3  | 2.45                     | 0.52              |
| 1:r:439:VAL:O    | 1:s:488:ALA:HB3  | 2.10                     | 0.52              |
| 1:t:486:VAL:HB   | 1:v:441:THR:HG22 | 1.92                     | 0.52              |
| 1:2:513:ASN:ND2  | 1:2:526:THR:HG22 | 2.10                     | 0.52              |
| 1:3:342:PRO:HB3  | 1:4:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:6:489:PHE:O    | 1:6:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:A:486:VAL:HB   | 1:I:441:THR:HG22 | 1.92                     | 0.52              |
| 1:D:421:GLN:NE2  | 1:N:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:D:513:ASN:ND2  | 1:D:526:THR:HG22 | 2.10                     | 0.52              |
| 1:F:486:VAL:HB   | 1:Q:441:THR:HG22 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:342:PRO:HB3  | 1:Y:421:GLN:NE2  | 2.24                     | 0.52              |
| 1:H:421:GLN:NE2  | 1:W:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:K:421:GLN:NE2  | 1:a:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:K:439:VAL:O    | 1:a:488:ALA:HB3  | 2.10                     | 0.52              |
| 1:M:342:PRO:HB3  | 1:b:421:GLN:NE2  | 2.25                     | 0.52              |
| 1:M:373:ARG:O    | 1:M:376:THR:OG1  | 2.19                     | 0.52              |
| 1:M:489:PHE:O    | 1:M:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:R:328:THR:CG2  | 1:V:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:R:488:ALA:HB3  | 1:U:439:VAL:O    | 2.10                     | 0.52              |
| 1:U:476:ASN:ND2  | 1:U:520:THR:OG1  | 2.43                     | 0.52              |
| 1:V:476:ASN:ND2  | 1:V:520:THR:OG1  | 2.43                     | 0.52              |
| 1:X:513:ASN:ND2  | 1:X:526:THR:HG22 | 2.10                     | 0.52              |
| 1:Z:421:GLN:NE2  | 1:4:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:d:489:PHE:O    | 1:d:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:g:328:THR:CG2  | 1:k:310:GLN:HG2  | 2.40                     | 0.52              |
| 1:j:310:GLN:HG2  | 1:x:328:THR:CG2  | 2.39                     | 0.52              |
| 1:m:476:ASN:ND2  | 1:m:520:THR:OG1  | 2.43                     | 0.52              |
| 1:o:421:GLN:NE2  | 1:p:342:PRO:HB3  | 2.25                     | 0.52              |
| 1:o:476:ASN:ND2  | 1:o:520:THR:OG1  | 2.43                     | 0.52              |
| 1:q:476:ASN:ND2  | 1:q:520:THR:OG1  | 2.43                     | 0.52              |
| 1:u:421:GLN:NE2  | 1:v:342:PRO:HB3  | 2.24                     | 0.52              |
| 1:x:476:ASN:ND2  | 1:x:520:THR:OG1  | 2.43                     | 0.52              |
| 1:4:489:PHE:O    | 1:4:494:ARG:NH1  | 2.37                     | 0.52              |
| 1:A:342:PRO:HB3  | 1:I:421:GLN:NE2  | 2.25                     | 0.51              |
| 1:C:342:PRO:HB3  | 1:M:421:GLN:NE2  | 2.25                     | 0.51              |
| 1:F:373:ARG:O    | 1:F:376:THR:OG1  | 2.19                     | 0.51              |
| 1:H:328:THR:CG2  | 1:Z:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:N:476:ASN:ND2  | 1:N:520:THR:OG1  | 2.43                     | 0.51              |
| 1:V:486:VAL:HB   | 1:X:441:THR:HG22 | 1.92                     | 0.51              |
| 1:X:328:THR:CG2  | 1:f:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:X:342:PRO:HB3  | 1:e:421:GLN:NE2  | 2.25                     | 0.51              |
| 1:Y:489:PHE:O    | 1:Y:494:ARG:NH1  | 2.37                     | 0.51              |
| 1:b:310:GLN:HG2  | 1:o:328:THR:CG2  | 2.40                     | 0.51              |
| 1:c:421:GLN:NE2  | 1:o:342:PRO:HB3  | 2.24                     | 0.51              |
| 1:c:476:ASN:ND2  | 1:c:520:THR:OG1  | 2.43                     | 0.51              |
| 1:f:476:ASN:ND2  | 1:f:520:THR:OG1  | 2.43                     | 0.51              |
| 1:p:619:HIS:HA   | 2:iA:997:DA:H2'  | 1.88                     | 0.51              |
| 1:w:441:THR:HG22 | 1:x:486:VAL:HB   | 1.92                     | 0.51              |
| 1:x:439:VAL:O    | 1:y:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:A:328:THR:CG2  | 1:B:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:A:421:GLN:NE2  | 1:G:342:PRO:HB3  | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:489:PHE:O    | 1:A:494:ARG:NH1  | 2.37                     | 0.51              |
| 1:A:596:TRP:NE1  | 1:A:598:GLU:OE2  | 2.41                     | 0.51              |
| 1:C:439:VAL:O    | 1:b:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:J:421:GLN:NE2  | 1:L:342:PRO:HB3  | 2.25                     | 0.51              |
| 1:N:310:GLN:HG2  | 1:m:328:THR:CG2  | 2.40                     | 0.51              |
| 1:O:439:VAL:O    | 1:m:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:S:596:TRP:NE1  | 1:S:598:GLU:OE2  | 2.41                     | 0.51              |
| 1:T:328:THR:CG2  | 1:i:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:T:486:VAL:HB   | 1:l:441:THR:HG22 | 1.92                     | 0.51              |
| 1:Z:619:HIS:HA   | 2:QA:997:DA:H2'  | 1.88                     | 0.51              |
| 1:e:489:PHE:O    | 1:e:494:ARG:NH1  | 2.37                     | 0.51              |
| 1:f:441:THR:HG22 | 1:h:486:VAL:HB   | 1.92                     | 0.51              |
| 1:f:488:ALA:HB3  | 1:g:439:VAL:O    | 2.11                     | 0.51              |
| 1:f:596:TRP:NE1  | 1:f:598:GLU:OE2  | 2.41                     | 0.51              |
| 1:h:476:ASN:ND2  | 1:h:520:THR:OG1  | 2.43                     | 0.51              |
| 1:i:441:THR:HG22 | 1:j:486:VAL:HB   | 1.92                     | 0.51              |
| 1:l:328:THR:CG2  | 1:n:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:m:421:GLN:NE2  | 1:n:342:PRO:HB3  | 2.24                     | 0.51              |
| 1:m:441:THR:HG22 | 1:n:486:VAL:HB   | 1.92                     | 0.51              |
| 1:n:476:ASN:ND2  | 1:n:520:THR:OG1  | 2.43                     | 0.51              |
| 1:z:342:PRO:HB3  | 1:2:421:GLN:NE2  | 2.25                     | 0.51              |
| 1:z:476:ASN:ND2  | 1:z:520:THR:OG1  | 2.43                     | 0.51              |
| 1:5:439:VAL:O    | 1:6:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:D:439:VAL:O    | 1:N:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:D:486:VAL:HB   | 1:P:441:THR:HG22 | 1.92                     | 0.51              |
| 1:K:488:ALA:HB3  | 1:8:439:VAL:O    | 2.11                     | 0.51              |
| 1:S:441:THR:HG22 | 1:U:486:VAL:HB   | 1.92                     | 0.51              |
| 1:Z:488:ALA:HB3  | 1:3:439:VAL:O    | 2.10                     | 0.51              |
| 1:a:439:VAL:O    | 1:8:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:f:421:GLN:NE2  | 1:h:342:PRO:HB3  | 2.24                     | 0.51              |
| 1:f:486:VAL:HB   | 1:g:441:THR:HG22 | 1.92                     | 0.51              |
| 1:h:310:GLN:HG2  | 1:i:328:THR:CG2  | 2.40                     | 0.51              |
| 1:i:476:ASN:ND2  | 1:i:520:THR:OG1  | 2.43                     | 0.51              |
| 1:j:328:THR:CG2  | 1:l:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:k:513:ASN:ND2  | 1:k:526:THR:HG22 | 2.10                     | 0.51              |
| 1:l:476:ASN:ND2  | 1:l:520:THR:OG1  | 2.43                     | 0.51              |
| 1:q:373:ARG:O    | 1:q:376:THR:OG1  | 2.19                     | 0.51              |
| 1:r:421:GLN:NE2  | 1:s:342:PRO:HB3  | 2.25                     | 0.51              |
| 1:r:476:ASN:ND2  | 1:r:520:THR:OG1  | 2.43                     | 0.51              |
| 1:w:476:ASN:ND2  | 1:w:520:THR:OG1  | 2.43                     | 0.51              |
| 1:z:488:ALA:HB3  | 1:2:439:VAL:O    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:476:ASN:ND2  | 1:2:520:THR:OG1  | 2.43                     | 0.51              |
| 1:5:489:PHE:O    | 1:5:494:ARG:NH1  | 2.37                     | 0.51              |
| 1:B:439:VAL:O    | 1:J:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:B:488:ALA:HB3  | 1:L:439:VAL:O    | 2.10                     | 0.51              |
| 1:D:476:ASN:ND2  | 1:D:520:THR:OG1  | 2.43                     | 0.51              |
| 1:R:441:THR:HG22 | 1:S:486:VAL:HB   | 1.93                     | 0.51              |
| 1:S:310:GLN:HG2  | 1:d:328:THR:CG2  | 2.40                     | 0.51              |
| 1:S:373:ARG:O    | 1:S:376:THR:OG1  | 2.19                     | 0.51              |
| 1:W:619:HIS:HA   | 2:NA:997:DA:H2'  | 1.88                     | 0.51              |
| 1:e:476:ASN:ND2  | 1:e:520:THR:OG1  | 2.43                     | 0.51              |
| 1:f:328:THR:CG2  | 1:z:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:m:596:TRP:NE1  | 1:m:598:GLU:OE2  | 2.41                     | 0.51              |
| 1:r:328:THR:CG2  | 1:x:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:r:441:THR:HG22 | 1:s:486:VAL:HB   | 1.91                     | 0.51              |
| 1:r:489:PHE:O    | 1:r:494:ARG:NH1  | 2.37                     | 0.51              |
| 1:t:421:GLN:NE2  | 1:u:342:PRO:HB3  | 2.24                     | 0.51              |
| 1:t:476:ASN:ND2  | 1:t:520:THR:OG1  | 2.43                     | 0.51              |
| 1:w:486:VAL:HB   | 1:y:441:THR:HG22 | 1.93                     | 0.51              |
| 1:w:596:TRP:NE1  | 1:w:598:GLU:OE2  | 2.41                     | 0.51              |
| 1:z:441:THR:HG22 | 1:1:486:VAL:HB   | 1.92                     | 0.51              |
| 1:1:439:VAL:O    | 1:2:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:1:441:THR:HG22 | 1:2:486:VAL:HB   | 1.92                     | 0.51              |
| 1:5:596:TRP:NE1  | 1:5:598:GLU:OE2  | 2.41                     | 0.51              |
| 1:A:476:ASN:ND2  | 1:A:520:THR:OG1  | 2.43                     | 0.51              |
| 1:D:488:ALA:HB3  | 1:P:439:VAL:O    | 2.11                     | 0.51              |
| 1:E:342:PRO:HB3  | 1:F:421:GLN:NE2  | 2.24                     | 0.51              |
| 1:E:486:VAL:HB   | 1:F:441:THR:HG22 | 1.92                     | 0.51              |
| 1:F:476:ASN:ND2  | 1:F:520:THR:OG1  | 2.43                     | 0.51              |
| 1:H:486:VAL:HB   | 1:Y:441:THR:HG22 | 1.92                     | 0.51              |
| 1:I:310:GLN:HG2  | 1:J:328:THR:CG2  | 2.40                     | 0.51              |
| 1:I:373:ARG:O    | 1:I:376:THR:OG1  | 2.19                     | 0.51              |
| 1:M:619:HIS:HA   | 2:CA:997:DA:H2'  | 1.88                     | 0.51              |
| 1:N:441:THR:HG22 | 1:P:486:VAL:HB   | 1.92                     | 0.51              |
| 1:O:441:THR:HG22 | 1:m:486:VAL:HB   | 1.92                     | 0.51              |
| 1:S:476:ASN:ND2  | 1:S:520:THR:OG1  | 2.43                     | 0.51              |
| 1:U:310:GLN:HG2  | 1:e:328:THR:CG2  | 2.40                     | 0.51              |
| 1:Z:486:VAL:HB   | 1:3:441:THR:HG22 | 1.92                     | 0.51              |
| 1:b:619:HIS:HA   | 2:SA:997:DA:H2'  | 1.88                     | 0.51              |
| 1:c:439:VAL:O    | 1:o:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:k:328:THR:CG2  | 1:w:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:l:513:ASN:ND2  | 1:l:526:THR:HG22 | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:342:PRO:HB3  | 1:y:421:GLN:NE2  | 2.25                     | 0.51              |
| 1:B:373:ARG:O    | 1:B:376:THR:OG1  | 2.19                     | 0.51              |
| 1:C:441:THR:HG22 | 1:b:486:VAL:HB   | 1.92                     | 0.51              |
| 1:H:488:ALA:HB3  | 1:Y:439:VAL:O    | 2.11                     | 0.51              |
| 1:M:310:GLN:HG2  | 1:N:328:THR:CG2  | 2.40                     | 0.51              |
| 1:X:488:ALA:HB3  | 1:e:439:VAL:O    | 2.10                     | 0.51              |
| 1:Y:310:GLN:HG2  | 1:4:328:THR:CG2  | 2.40                     | 0.51              |
| 1:c:441:THR:HG22 | 1:o:486:VAL:HB   | 1.92                     | 0.51              |
| 1:d:476:ASN:ND2  | 1:d:520:THR:OG1  | 2.43                     | 0.51              |
| 1:g:310:GLN:HG2  | 1:1:328:THR:CG2  | 2.39                     | 0.51              |
| 1:k:476:ASN:ND2  | 1:k:520:THR:OG1  | 2.43                     | 0.51              |
| 1:q:488:ALA:HB3  | 1:s:439:VAL:O    | 2.11                     | 0.51              |
| 1:s:513:ASN:ND2  | 1:s:526:THR:HG22 | 2.10                     | 0.51              |
| 1:w:439:VAL:O    | 1:x:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:7:513:ASN:ND2  | 1:7:526:THR:HG22 | 2.10                     | 0.51              |
| 1:C:498:GLU:HA   | 1:M:515:LEU:HD21 | 1.93                     | 0.51              |
| 1:G:439:VAL:O    | 1:I:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:I:513:ASN:ND2  | 1:I:526:THR:HG22 | 2.10                     | 0.51              |
| 1:J:441:THR:HG22 | 1:L:486:VAL:HB   | 1.92                     | 0.51              |
| 1:K:328:THR:CG2  | 1:7:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:K:441:THR:HG22 | 1:a:486:VAL:HB   | 1.92                     | 0.51              |
| 1:O:310:GLN:HG2  | 1:P:328:THR:CG2  | 2.39                     | 0.51              |
| 1:R:421:GLN:NE2  | 1:S:342:PRO:HB3  | 2.25                     | 0.51              |
| 1:W:373:ARG:O    | 1:W:376:THR:OG1  | 2.19                     | 0.51              |
| 1:Z:498:GLU:HA   | 1:3:515:LEU:HD21 | 1.93                     | 0.51              |
| 1:t:441:THR:HG22 | 1:u:486:VAL:HB   | 1.92                     | 0.51              |
| 1:z:328:THR:CG2  | 1:4:310:GLN:HG2  | 2.40                     | 0.51              |
| 1:3:498:GLU:HA   | 1:4:515:LEU:HD21 | 1.93                     | 0.51              |
| 1:5:476:ASN:ND2  | 1:5:520:THR:OG1  | 2.43                     | 0.51              |
| 1:8:373:ARG:O    | 1:8:376:THR:OG1  | 2.19                     | 0.51              |
| 1:C:515:LEU:HD21 | 1:b:498:GLU:HA   | 1.93                     | 0.51              |
| 1:E:441:THR:HG22 | 1:Q:486:VAL:HB   | 1.92                     | 0.51              |
| 1:J:513:ASN:ND2  | 1:J:526:THR:HG22 | 2.10                     | 0.51              |
| 1:O:486:VAL:HB   | 1:n:441:THR:HG22 | 1.92                     | 0.51              |
| 1:O:488:ALA:HB3  | 1:n:439:VAL:O    | 2.11                     | 0.51              |
| 1:R:498:GLU:HA   | 1:U:515:LEU:HD21 | 1.93                     | 0.51              |
| 1:S:439:VAL:O    | 1:U:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:Z:439:VAL:O    | 1:4:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:d:513:ASN:ND2  | 1:d:526:THR:HG22 | 2.10                     | 0.51              |
| 1:g:488:ALA:HB3  | 1:h:439:VAL:O    | 2.10                     | 0.51              |
| 1:u:441:THR:HG22 | 1:v:486:VAL:HB   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:513:ASN:ND2  | 1:u:526:THR:HG22 | 2.10                     | 0.51              |
| 1:x:515:LEU:HD21 | 1:y:498:GLU:HA   | 1.93                     | 0.51              |
| 1:6:439:VAL:O    | 1:7:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:D:498:GLU:HA   | 1:P:515:LEU:HD21 | 1.93                     | 0.51              |
| 1:M:488:ALA:HB3  | 1:b:439:VAL:O    | 2.10                     | 0.51              |
| 1:d:439:VAL:O    | 1:l:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:d:441:THR:HG22 | 1:l:486:VAL:HB   | 1.92                     | 0.51              |
| 1:f:439:VAL:O    | 1:h:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:g:486:VAL:HB   | 1:h:441:THR:HG22 | 1.92                     | 0.51              |
| 1:i:488:ALA:HB3  | 1:k:439:VAL:O    | 2.11                     | 0.51              |
| 1:6:515:LEU:HD21 | 1:7:498:GLU:HA   | 1.93                     | 0.51              |
| 1:F:488:ALA:HB3  | 1:Q:439:VAL:O    | 2.10                     | 0.51              |
| 1:G:515:LEU:HD21 | 1:I:498:GLU:HA   | 1.93                     | 0.51              |
| 1:J:310:GLN:HG2  | 1:a:328:THR:CG2  | 2.40                     | 0.51              |
| 1:K:515:LEU:HD21 | 1:a:498:GLU:HA   | 1.93                     | 0.51              |
| 1:R:439:VAL:O    | 1:S:488:ALA:HB3  | 2.10                     | 0.51              |
| 1:W:489:PHE:O    | 1:W:494:ARG:NH1  | 2.37                     | 0.51              |
| 1:o:310:GLN:HG2  | 1:7:328:THR:CG2  | 2.40                     | 0.51              |
| 1:z:439:VAL:O    | 1:l:488:ALA:HB3  | 2.11                     | 0.51              |
| 1:l:515:LEU:HD21 | 1:2:498:GLU:HA   | 1.93                     | 0.51              |
| 1:B:441:THR:HG22 | 1:J:486:VAL:HB   | 1.92                     | 0.50              |
| 1:N:439:VAL:O    | 1:P:488:ALA:HB3  | 2.11                     | 0.50              |
| 1:T:439:VAL:O    | 1:d:488:ALA:HB3  | 2.10                     | 0.50              |
| 1:a:441:THR:HG22 | 1:8:486:VAL:HB   | 1.92                     | 0.50              |
| 1:i:513:ASN:ND2  | 1:i:526:THR:HG22 | 2.10                     | 0.50              |
| 1:j:439:VAL:O    | 1:k:488:ALA:HB3  | 2.10                     | 0.50              |
| 1:m:439:VAL:O    | 1:n:488:ALA:HB3  | 2.11                     | 0.50              |
| 1:t:488:ALA:HB3  | 1:v:439:VAL:O    | 2.10                     | 0.50              |
| 1:w:488:ALA:HB3  | 1:y:439:VAL:O    | 2.10                     | 0.50              |
| 1:5:441:THR:HG22 | 1:6:486:VAL:HB   | 1.92                     | 0.50              |
| 1:7:373:ARG:O    | 1:7:376:THR:OG1  | 2.19                     | 0.50              |
| 1:A:441:THR:HG22 | 1:G:486:VAL:HB   | 1.92                     | 0.50              |
| 1:A:488:ALA:HB3  | 1:I:439:VAL:O    | 2.11                     | 0.50              |
| 1:B:486:VAL:HB   | 1:L:441:THR:HG22 | 1.92                     | 0.50              |
| 1:E:513:ASN:ND2  | 1:E:526:THR:HG22 | 2.10                     | 0.50              |
| 1:H:310:GLN:HG2  | 1:I:328:THR:CG2  | 2.40                     | 0.50              |
| 1:H:441:THR:HG22 | 1:W:486:VAL:HB   | 1.92                     | 0.50              |
| 1:I:476:ASN:ND2  | 1:I:520:THR:OG1  | 2.43                     | 0.50              |
| 1:J:515:LEU:HD21 | 1:L:498:GLU:HA   | 1.93                     | 0.50              |
| 1:K:310:GLN:HG2  | 1:L:328:THR:CG2  | 2.40                     | 0.50              |
| 1:K:486:VAL:HB   | 1:8:441:THR:HG22 | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:441:THR:HG22 | 1:4:486:VAL:HB   | 1.92                     | 0.50              |
| 1:i:486:VAL:HB   | 1:k:441:THR:HG22 | 1.92                     | 0.50              |
| 1:m:699:VAL:HG23 | 1:m:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:o:441:THR:HG22 | 1:p:486:VAL:HB   | 1.92                     | 0.50              |
| 1:p:699:VAL:HG23 | 1:p:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:t:328:THR:CG2  | 1:y:310:GLN:HG2  | 2.40                     | 0.50              |
| 1:5:498:GLU:HA   | 1:7:515:LEU:HD21 | 1.93                     | 0.50              |
| 1:B:515:LEU:HD21 | 1:J:498:GLU:HA   | 1.94                     | 0.50              |
| 1:F:328:THR:CG2  | 1:R:310:GLN:HG2  | 2.40                     | 0.50              |
| 1:G:441:THR:HG22 | 1:I:486:VAL:HB   | 1.92                     | 0.50              |
| 1:H:439:VAL:O    | 1:W:488:ALA:HB3  | 2.10                     | 0.50              |
| 1:K:498:GLU:HA   | 1:8:515:LEU:HD21 | 1.94                     | 0.50              |
| 1:M:486:VAL:HB   | 1:b:441:THR:HG22 | 1.92                     | 0.50              |
| 1:T:488:ALA:HB3  | 1:l:439:VAL:O    | 2.10                     | 0.50              |
| 1:T:699:VAL:HG23 | 1:T:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:W:699:VAL:HG23 | 1:W:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:a:515:LEU:HD21 | 1:8:498:GLU:HA   | 1.94                     | 0.50              |
| 1:i:439:VAL:O    | 1:j:488:ALA:HB3  | 2.10                     | 0.50              |
| 1:i:515:LEU:HD21 | 1:j:498:GLU:HA   | 1.93                     | 0.50              |
| 1:o:439:VAL:O    | 1:p:488:ALA:HB3  | 2.10                     | 0.50              |
| 1:6:441:THR:HG22 | 1:7:486:VAL:HB   | 1.92                     | 0.50              |
| 1:7:476:ASN:ND2  | 1:7:520:THR:OG1  | 2.43                     | 0.50              |
| 1:B:498:GLU:HA   | 1:L:515:LEU:HD21 | 1.94                     | 0.50              |
| 1:E:699:VAL:HG23 | 1:E:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:K:513:ASN:ND2  | 1:K:526:THR:HG22 | 2.10                     | 0.50              |
| 1:R:486:VAL:HB   | 1:U:441:THR:HG22 | 1.92                     | 0.50              |
| 1:X:486:VAL:HB   | 1:e:441:THR:HG22 | 1.92                     | 0.50              |
| 1:f:699:VAL:HG23 | 1:f:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:j:699:VAL:HG23 | 1:j:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:p:489:PHE:O    | 1:p:494:ARG:NH1  | 2.37                     | 0.50              |
| 1:t:699:VAL:HG23 | 1:t:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:u:699:VAL:HG23 | 1:u:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:w:498:GLU:HA   | 1:y:515:LEU:HD21 | 1.93                     | 0.50              |
| 1:1:513:ASN:ND2  | 1:1:526:THR:HG22 | 2.10                     | 0.50              |
| 1:5:488:ALA:HB3  | 1:7:439:VAL:O    | 2.11                     | 0.50              |
| 1:C:486:VAL:HB   | 1:M:441:THR:HG22 | 1.92                     | 0.50              |
| 1:D:441:THR:HG22 | 1:N:486:VAL:HB   | 1.92                     | 0.50              |
| 1:F:699:VAL:HG23 | 1:F:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:R:515:LEU:HD21 | 1:S:498:GLU:HA   | 1.93                     | 0.50              |
| 1:T:498:GLU:HA   | 1:l:515:LEU:HD21 | 1.93                     | 0.50              |
| 1:V:498:GLU:HA   | 1:X:515:LEU:HD21 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:441:THR:HG22 | 1:r:486:VAL:HB   | 1.92                     | 0.50              |
| 1:A:439:VAL:O    | 1:G:488:ALA:HB3  | 2.12                     | 0.50              |
| 1:E:498:GLU:HA   | 1:F:515:LEU:HD21 | 1.94                     | 0.50              |
| 1:E:628:GLY:C    | 2:qA:997:DA:N1   | 2.66                     | 0.50              |
| 1:Q:699:VAL:HG23 | 1:Q:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:V:439:VAL:O    | 1:e:488:ALA:HB3  | 2.11                     | 0.50              |
| 1:V:441:THR:HG22 | 1:e:486:VAL:HB   | 1.92                     | 0.50              |
| 1:Z:589:GLU:OE2  | 1:3:588:GLN:HG3  | 2.12                     | 0.50              |
| 1:Z:699:VAL:HG23 | 1:Z:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:b:699:VAL:HG23 | 1:b:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:q:349:THR:HA   | 1:s:433:GLN:HA   | 1.93                     | 0.50              |
| 1:q:439:VAL:O    | 1:r:488:ALA:HB3  | 2.11                     | 0.50              |
| 1:z:486:VAL:HB   | 1:2:441:THR:HG22 | 1.92                     | 0.50              |
| 1:3:486:VAL:HB   | 1:4:441:THR:HG22 | 1.93                     | 0.50              |
| 1:C:588:GLN:HG3  | 1:b:589:GLU:OE2  | 2.12                     | 0.50              |
| 1:M:699:VAL:HG23 | 1:M:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:O:498:GLU:HA   | 1:n:515:LEU:HD21 | 1.93                     | 0.50              |
| 1:U:513:ASN:ND2  | 1:U:526:THR:HG22 | 2.10                     | 0.50              |
| 1:n:628:GLY:C    | 2:gA:997:DA:N1   | 2.66                     | 0.50              |
| 1:t:515:LEU:HD21 | 1:u:498:GLU:HA   | 1.94                     | 0.50              |
| 1:v:328:THR:CG2  | 1:1:310:GLN:HG2  | 2.40                     | 0.50              |
| 1:v:699:VAL:HG23 | 1:v:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:4:699:VAL:HG23 | 1:4:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:D:349:THR:HA   | 1:P:433:GLN:HA   | 1.94                     | 0.50              |
| 1:I:415:SER:HB2  | 1:I:417:PHE:CE2  | 2.47                     | 0.50              |
| 1:J:699:VAL:HG23 | 1:J:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:P:310:GLN:HG2  | 1:Q:328:THR:CG2  | 2.40                     | 0.50              |
| 1:P:699:VAL:HG23 | 1:P:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:S:515:LEU:HD21 | 1:U:498:GLU:HA   | 1.93                     | 0.50              |
| 1:S:699:VAL:HG23 | 1:S:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:g:498:GLU:HA   | 1:h:515:LEU:HD21 | 1.93                     | 0.50              |
| 1:h:628:GLY:C    | 2:ZA:997:DA:N1   | 2.66                     | 0.50              |
| 1:u:628:GLY:C    | 2:nA:997:DA:N1   | 2.66                     | 0.50              |
| 1:w:515:LEU:HD21 | 1:x:498:GLU:HA   | 1.93                     | 0.50              |
| 1:w:699:VAL:HG23 | 1:w:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:x:441:THR:HG22 | 1:y:486:VAL:HB   | 1.93                     | 0.50              |
| 1:1:433:GLN:HA   | 1:2:349:THR:HA   | 1.94                     | 0.50              |
| 1:6:699:VAL:HG23 | 1:6:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:E:349:THR:HA   | 1:F:433:GLN:HA   | 1.94                     | 0.50              |
| 1:G:699:VAL:HG23 | 1:G:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:K:699:VAL:HG23 | 1:K:702:ALA:HB3  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:513:ASN:ND2  | 1:P:526:THR:HG22 | 2.10                     | 0.50              |
| 1:R:349:THR:HA   | 1:U:433:GLN:HA   | 1.94                     | 0.50              |
| 1:R:588:GLN:HG3  | 1:S:589:GLU:OE2  | 2.12                     | 0.50              |
| 1:X:503:GLN:O    | 1:X:505:PRO:HD3  | 2.12                     | 0.50              |
| 1:c:486:VAL:HB   | 1:p:441:THR:HG22 | 1.92                     | 0.50              |
| 1:d:433:GLN:HA   | 1:l:349:THR:HA   | 1.94                     | 0.50              |
| 1:f:415:SER:HB2  | 1:f:417:PHE:CE2  | 2.47                     | 0.50              |
| 1:f:498:GLU:HA   | 1:g:515:LEU:HD21 | 1.93                     | 0.50              |
| 1:f:515:LEU:HD21 | 1:h:498:GLU:HA   | 1.93                     | 0.50              |
| 1:i:415:SER:HB2  | 1:i:417:PHE:CE2  | 2.47                     | 0.50              |
| 1:i:628:GLY:C    | 2:aA:997:DA:N1   | 2.66                     | 0.50              |
| 1:m:415:SER:HB2  | 1:m:417:PHE:CE2  | 2.47                     | 0.50              |
| 1:m:515:LEU:HD21 | 1:n:498:GLU:HA   | 1.94                     | 0.50              |
| 1:q:503:GLN:O    | 1:q:505:PRO:HD3  | 2.12                     | 0.50              |
| 1:s:503:GLN:O    | 1:s:505:PRO:HD3  | 2.12                     | 0.50              |
| 1:t:433:GLN:HA   | 1:u:349:THR:HA   | 1.94                     | 0.50              |
| 1:w:589:GLU:OE2  | 1:y:588:GLN:HG3  | 2.12                     | 0.50              |
| 1:x:433:GLN:HA   | 1:y:349:THR:HA   | 1.94                     | 0.50              |
| 1:z:699:VAL:HG23 | 1:z:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:1:588:GLN:HG3  | 1:2:589:GLU:OE2  | 2.12                     | 0.50              |
| 1:1:699:VAL:HG23 | 1:1:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:3:349:THR:HA   | 1:4:433:GLN:HA   | 1.94                     | 0.50              |
| 1:3:699:VAL:HG23 | 1:3:702:ALA:HB3  | 1.94                     | 0.50              |
| 1:5:415:SER:HB2  | 1:5:417:PHE:CE2  | 2.47                     | 0.50              |
| 1:7:415:SER:HB2  | 1:7:417:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:415:SER:HB2  | 1:A:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:498:GLU:HA   | 1:I:515:LEU:HD21 | 1.94                     | 0.49              |
| 1:B:415:SER:HB2  | 1:B:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:B:433:GLN:HA   | 1:J:349:THR:HA   | 1.94                     | 0.49              |
| 1:C:349:THR:HA   | 1:M:433:GLN:HA   | 1.94                     | 0.49              |
| 1:C:415:SER:HB2  | 1:C:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:C:699:VAL:HG23 | 1:C:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:D:589:GLU:OE2  | 1:P:588:GLN:HG3  | 2.13                     | 0.49              |
| 1:M:498:GLU:HA   | 1:b:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:N:415:SER:HB2  | 1:N:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:V:503:GLN:O    | 1:V:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:W:441:THR:HG22 | 1:Y:486:VAL:HB   | 1.92                     | 0.49              |
| 1:W:503:GLN:O    | 1:W:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:l:415:SER:HB2  | 1:l:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:u:439:VAL:O    | 1:v:488:ALA:HB3  | 2.11                     | 0.49              |
| 1:z:415:SER:HB2  | 1:z:417:PHE:CE2  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:z:498:GLU:HA   | 1:2:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:3:415:SER:HB2  | 1:3:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:8:415:SER:HB2  | 1:8:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:D:433:GLN:HA   | 1:N:349:THR:HA   | 1.94                     | 0.49              |
| 1:E:439:VAL:O    | 1:Q:488:ALA:HB3  | 2.11                     | 0.49              |
| 1:F:589:GLU:OE2  | 1:Q:588:GLN:HG3  | 2.13                     | 0.49              |
| 1:G:291:ILE:HD12 | 1:G:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:H:498:GLU:HA   | 1:Y:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:I:699:VAL:HG23 | 1:I:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:K:349:THR:HA   | 1:8:433:GLN:HA   | 1.94                     | 0.49              |
| 1:N:699:VAL:HG23 | 1:N:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:O:515:LEU:HD21 | 1:m:498:GLU:HA   | 1.93                     | 0.49              |
| 1:T:349:THR:HA   | 1:l:433:GLN:HA   | 1.95                     | 0.49              |
| 1:V:515:LEU:HD21 | 1:e:498:GLU:HA   | 1.93                     | 0.49              |
| 1:Y:699:VAL:HG23 | 1:Y:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:Z:515:LEU:HD21 | 1:4:498:GLU:HA   | 1.93                     | 0.49              |
| 1:a:433:GLN:HA   | 1:8:349:THR:HA   | 1.94                     | 0.49              |
| 1:a:699:VAL:HG23 | 1:a:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:b:291:ILE:HD12 | 1:b:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:c:699:VAL:HG23 | 1:c:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:i:349:THR:HA   | 1:k:433:GLN:HA   | 1.94                     | 0.49              |
| 1:i:433:GLN:HA   | 1:j:349:THR:HA   | 1.95                     | 0.49              |
| 1:i:503:GLN:O    | 1:i:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:l:503:GLN:O    | 1:l:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:p:503:GLN:O    | 1:p:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:q:498:GLU:HA   | 1:s:515:LEU:HD21 | 1.94                     | 0.49              |
| 1:v:503:GLN:O    | 1:v:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:z:349:THR:HA   | 1:2:433:GLN:HA   | 1.94                     | 0.49              |
| 1:5:699:VAL:HG23 | 1:5:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:A:349:THR:HA   | 1:I:433:GLN:HA   | 1.94                     | 0.49              |
| 1:B:349:THR:HA   | 1:L:433:GLN:HA   | 1.94                     | 0.49              |
| 1:B:588:GLN:HG3  | 1:J:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:C:503:GLN:O    | 1:C:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:D:415:SER:HB2  | 1:D:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:D:515:LEU:HD21 | 1:N:498:GLU:HA   | 1.93                     | 0.49              |
| 1:H:349:THR:HA   | 1:Y:433:GLN:HA   | 1.94                     | 0.49              |
| 1:I:503:GLN:O    | 1:I:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:K:589:GLU:OE2  | 1:8:588:GLN:HG3  | 2.13                     | 0.49              |
| 1:L:699:VAL:HG23 | 1:L:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:P:503:GLN:O    | 1:P:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:Q:503:GLN:O    | 1:Q:505:PRO:HD3  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:R:415:SER:HB2  | 1:R:417:PHE:CE2 | 2.47                     | 0.49              |
| 1:R:433:GLN:HA   | 1:S:349:THR:HA  | 1.94                     | 0.49              |
| 1:R:589:GLU:OE2  | 1:U:588:GLN:HG3 | 2.12                     | 0.49              |
| 1:S:291:ILE:HD12 | 1:S:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:T:291:ILE:HD12 | 1:T:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:U:415:SER:HB2  | 1:U:417:PHE:CE2 | 2.47                     | 0.49              |
| 1:Z:291:ILE:HD12 | 1:Z:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:Z:503:GLN:O    | 1:Z:505:PRO:HD3 | 2.12                     | 0.49              |
| 1:b:503:GLN:O    | 1:b:505:PRO:HD3 | 2.12                     | 0.49              |
| 1:c:588:GLN:HG3  | 1:o:589:GLU:OE2 | 2.13                     | 0.49              |
| 1:c:628:GLY:C    | 2:TA:997:DA:N1  | 2.66                     | 0.49              |
| 1:f:503:GLN:O    | 1:f:505:PRO:HD3 | 2.12                     | 0.49              |
| 1:j:291:ILE:HD12 | 1:j:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:k:291:ILE:HD12 | 1:k:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:l:628:GLY:C    | 2:dA:997:DA:N1  | 2.67                     | 0.49              |
| 1:n:291:ILE:HD12 | 1:n:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:t:291:ILE:HD12 | 1:t:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:t:589:GLU:OE2  | 1:v:588:GLN:HG3 | 2.13                     | 0.49              |
| 1:w:291:ILE:HD12 | 1:w:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:x:415:SER:HB2  | 1:x:417:PHE:CE2 | 2.47                     | 0.49              |
| 1:x:588:GLN:HG3  | 1:y:589:GLU:OE2 | 2.12                     | 0.49              |
| 1:y:415:SER:HB2  | 1:y:417:PHE:CE2 | 2.47                     | 0.49              |
| 1:z:619:HIS:HA   | 2:tA:997:DA:H2' | 1.87                     | 0.49              |
| 1:1:503:GLN:O    | 1:1:505:PRO:HD3 | 2.12                     | 0.49              |
| 1:2:503:GLN:O    | 1:2:505:PRO:HD3 | 2.12                     | 0.49              |
| 1:5:349:THR:HA   | 1:7:433:GLN:HA  | 1.95                     | 0.49              |
| 1:5:515:LEU:HD21 | 1:6:498:GLU:HA  | 1.93                     | 0.49              |
| 1:6:291:ILE:HD12 | 1:6:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:6:628:GLY:C    | 2:zA:997:DA:N1  | 2.66                     | 0.49              |
| 1:7:503:GLN:O    | 1:7:505:PRO:HD3 | 2.12                     | 0.49              |
| 1:A:699:VAL:HG23 | 1:A:702:ALA:HB3 | 1.94                     | 0.49              |
| 1:C:589:GLU:OE2  | 1:M:588:GLN:HG3 | 2.12                     | 0.49              |
| 1:D:503:GLN:O    | 1:D:505:PRO:HD3 | 2.13                     | 0.49              |
| 1:F:291:ILE:HD12 | 1:F:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:H:291:ILE:HD12 | 1:H:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:H:589:GLU:OE2  | 1:Y:588:GLN:HG3 | 2.12                     | 0.49              |
| 1:O:588:GLN:HG3  | 1:m:589:GLU:OE2 | 2.13                     | 0.49              |
| 1:S:415:SER:HB2  | 1:S:417:PHE:CE2 | 2.47                     | 0.49              |
| 1:Z:588:GLN:HG3  | 1:4:589:GLU:OE2 | 2.12                     | 0.49              |
| 1:d:291:ILE:HD12 | 1:d:719:TYR:CE2 | 2.48                     | 0.49              |
| 1:e:699:VAL:HG23 | 1:e:702:ALA:HB3 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:291:ILE:HD12 | 1:f:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:h:291:ILE:HD12 | 1:h:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:m:503:GLN:O    | 1:m:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:o:291:ILE:HD12 | 1:o:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:q:291:ILE:HD12 | 1:q:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:q:515:LEU:HD21 | 1:r:498:GLU:HA   | 1.94                     | 0.49              |
| 1:r:699:VAL:HG23 | 1:r:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:t:498:GLU:HA   | 1:v:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:w:349:THR:HA   | 1:y:433:GLN:HA   | 1.94                     | 0.49              |
| 1:w:415:SER:HB2  | 1:w:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:x:513:ASN:ND2  | 1:x:526:THR:HG22 | 2.10                     | 0.49              |
| 1:2:415:SER:HB2  | 1:2:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:3:503:GLN:O    | 1:3:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:7:699:VAL:HG23 | 1:7:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:8:699:VAL:HG23 | 1:8:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:A:286:ASP:OD2  | 1:E:390:TYR:OH   | 2.31                     | 0.49              |
| 1:D:628:GLY:C    | 2:fA:997:DA:N1   | 2.66                     | 0.49              |
| 1:E:515:LEU:HD21 | 1:Q:498:GLU:HA   | 1.93                     | 0.49              |
| 1:F:498:GLU:HA   | 1:Q:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:G:503:GLN:O    | 1:G:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:G:628:GLY:C    | 2:3A:997:DA:N1   | 2.66                     | 0.49              |
| 1:J:415:SER:HB2  | 1:J:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:K:415:SER:HB2  | 1:K:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:L:291:ILE:HD12 | 1:L:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:M:589:GLU:OE2  | 1:b:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:S:588:GLN:HG3  | 1:U:589:GLU:OE2  | 2.12                     | 0.49              |
| 1:U:503:GLN:O    | 1:U:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:V:291:ILE:HD12 | 1:V:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:V:699:VAL:HG23 | 1:V:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:W:291:ILE:HD12 | 1:W:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:c:433:GLN:HA   | 1:o:349:THR:HA   | 1.94                     | 0.49              |
| 1:c:515:LEU:HD21 | 1:o:498:GLU:HA   | 1.93                     | 0.49              |
| 1:f:589:GLU:OE2  | 1:g:588:GLN:HG3  | 2.13                     | 0.49              |
| 1:g:503:GLN:O    | 1:g:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:g:589:GLU:OE2  | 1:h:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:j:515:LEU:HD21 | 1:k:498:GLU:HA   | 1.94                     | 0.49              |
| 1:m:291:ILE:HD12 | 1:m:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:m:433:GLN:HA   | 1:n:349:THR:HA   | 1.95                     | 0.49              |
| 1:p:415:SER:HB2  | 1:p:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:t:439:VAL:O    | 1:u:488:ALA:HB3  | 2.11                     | 0.49              |
| 1:u:515:LEU:HD21 | 1:v:498:GLU:HA   | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:588:GLN:HG3  | 1:x:589:GLU:OE2  | 2.12                     | 0.49              |
| 1:2:628:GLY:C    | 2:vA:997:DA:N1   | 2.66                     | 0.49              |
| 1:2:699:VAL:HG23 | 1:2:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:3:589:GLU:OE2  | 1:4:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:6:503:GLN:O    | 1:6:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:B:699:VAL:HG23 | 1:B:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:D:699:VAL:HG23 | 1:D:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:N:619:HIS:HA   | 2:DA:997:DA:H2'  | 1.88                     | 0.49              |
| 1:O:503:GLN:O    | 1:O:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:O:589:GLU:OE2  | 1:n:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:P:415:SER:HB2  | 1:P:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:R:503:GLN:O    | 1:R:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:V:588:GLN:HG3  | 1:e:589:GLU:OE2  | 2.12                     | 0.49              |
| 1:W:415:SER:HB2  | 1:W:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:X:349:THR:HA   | 1:e:433:GLN:HA   | 1.94                     | 0.49              |
| 1:Y:628:GLY:C    | 2:PA:997:DA:N1   | 2.66                     | 0.49              |
| 1:a:291:ILE:HD12 | 1:a:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:c:390:TYR:OH   | 1:s:286:ASP:OD2  | 2.31                     | 0.49              |
| 1:c:498:GLU:HA   | 1:p:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:d:415:SER:HB2  | 1:d:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:f:433:GLN:HA   | 1:h:349:THR:HA   | 1.95                     | 0.49              |
| 1:h:415:SER:HB2  | 1:h:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:k:415:SER:HB2  | 1:k:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:n:415:SER:HB2  | 1:n:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:o:503:GLN:O    | 1:o:505:PRO:HD3  | 2.13                     | 0.49              |
| 1:p:291:ILE:HD12 | 1:p:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:s:415:SER:HB2  | 1:s:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:s:699:VAL:HG23 | 1:s:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:u:291:ILE:HD12 | 1:u:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:z:291:ILE:HD12 | 1:z:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:A:503:GLN:O    | 1:A:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:E:291:ILE:HD12 | 1:E:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:E:415:SER:HB2  | 1:E:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:E:488:ALA:HB3  | 1:F:439:VAL:O    | 2.11                     | 0.49              |
| 1:H:503:GLN:O    | 1:H:505:PRO:HD3  | 2.13                     | 0.49              |
| 1:H:699:VAL:HG23 | 1:H:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:J:291:ILE:HD12 | 1:J:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:K:291:ILE:HD12 | 1:K:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:N:291:ILE:HD12 | 1:N:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:Q:291:ILE:HD12 | 1:Q:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:S:503:GLN:O    | 1:S:505:PRO:HD3  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:515:LEU:HD21 | 1:d:498:GLU:HA   | 1.94                     | 0.49              |
| 1:T:588:GLN:HG3  | 1:d:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:W:515:LEU:HD21 | 1:Y:498:GLU:HA   | 1.93                     | 0.49              |
| 1:X:415:SER:HB2  | 1:X:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:X:498:GLU:HA   | 1:e:515:LEU:HD21 | 1.93                     | 0.49              |
| 1:f:588:GLN:HG3  | 1:h:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:n:619:HIS:HA   | 2:gA:997:DA:H2'  | 1.88                     | 0.49              |
| 1:q:513:ASN:ND2  | 1:q:526:THR:HG22 | 2.10                     | 0.49              |
| 1:q:628:GLY:C    | 2:jA:997:DA:N1   | 2.66                     | 0.49              |
| 1:q:699:VAL:HG23 | 1:q:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:r:515:LEU:HD21 | 1:s:498:GLU:HA   | 1.94                     | 0.49              |
| 1:u:415:SER:HB2  | 1:u:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:w:503:GLN:O    | 1:w:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:x:503:GLN:O    | 1:x:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:y:503:GLN:O    | 1:y:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:z:589:GLU:OE2  | 1:2:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:5:503:GLN:O    | 1:5:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:6:415:SER:HB2  | 1:6:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:7:619:HIS:C    | 2:0A:997:DA:H2'  | 2.38                     | 0.49              |
| 1:D:588:GLN:HG3  | 1:N:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:E:619:HIS:HA   | 2:qA:997:DA:H2'  | 1.88                     | 0.49              |
| 1:G:415:SER:HB2  | 1:G:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:H:515:LEU:HD21 | 1:W:498:GLU:HA   | 1.93                     | 0.49              |
| 1:I:619:HIS:C    | 2:5A:997:DA:H2'  | 2.38                     | 0.49              |
| 1:J:433:GLN:HA   | 1:L:349:THR:HA   | 1.95                     | 0.49              |
| 1:T:433:GLN:HA   | 1:d:349:THR:HA   | 1.94                     | 0.49              |
| 1:U:699:VAL:HG23 | 1:U:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:V:373:ARG:O    | 1:V:376:THR:OG1  | 2.19                     | 0.49              |
| 1:V:589:GLU:OE2  | 1:X:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:W:619:HIS:C    | 2:NA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:X:619:HIS:C    | 2:OA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:X:699:VAL:HG23 | 1:X:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:c:503:GLN:O    | 1:c:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:c:678:GLU:OE2  | 1:c:680:SER:OG   | 2.24                     | 0.49              |
| 1:i:588:GLN:HG3  | 1:j:589:GLU:OE2  | 2.12                     | 0.49              |
| 1:i:699:VAL:HG23 | 1:i:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:j:513:ASN:ND2  | 1:j:526:THR:HG22 | 2.10                     | 0.49              |
| 1:j:588:GLN:HG3  | 1:k:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:l:699:VAL:HG23 | 1:l:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:m:588:GLN:HG3  | 1:n:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:o:515:LEU:HD21 | 1:p:498:GLU:HA   | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:699:VAL:HG23 | 1:o:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:p:678:GLU:OE2  | 1:p:680:SER:OG   | 2.24                     | 0.49              |
| 1:q:588:GLN:HG3  | 1:r:589:GLU:OE2  | 2.13                     | 0.49              |
| 1:r:291:ILE:HD12 | 1:r:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:s:619:HIS:C    | 2:lA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:v:415:SER:HB2  | 1:v:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:x:699:VAL:HG23 | 1:x:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:1:415:SER:HB2  | 1:1:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:1:619:HIS:C    | 2:uA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:6:433:GLN:HA   | 1:7:349:THR:HA   | 1.95                     | 0.49              |
| 1:A:291:ILE:HD12 | 1:A:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:B:628:GLY:C    | 2:JA:997:DA:N1   | 2.66                     | 0.49              |
| 1:G:433:GLN:HA   | 1:I:349:THR:HA   | 1.95                     | 0.49              |
| 1:G:619:HIS:C    | 2:3A:997:DA:H2'  | 2.38                     | 0.49              |
| 1:K:433:GLN:HA   | 1:a:349:THR:HA   | 1.95                     | 0.49              |
| 1:N:503:GLN:O    | 1:N:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:P:619:HIS:C    | 2:FA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:S:619:HIS:C    | 2:IA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:T:415:SER:HB2  | 1:T:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:U:619:HIS:C    | 2:LA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:W:678:GLU:OE2  | 1:W:680:SER:OG   | 2.24                     | 0.49              |
| 1:X:628:GLY:C    | 2:OA:997:DA:N1   | 2.66                     | 0.49              |
| 1:e:291:ILE:HD12 | 1:e:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:i:291:ILE:HD12 | 1:i:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:j:415:SER:HB2  | 1:j:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:j:433:GLN:HA   | 1:k:349:THR:HA   | 1.94                     | 0.49              |
| 1:o:433:GLN:HA   | 1:p:349:THR:HA   | 1.94                     | 0.49              |
| 1:p:619:HIS:C    | 2:iA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:v:291:ILE:HD12 | 1:v:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:w:513:ASN:ND2  | 1:w:526:THR:HG22 | 2.10                     | 0.49              |
| 1:w:619:HIS:C    | 2:pA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:z:503:GLN:O    | 1:z:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:5:589:GLU:OE2  | 1:7:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:H:433:GLN:HA   | 1:W:349:THR:HA   | 1.94                     | 0.49              |
| 1:J:588:GLN:HG3  | 1:L:589:GLU:OE2  | 2.12                     | 0.49              |
| 1:L:332:GLN:HE21 | 1:L:395:MET:HE3  | 1.78                     | 0.49              |
| 1:O:699:VAL:HG23 | 1:O:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:Q:415:SER:HB2  | 1:Q:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:T:589:GLU:OE2  | 1:l:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:T:628:GLY:C    | 2:KA:997:DA:N1   | 2.66                     | 0.49              |
| 1:V:415:SER:HB2  | 1:V:417:PHE:CE2  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:503:GLN:O    | 1:Y:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:b:513:ASN:ND2  | 1:b:526:THR:HG22 | 2.10                     | 0.49              |
| 1:c:589:GLU:OE2  | 1:p:588:GLN:HG3  | 2.12                     | 0.49              |
| 1:d:503:GLN:O    | 1:d:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:d:515:LEU:HD21 | 1:l:498:GLU:HA   | 1.94                     | 0.49              |
| 1:f:349:THR:HA   | 1:g:433:GLN:HA   | 1.95                     | 0.49              |
| 1:g:699:VAL:HG23 | 1:g:702:ALA:HB3  | 1.94                     | 0.49              |
| 1:h:619:HIS:C    | 2:ZA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:k:503:GLN:O    | 1:k:505:PRO:HD3  | 2.12                     | 0.49              |
| 1:l:291:ILE:HD12 | 1:l:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:n:619:HIS:C    | 2:gA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:q:332:GLN:HE21 | 1:q:395:MET:HE3  | 1.78                     | 0.49              |
| 1:q:415:SER:HB2  | 1:q:417:PHE:CE2  | 2.47                     | 0.49              |
| 1:q:589:GLU:OE2  | 1:s:588:GLN:HG3  | 2.13                     | 0.49              |
| 1:r:433:GLN:HA   | 1:s:349:THR:HA   | 1.95                     | 0.49              |
| 1:r:588:GLN:HG3  | 1:s:589:GLU:OE2  | 2.12                     | 0.49              |
| 1:u:619:HIS:HA   | 2:nA:997:DA:H2'  | 1.88                     | 0.49              |
| 1:x:619:HIS:C    | 2:rA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:4:619:HIS:C    | 2:xA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:5:291:ILE:HD12 | 1:5:719:TYR:CE2  | 2.48                     | 0.49              |
| 1:5:619:HIS:HA   | 2:yA:997:DA:H2'  | 1.88                     | 0.49              |
| 1:6:619:HIS:C    | 2:zA:997:DA:H2'  | 2.38                     | 0.49              |
| 1:C:489:PHE:O    | 1:C:494:ARG:NH1  | 2.37                     | 0.48              |
| 1:H:415:SER:HB2  | 1:H:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:J:332:GLN:HE21 | 1:J:395:MET:HE3  | 1.78                     | 0.48              |
| 1:K:332:GLN:HE21 | 1:K:395:MET:HE3  | 1.78                     | 0.48              |
| 1:K:588:GLN:HG3  | 1:a:589:GLU:OE2  | 2.12                     | 0.48              |
| 1:M:415:SER:HB2  | 1:M:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:M:619:HIS:C    | 2:CA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:N:619:HIS:C    | 2:DA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:O:433:GLN:HA   | 1:m:349:THR:HA   | 1.94                     | 0.48              |
| 1:O:619:HIS:C    | 2:EA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:S:332:GLN:HE21 | 1:S:395:MET:HE3  | 1.78                     | 0.48              |
| 1:S:513:ASN:ND2  | 1:S:526:THR:HG22 | 2.10                     | 0.48              |
| 1:V:332:GLN:HE21 | 1:V:395:MET:HE3  | 1.78                     | 0.48              |
| 1:V:628:GLY:C    | 2:MA:997:DA:N1   | 2.66                     | 0.48              |
| 1:W:588:GLN:HG3  | 1:Y:589:GLU:OE2  | 2.12                     | 0.48              |
| 1:Y:415:SER:HB2  | 1:Y:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:a:332:GLN:HE21 | 1:a:395:MET:HE3  | 1.78                     | 0.48              |
| 1:a:415:SER:HB2  | 1:a:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:g:619:HIS:C    | 2:YA:997:DA:H2'  | 2.38                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:332:GLN:HE21 | 1:r:395:MET:HE3  | 1.78                     | 0.48              |
| 1:s:628:GLY:C    | 2:lA:997:DA:N1   | 2.66                     | 0.48              |
| 1:z:515:LEU:HD21 | 1:1:498:GLU:HA   | 1.94                     | 0.48              |
| 1:z:619:HIS:C    | 2:tA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:B:619:HIS:C    | 2:JA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:D:291:ILE:HD12 | 1:D:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:D:390:TYR:OH   | 1:E:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:E:433:GLN:HA   | 1:Q:349:THR:HA   | 1.94                     | 0.48              |
| 1:E:503:GLN:O    | 1:E:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:G:588:GLN:HG3  | 1:I:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:L:415:SER:HB2  | 1:L:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:N:515:LEU:HD21 | 1:P:498:GLU:HA   | 1.94                     | 0.48              |
| 1:O:415:SER:HB2  | 1:O:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:Q:619:HIS:C    | 2:GA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:X:332:GLN:HE21 | 1:X:395:MET:HE3  | 1.78                     | 0.48              |
| 1:Y:678:GLU:OE2  | 1:Y:680:SER:OG   | 2.24                     | 0.48              |
| 1:Z:415:SER:HB2  | 1:Z:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:b:415:SER:HB2  | 1:b:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:e:503:GLN:O    | 1:e:505:PRO:HD3  | 2.13                     | 0.48              |
| 1:e:619:HIS:C    | 2:WA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:g:415:SER:HB2  | 1:g:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:i:498:GLU:HA   | 1:k:515:LEU:HD21 | 1.94                     | 0.48              |
| 1:j:628:GLY:C    | 2:bA:997:DA:N1   | 2.66                     | 0.48              |
| 1:l:332:GLN:HE21 | 1:l:395:MET:HE3  | 1.78                     | 0.48              |
| 1:o:415:SER:HB2  | 1:o:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:q:433:GLN:HA   | 1:r:349:THR:HA   | 1.94                     | 0.48              |
| 1:s:332:GLN:HE21 | 1:s:395:MET:HE3  | 1.78                     | 0.48              |
| 1:u:286:ASP:OD2  | 1:2:390:TYR:OH   | 2.32                     | 0.48              |
| 1:u:433:GLN:HA   | 1:v:349:THR:HA   | 1.94                     | 0.48              |
| 1:v:619:HIS:C    | 2:oA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:w:332:GLN:HE21 | 1:w:395:MET:HE3  | 1.78                     | 0.48              |
| 1:1:291:ILE:HD12 | 1:1:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:3:513:ASN:ND2  | 1:3:526:THR:HG22 | 2.10                     | 0.48              |
| 1:8:628:GLY:C    | 2:2A:997:DA:N1   | 2.66                     | 0.48              |
| 1:B:291:ILE:HD12 | 1:B:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:B:503:GLN:O    | 1:B:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:E:332:GLN:HE21 | 1:E:395:MET:HE3  | 1.78                     | 0.48              |
| 1:G:332:GLN:HE21 | 1:G:395:MET:HE3  | 1.78                     | 0.48              |
| 1:G:513:ASN:ND2  | 1:G:526:THR:HG22 | 2.10                     | 0.48              |
| 1:H:588:GLN:HG3  | 1:W:589:GLU:OE2  | 2.12                     | 0.48              |
| 1:M:291:ILE:HD12 | 1:M:719:TYR:CE2  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:349:THR:HA   | 1:b:433:GLN:HA   | 1.94                     | 0.48              |
| 1:M:503:GLN:O    | 1:M:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:P:291:ILE:HD12 | 1:P:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:R:628:GLY:C    | 2:HA:997:DA:N1   | 2.66                     | 0.48              |
| 1:T:332:GLN:HE21 | 1:T:395:MET:HE3  | 1.78                     | 0.48              |
| 1:T:513:ASN:ND2  | 1:T:526:THR:HG22 | 2.10                     | 0.48              |
| 1:W:332:GLN:HE21 | 1:W:395:MET:HE3  | 1.78                     | 0.48              |
| 1:X:589:GLU:OE2  | 1:e:588:GLN:HG3  | 2.12                     | 0.48              |
| 1:c:330:THR:HG21 | 1:c:395:MET:HE2  | 1.96                     | 0.48              |
| 1:c:415:SER:HB2  | 1:c:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:e:330:THR:HG21 | 1:e:395:MET:HE2  | 1.96                     | 0.48              |
| 1:e:332:GLN:HE21 | 1:e:395:MET:HE3  | 1.78                     | 0.48              |
| 1:f:332:GLN:HE21 | 1:f:395:MET:HE3  | 1.78                     | 0.48              |
| 1:i:332:GLN:HE21 | 1:i:395:MET:HE3  | 1.78                     | 0.48              |
| 1:j:332:GLN:HE21 | 1:j:395:MET:HE3  | 1.78                     | 0.48              |
| 1:j:619:HIS:C    | 2:bA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:m:332:GLN:HE21 | 1:m:395:MET:HE3  | 1.78                     | 0.48              |
| 1:n:699:VAL:HG23 | 1:n:702:ALA:HB3  | 1.94                     | 0.48              |
| 1:r:330:THR:HG21 | 1:r:395:MET:HE2  | 1.96                     | 0.48              |
| 1:r:503:GLN:O    | 1:r:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:r:619:HIS:C    | 2:kA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:u:332:GLN:HE21 | 1:u:395:MET:HE3  | 1.78                     | 0.48              |
| 1:u:503:GLN:O    | 1:u:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:2:291:ILE:HD12 | 1:2:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:4:415:SER:HB2  | 1:4:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:6:332:GLN:HE21 | 1:6:395:MET:HE3  | 1.78                     | 0.48              |
| 1:6:588:GLN:HG3  | 1:7:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:8:619:HIS:C    | 2:2A:997:DA:H2'  | 2.38                     | 0.48              |
| 1:C:513:ASN:ND2  | 1:C:526:THR:HG22 | 2.10                     | 0.48              |
| 1:P:286:ASP:OD2  | 1:Q:390:TYR:OH   | 2.32                     | 0.48              |
| 1:S:286:ASP:OD2  | 1:d:390:TYR:OH   | 2.32                     | 0.48              |
| 1:T:503:GLN:O    | 1:T:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:T:619:HIS:C    | 2:KA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:U:330:THR:HG21 | 1:U:395:MET:HE2  | 1.96                     | 0.48              |
| 1:V:349:THR:HA   | 1:X:433:GLN:HA   | 1.95                     | 0.48              |
| 1:Y:291:ILE:HD12 | 1:Y:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:Z:433:GLN:HA   | 1:4:349:THR:HA   | 1.94                     | 0.48              |
| 1:Z:513:ASN:ND2  | 1:Z:526:THR:HG22 | 2.10                     | 0.48              |
| 1:Z:619:HIS:C    | 2:QA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:d:699:VAL:HG23 | 1:d:702:ALA:HB3  | 1.94                     | 0.48              |
| 1:h:330:THR:HG21 | 1:h:395:MET:HE2  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:699:VAL:HG23 | 1:h:702:ALA:HB3  | 1.94                     | 0.48              |
| 1:o:588:GLN:HG3  | 1:p:589:GLU:OE2  | 2.12                     | 0.48              |
| 1:p:332:GLN:HE21 | 1:p:395:MET:HE3  | 1.78                     | 0.48              |
| 1:t:503:GLN:O    | 1:t:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:v:286:ASP:OD2  | 1:w:390:TYR:OH   | 2.32                     | 0.48              |
| 1:v:390:TYR:OH   | 1:1:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:w:330:THR:HG21 | 1:w:395:MET:HE2  | 1.96                     | 0.48              |
| 1:y:291:ILE:HD12 | 1:y:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:z:588:GLN:HG3  | 1:1:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:2:372:ASN:ND2  | 1:2:376:THR:O    | 2.44                     | 0.48              |
| 1:4:291:ILE:HD12 | 1:4:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:5:588:GLN:HG3  | 1:6:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:A:330:THR:HG21 | 1:A:395:MET:HE2  | 1.96                     | 0.48              |
| 1:C:433:GLN:HA   | 1:b:349:THR:HA   | 1.94                     | 0.48              |
| 1:D:372:ASN:ND2  | 1:D:376:THR:O    | 2.44                     | 0.48              |
| 1:F:503:GLN:O    | 1:F:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:L:286:ASP:OD2  | 1:b:390:TYR:OH   | 2.32                     | 0.48              |
| 1:Q:286:ASP:OD2  | 1:S:390:TYR:OH   | 2.32                     | 0.48              |
| 1:R:291:ILE:HD12 | 1:R:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:R:699:VAL:HG23 | 1:R:702:ALA:HB3  | 1.94                     | 0.48              |
| 1:S:330:THR:HG21 | 1:S:395:MET:HE2  | 1.96                     | 0.48              |
| 1:W:330:THR:HG21 | 1:W:395:MET:HE2  | 1.96                     | 0.48              |
| 1:Y:330:THR:HG21 | 1:Y:395:MET:HE2  | 1.96                     | 0.48              |
| 1:Y:619:HIS:C    | 2:PA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:a:503:GLN:O    | 1:a:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:b:619:HIS:C    | 2:SA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:f:678:GLU:OE2  | 1:f:680:SER:OG   | 2.24                     | 0.48              |
| 1:g:330:THR:HG21 | 1:g:395:MET:HE2  | 1.96                     | 0.48              |
| 1:j:503:GLN:O    | 1:j:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:k:390:TYR:OH   | 1:w:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:k:699:VAL:HG23 | 1:k:702:ALA:HB3  | 1.94                     | 0.48              |
| 1:p:330:THR:HG21 | 1:p:395:MET:HE2  | 1.96                     | 0.48              |
| 1:u:330:THR:HG21 | 1:u:395:MET:HE2  | 1.96                     | 0.48              |
| 1:x:330:THR:HG21 | 1:x:395:MET:HE2  | 1.96                     | 0.48              |
| 1:8:291:ILE:HD12 | 1:8:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:8:503:GLN:O    | 1:8:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:B:488:ALA:O    | 1:B:492:THR:HG23 | 2.14                     | 0.48              |
| 1:E:330:THR:HG21 | 1:E:395:MET:HE2  | 1.96                     | 0.48              |
| 1:K:619:HIS:C    | 2:AA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:M:390:TYR:OH   | 1:c:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:N:588:GLN:HG3  | 1:P:589:GLU:OE2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:330:THR:HG21 | 1:O:395:MET:HE2  | 1.96                     | 0.48              |
| 1:T:390:TYR:OH   | 1:i:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:V:433:GLN:HA   | 1:e:349:THR:HA   | 1.94                     | 0.48              |
| 1:Z:390:TYR:OH   | 1:a:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:c:291:ILE:HD12 | 1:c:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:c:619:HIS:C    | 2:TA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:d:332:GLN:HE21 | 1:d:395:MET:HE3  | 1.78                     | 0.48              |
| 1:e:513:ASN:ND2  | 1:e:526:THR:HG22 | 2.10                     | 0.48              |
| 1:f:390:TYR:OH   | 1:z:286:ASP:OD2  | 2.31                     | 0.48              |
| 1:g:291:ILE:HD12 | 1:g:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:g:513:ASN:ND2  | 1:g:526:THR:HG22 | 2.10                     | 0.48              |
| 1:h:332:GLN:HE21 | 1:h:395:MET:HE3  | 1.78                     | 0.48              |
| 1:i:330:THR:HG21 | 1:i:395:MET:HE2  | 1.96                     | 0.48              |
| 1:k:332:GLN:HE21 | 1:k:395:MET:HE3  | 1.78                     | 0.48              |
| 1:l:619:HIS:C    | 2:dA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:n:330:THR:HG21 | 1:n:395:MET:HE2  | 1.96                     | 0.48              |
| 1:q:619:HIS:C    | 2:jA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:r:415:SER:HB2  | 1:r:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:r:681:LYS:HG3  | 1:s:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:u:390:TYR:OH   | 1:5:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:u:588:GLN:HG3  | 1:v:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:2:286:ASP:OD2  | 1:3:390:TYR:OH   | 2.32                     | 0.48              |
| 1:4:503:GLN:O    | 1:4:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:7:332:GLN:HE21 | 1:7:395:MET:HE3  | 1.78                     | 0.48              |
| 1:8:488:ALA:O    | 1:8:492:THR:HG23 | 2.14                     | 0.48              |
| 1:A:410:GLU:OE2  | 2:0:996:DA:N6    | 2.47                     | 0.48              |
| 1:A:453:LEU:HD22 | 1:G:537:GLY:HA2  | 1.96                     | 0.48              |
| 1:C:390:TYR:OH   | 1:D:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:D:330:THR:HG21 | 1:D:395:MET:HE2  | 1.96                     | 0.48              |
| 1:E:588:GLN:HG3  | 1:Q:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:F:286:ASP:OD2  | 1:G:390:TYR:OH   | 2.31                     | 0.48              |
| 1:I:291:ILE:HD12 | 1:I:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:J:619:HIS:C    | 2:9:997:DA:H2'   | 2.38                     | 0.48              |
| 1:L:503:GLN:O    | 1:L:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:N:286:ASP:OD2  | 1:m:390:TYR:OH   | 2.31                     | 0.48              |
| 1:O:291:ILE:HD12 | 1:O:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:R:332:GLN:HE21 | 1:R:395:MET:HE3  | 1.78                     | 0.48              |
| 1:V:619:HIS:C    | 2:MA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:X:286:ASP:OD2  | 1:Y:390:TYR:OH   | 2.32                     | 0.48              |
| 1:Y:286:ASP:OD2  | 1:4:390:TYR:OH   | 2.32                     | 0.48              |
| 1:Z:349:THR:HA   | 1:3:433:GLN:HA   | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:588:GLN:HG3  | 1:l:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:e:415:SER:HB2  | 1:e:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:i:619:HIS:C    | 2:aA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:j:390:TYR:OH   | 1:l:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:l:330:THR:HG21 | 1:l:395:MET:HE2  | 1.96                     | 0.48              |
| 1:s:291:ILE:HD12 | 1:s:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:x:628:GLY:C    | 2:rA:997:DA:N1   | 2.67                     | 0.48              |
| 1:y:628:GLY:C    | 2:sA:997:DA:N1   | 2.66                     | 0.48              |
| 1:y:699:VAL:HG23 | 1:y:702:ALA:HB3  | 1.94                     | 0.48              |
| 1:1:332:GLN:HE21 | 1:1:395:MET:HE3  | 1.78                     | 0.48              |
| 1:4:332:GLN:HE21 | 1:4:395:MET:HE3  | 1.78                     | 0.48              |
| 1:5:330:THR:HG21 | 1:5:395:MET:HE2  | 1.96                     | 0.48              |
| 1:5:681:LYS:HG3  | 1:6:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:6:513:ASN:ND2  | 1:6:526:THR:HG22 | 2.10                     | 0.48              |
| 1:A:515:LEU:HD21 | 1:G:498:GLU:HA   | 1.95                     | 0.48              |
| 1:A:589:GLU:OE2  | 1:I:588:GLN:HG3  | 2.13                     | 0.48              |
| 1:B:330:THR:HG21 | 1:B:395:MET:HE2  | 1.96                     | 0.48              |
| 1:F:349:THR:HA   | 1:Q:433:GLN:HA   | 1.94                     | 0.48              |
| 1:F:410:GLU:OE2  | 2:1A:996:DA:N6   | 2.47                     | 0.48              |
| 1:L:410:GLU:OE2  | 2:BA:996:DA:N6   | 2.47                     | 0.48              |
| 1:M:332:GLN:HE21 | 1:M:395:MET:HE3  | 1.78                     | 0.48              |
| 1:O:513:ASN:ND2  | 1:O:526:THR:HG22 | 2.10                     | 0.48              |
| 1:P:332:GLN:HE21 | 1:P:395:MET:HE3  | 1.78                     | 0.48              |
| 1:P:410:GLU:OE2  | 2:FA:996:DA:N6   | 2.47                     | 0.48              |
| 1:Q:332:GLN:HE21 | 1:Q:395:MET:HE3  | 1.78                     | 0.48              |
| 1:X:291:ILE:HD12 | 1:X:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:Z:488:ALA:O    | 1:Z:492:THR:HG23 | 2.14                     | 0.48              |
| 1:a:588:GLN:HG3  | 1:8:589:GLU:OE2  | 2.13                     | 0.48              |
| 1:b:332:GLN:HE21 | 1:b:395:MET:HE3  | 1.78                     | 0.48              |
| 1:b:488:ALA:O    | 1:b:492:THR:HG23 | 2.14                     | 0.48              |
| 1:f:488:ALA:O    | 1:f:492:THR:HG23 | 2.14                     | 0.48              |
| 1:i:589:GLU:OE2  | 1:k:588:GLN:HG3  | 2.13                     | 0.48              |
| 1:m:488:ALA:O    | 1:m:492:THR:HG23 | 2.14                     | 0.48              |
| 1:m:678:GLU:OE2  | 1:m:680:SER:OG   | 2.24                     | 0.48              |
| 1:n:332:GLN:HE21 | 1:n:395:MET:HE3  | 1.78                     | 0.48              |
| 1:t:286:ASP:OD2  | 1:6:390:TYR:OH   | 2.31                     | 0.48              |
| 1:t:349:THR:HA   | 1:v:433:GLN:HA   | 1.94                     | 0.48              |
| 1:t:410:GLU:OE2  | 2:mA:996:DA:N6   | 2.47                     | 0.48              |
| 1:t:619:HIS:C    | 2:mA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:v:332:GLN:HE21 | 1:v:395:MET:HE3  | 1.78                     | 0.48              |
| 1:x:291:ILE:HD12 | 1:x:719:TYR:CE2  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:y:332:GLN:HE21 | 1:y:395:MET:HE3  | 1.78                     | 0.48              |
| 1:2:330:THR:HG21 | 1:2:395:MET:HE2  | 1.96                     | 0.48              |
| 1:5:410:GLU:OE2  | 2:yA:996:DA:N6   | 2.47                     | 0.48              |
| 1:5:433:GLN:HA   | 1:6:349:THR:HA   | 1.95                     | 0.48              |
| 1:5:488:ALA:O    | 1:5:492:THR:HG23 | 2.14                     | 0.48              |
| 1:7:291:ILE:HD12 | 1:7:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:A:488:ALA:O    | 1:A:492:THR:HG23 | 2.14                     | 0.48              |
| 1:C:332:GLN:HE21 | 1:C:395:MET:HE3  | 1.78                     | 0.48              |
| 1:E:391:PHE:CE1  | 1:F:681:LYS:HG3  | 2.49                     | 0.48              |
| 1:G:330:THR:HG21 | 1:G:395:MET:HE2  | 1.96                     | 0.48              |
| 1:G:681:LYS:HG3  | 1:I:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:H:332:GLN:HE21 | 1:H:395:MET:HE3  | 1.78                     | 0.48              |
| 1:I:332:GLN:HE21 | 1:I:395:MET:HE3  | 1.78                     | 0.48              |
| 1:J:503:GLN:O    | 1:J:505:PRO:HD3  | 2.12                     | 0.48              |
| 1:L:619:HIS:C    | 2:BA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:N:433:GLN:HA   | 1:P:349:THR:HA   | 1.94                     | 0.48              |
| 1:U:291:ILE:HD12 | 1:U:719:TYR:CE2  | 2.48                     | 0.48              |
| 1:U:488:ALA:O    | 1:U:492:THR:HG23 | 2.14                     | 0.48              |
| 1:U:628:GLY:C    | 2:LA:997:DA:N1   | 2.67                     | 0.48              |
| 1:X:330:THR:HG21 | 1:X:395:MET:HE2  | 1.96                     | 0.48              |
| 1:Z:332:GLN:HE21 | 1:Z:395:MET:HE3  | 1.78                     | 0.48              |
| 1:a:410:GLU:OE2  | 2:RA:996:DA:N6   | 2.47                     | 0.48              |
| 1:d:330:THR:HG21 | 1:d:395:MET:HE2  | 1.96                     | 0.48              |
| 1:i:681:LYS:HG3  | 1:j:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:m:286:ASP:OD2  | 1:s:390:TYR:OH   | 2.31                     | 0.48              |
| 1:m:681:LYS:HG3  | 1:n:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:o:332:GLN:HE21 | 1:o:395:MET:HE3  | 1.78                     | 0.48              |
| 1:t:681:LYS:HG3  | 1:u:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:w:433:GLN:HA   | 1:x:349:THR:HA   | 1.94                     | 0.48              |
| 1:x:488:ALA:O    | 1:x:492:THR:HG23 | 2.14                     | 0.48              |
| 1:1:410:GLU:OE2  | 2:uA:996:DA:N6   | 2.47                     | 0.48              |
| 1:4:488:ALA:O    | 1:4:492:THR:HG23 | 2.14                     | 0.48              |
| 1:5:391:PHE:CE1  | 1:7:681:LYS:HG3  | 2.49                     | 0.48              |
| 1:6:681:LYS:HG3  | 1:7:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:8:330:THR:HG21 | 1:8:395:MET:HE2  | 1.96                     | 0.48              |
| 1:A:332:GLN:HE21 | 1:A:395:MET:HE3  | 1.78                     | 0.48              |
| 1:B:390:TYR:OH   | 1:C:286:ASP:OD2  | 2.32                     | 0.48              |
| 1:B:589:GLU:OE2  | 1:L:588:GLN:HG3  | 2.13                     | 0.48              |
| 1:C:488:ALA:O    | 1:C:492:THR:HG23 | 2.14                     | 0.48              |
| 1:D:619:HIS:C    | 2:fA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:F:332:GLN:HE21 | 1:F:395:MET:HE3  | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:415:SER:HB2  | 1:F:417:PHE:CE2  | 2.47                     | 0.48              |
| 1:F:619:HIS:C    | 2:1A:997:DA:H2'  | 2.38                     | 0.48              |
| 1:M:488:ALA:O    | 1:M:492:THR:HG23 | 2.14                     | 0.48              |
| 1:T:391:PHE:CE1  | 1:l:681:LYS:HG3  | 2.49                     | 0.48              |
| 1:W:488:ALA:O    | 1:W:492:THR:HG23 | 2.14                     | 0.48              |
| 1:a:619:HIS:C    | 2:RA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:j:681:LYS:HG3  | 1:k:391:PHE:CE1  | 2.49                     | 0.48              |
| 1:k:330:THR:HG21 | 1:k:395:MET:HE2  | 1.96                     | 0.48              |
| 1:k:619:HIS:C    | 2:cA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:m:619:HIS:C    | 2:eA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:p:488:ALA:O    | 1:p:492:THR:HG23 | 2.14                     | 0.48              |
| 1:s:330:THR:HG21 | 1:s:395:MET:HE2  | 1.96                     | 0.48              |
| 1:t:332:GLN:HE21 | 1:t:395:MET:HE3  | 1.78                     | 0.48              |
| 1:z:433:GLN:HA   | 1:1:349:THR:HA   | 1.94                     | 0.48              |
| 1:2:332:GLN:HE21 | 1:2:395:MET:HE3  | 1.78                     | 0.48              |
| 1:2:619:HIS:C    | 2:vA:997:DA:H2'  | 2.38                     | 0.48              |
| 1:3:286:ASP:OD2  | 1:8:390:TYR:OH   | 2.32                     | 0.48              |
| 1:3:332:GLN:HE21 | 1:3:395:MET:HE3  | 1.78                     | 0.48              |
| 1:5:332:GLN:HE21 | 1:5:395:MET:HE3  | 1.78                     | 0.48              |
| 1:6:330:THR:HG21 | 1:6:395:MET:HE2  | 1.96                     | 0.48              |
| 1:A:433:GLN:HA   | 1:G:349:THR:HA   | 1.94                     | 0.47              |
| 1:C:619:HIS:C    | 2:UA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:D:332:GLN:HE21 | 1:D:395:MET:HE3  | 1.78                     | 0.47              |
| 1:I:488:ALA:O    | 1:I:492:THR:HG23 | 2.14                     | 0.47              |
| 1:J:681:LYS:HG3  | 1:L:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:K:503:GLN:O    | 1:K:505:PRO:HD3  | 2.12                     | 0.47              |
| 1:K:681:LYS:HG3  | 1:a:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:S:433:GLN:HA   | 1:U:349:THR:HA   | 1.94                     | 0.47              |
| 1:T:681:LYS:HG3  | 1:d:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:f:619:HIS:C    | 2:XA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:f:681:LYS:HG3  | 1:h:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:j:330:THR:HG21 | 1:j:395:MET:HE2  | 1.96                     | 0.47              |
| 1:q:488:ALA:O    | 1:q:492:THR:HG23 | 2.14                     | 0.47              |
| 1:r:390:TYR:OH   | 1:x:286:ASP:OD2  | 2.31                     | 0.47              |
| 1:t:415:SER:HB2  | 1:t:417:PHE:CE2  | 2.47                     | 0.47              |
| 1:y:330:THR:HG21 | 1:y:395:MET:HE2  | 1.96                     | 0.47              |
| 1:1:681:LYS:HG3  | 1:2:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:3:330:THR:HG21 | 1:3:395:MET:HE2  | 1.96                     | 0.47              |
| 1:3:488:ALA:O    | 1:3:492:THR:HG23 | 2.14                     | 0.47              |
| 1:3:619:HIS:C    | 2:wA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:6:410:GLU:OE2  | 2:zA:996:DA:N6   | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:7:488:ALA:O    | 1:7:492:THR:HG23 | 2.14                     | 0.47              |
| 1:C:330:THR:HG21 | 1:C:395:MET:HE2  | 1.96                     | 0.47              |
| 1:D:391:PHE:CE1  | 1:P:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:F:488:ALA:O    | 1:F:492:THR:HG23 | 2.14                     | 0.47              |
| 1:H:681:LYS:HG3  | 1:W:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:M:286:ASP:OD2  | 1:N:390:TYR:OH   | 2.32                     | 0.47              |
| 1:N:628:GLY:C    | 2:DA:997:DA:N1   | 2.66                     | 0.47              |
| 1:O:349:THR:HA   | 1:n:433:GLN:HA   | 1.95                     | 0.47              |
| 1:O:681:LYS:HG3  | 1:m:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:T:330:THR:HG21 | 1:T:395:MET:HE2  | 1.96                     | 0.47              |
| 1:W:433:GLN:HA   | 1:Y:349:THR:HA   | 1.95                     | 0.47              |
| 1:a:488:ALA:O    | 1:a:492:THR:HG23 | 2.14                     | 0.47              |
| 1:d:488:ALA:O    | 1:d:492:THR:HG23 | 2.14                     | 0.47              |
| 1:d:619:HIS:C    | 2:VA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:g:349:THR:HA   | 1:h:433:GLN:HA   | 1.95                     | 0.47              |
| 1:n:503:GLN:O    | 1:n:505:PRO:HD3  | 2.12                     | 0.47              |
| 1:o:681:LYS:HG3  | 1:p:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:q:286:ASP:OD2  | 1:y:390:TYR:OH   | 2.32                     | 0.47              |
| 1:q:681:LYS:HG3  | 1:r:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:r:513:ASN:ND2  | 1:r:526:THR:HG22 | 2.10                     | 0.47              |
| 1:t:488:ALA:O    | 1:t:492:THR:HG23 | 2.14                     | 0.47              |
| 1:y:488:ALA:O    | 1:y:492:THR:HG23 | 2.14                     | 0.47              |
| 1:z:628:GLY:C    | 2:tA:997:DA:N1   | 2.66                     | 0.47              |
| 1:3:291:ILE:HD12 | 1:3:719:TYR:CE2  | 2.48                     | 0.47              |
| 1:C:291:ILE:HD12 | 1:C:719:TYR:CE2  | 2.48                     | 0.47              |
| 1:C:681:LYS:HG3  | 1:b:391:PHE:CE1  | 2.50                     | 0.47              |
| 1:G:410:GLU:OE2  | 2:3A:996:DA:N6   | 2.47                     | 0.47              |
| 1:J:330:THR:HG21 | 1:J:395:MET:HE2  | 1.96                     | 0.47              |
| 1:J:488:ALA:O    | 1:J:492:THR:HG23 | 2.14                     | 0.47              |
| 1:K:488:ALA:O    | 1:K:492:THR:HG23 | 2.14                     | 0.47              |
| 1:L:488:ALA:O    | 1:L:492:THR:HG23 | 2.14                     | 0.47              |
| 1:L:678:GLU:OE2  | 1:L:680:SER:OG   | 2.24                     | 0.47              |
| 1:N:488:ALA:O    | 1:N:492:THR:HG23 | 2.14                     | 0.47              |
| 1:N:619:HIS:CA   | 2:DA:997:DA:O3'  | 2.60                     | 0.47              |
| 1:O:391:PHE:CE1  | 1:n:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:Q:410:GLU:OE2  | 2:GA:996:DA:N6   | 2.47                     | 0.47              |
| 1:R:488:ALA:O    | 1:R:492:THR:HG23 | 2.14                     | 0.47              |
| 1:U:286:ASP:OD2  | 1:e:390:TYR:OH   | 2.32                     | 0.47              |
| 1:V:390:TYR:OH   | 1:W:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:V:410:GLU:OE2  | 2:MA:996:DA:N6   | 2.47                     | 0.47              |
| 1:V:488:ALA:O    | 1:V:492:THR:HG23 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:391:PHE:CE1  | 1:e:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:Y:332:GLN:HE21 | 1:Y:395:MET:HE3  | 1.78                     | 0.47              |
| 1:Z:391:PHE:CE1  | 1:3:681:LYS:HG3  | 2.50                     | 0.47              |
| 1:b:380:THR:HG22 | 1:b:381:GLU:N    | 2.30                     | 0.47              |
| 1:c:332:GLN:HE21 | 1:c:395:MET:HE3  | 1.78                     | 0.47              |
| 1:c:349:THR:HA   | 1:p:433:GLN:HA   | 1.95                     | 0.47              |
| 1:g:391:PHE:CE1  | 1:h:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:h:503:GLN:O    | 1:h:505:PRO:HD3  | 2.12                     | 0.47              |
| 1:i:410:GLU:OE2  | 2:aA:996:DA:N6   | 2.47                     | 0.47              |
| 1:l:410:GLU:OE2  | 2:dA:996:DA:N6   | 2.47                     | 0.47              |
| 1:p:380:THR:HG22 | 1:p:381:GLU:N    | 2.30                     | 0.47              |
| 1:r:410:GLU:OE2  | 2:kA:996:DA:N6   | 2.47                     | 0.47              |
| 1:w:391:PHE:CE1  | 1:y:681:LYS:HG3  | 2.50                     | 0.47              |
| 1:z:390:TYR:OH   | 1:4:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:E:619:HIS:C    | 2:qA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:K:330:THR:HG21 | 1:K:395:MET:HE2  | 1.96                     | 0.47              |
| 1:R:330:THR:HG21 | 1:R:395:MET:HE2  | 1.96                     | 0.47              |
| 1:R:390:TYR:OH   | 1:V:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:R:681:LYS:HG3  | 1:S:391:PHE:CE1  | 2.50                     | 0.47              |
| 1:T:286:ASP:OD2  | 1:U:390:TYR:OH   | 2.32                     | 0.47              |
| 1:V:330:THR:HG21 | 1:V:395:MET:HE2  | 1.96                     | 0.47              |
| 1:V:391:PHE:CE1  | 1:X:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:V:681:LYS:HG3  | 1:e:391:PHE:CE1  | 2.50                     | 0.47              |
| 1:W:380:THR:HG22 | 1:W:381:GLU:N    | 2.30                     | 0.47              |
| 1:Z:380:THR:HG22 | 1:Z:381:GLU:N    | 2.30                     | 0.47              |
| 1:a:681:LYS:HG3  | 1:8:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:d:380:THR:HG22 | 1:d:381:GLU:N    | 2.30                     | 0.47              |
| 1:d:681:LYS:HG3  | 1:l:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:e:410:GLU:OE2  | 2:WA:996:DA:N6   | 2.47                     | 0.47              |
| 1:f:391:PHE:CE1  | 1:g:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:k:380:THR:HG22 | 1:k:381:GLU:N    | 2.30                     | 0.47              |
| 1:q:330:THR:HG21 | 1:q:395:MET:HE2  | 1.96                     | 0.47              |
| 1:q:410:GLU:OE2  | 2:jA:996:DA:N6   | 2.47                     | 0.47              |
| 1:t:380:THR:HG22 | 1:t:381:GLU:N    | 2.30                     | 0.47              |
| 1:t:391:PHE:CE1  | 1:v:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:t:588:GLN:HG3  | 1:u:589:GLU:OE2  | 2.13                     | 0.47              |
| 1:v:410:GLU:OE2  | 2:oA:996:DA:N6   | 2.47                     | 0.47              |
| 1:v:488:ALA:O    | 1:v:492:THR:HG23 | 2.14                     | 0.47              |
| 1:y:619:HIS:C    | 2:sA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:z:488:ALA:O    | 1:z:492:THR:HG23 | 2.14                     | 0.47              |
| 1:4:380:THR:HG22 | 1:4:381:GLU:N    | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:5:619:HIS:C    | 2:yA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:7:330:THR:HG21 | 1:7:395:MET:HE2  | 1.96                     | 0.47              |
| 1:A:619:HIS:C    | 2:0:997:DA:H2'   | 2.38                     | 0.47              |
| 1:B:391:PHE:CE1  | 1:L:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:E:589:GLU:OE2  | 1:F:588:GLN:HG3  | 2.13                     | 0.47              |
| 1:E:681:LYS:HG3  | 1:Q:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:F:380:THR:HG22 | 1:F:381:GLU:N    | 2.30                     | 0.47              |
| 1:F:391:PHE:CE1  | 1:Q:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:H:330:THR:HG21 | 1:H:395:MET:HE2  | 1.96                     | 0.47              |
| 1:H:488:ALA:O    | 1:H:492:THR:HG23 | 2.14                     | 0.47              |
| 1:I:330:THR:HG21 | 1:I:395:MET:HE2  | 1.96                     | 0.47              |
| 1:J:286:ASP:OD2  | 1:a:390:TYR:OH   | 2.32                     | 0.47              |
| 1:K:286:ASP:OD2  | 1:L:390:TYR:OH   | 2.32                     | 0.47              |
| 1:M:380:THR:HG22 | 1:M:381:GLU:N    | 2.30                     | 0.47              |
| 1:P:380:THR:HG22 | 1:P:381:GLU:N    | 2.30                     | 0.47              |
| 1:Q:488:ALA:O    | 1:Q:492:THR:HG23 | 2.14                     | 0.47              |
| 1:R:619:HIS:C    | 2:HA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:V:372:ASN:ND2  | 1:V:376:THR:O    | 2.44                     | 0.47              |
| 1:X:410:GLU:OE2  | 2:OA:996:DA:N6   | 2.47                     | 0.47              |
| 1:g:380:THR:HG22 | 1:g:381:GLU:N    | 2.30                     | 0.47              |
| 1:i:391:PHE:CE1  | 1:k:681:LYS:HG3  | 2.50                     | 0.47              |
| 1:i:678:GLU:OE2  | 1:i:680:SER:OG   | 2.24                     | 0.47              |
| 1:j:286:ASP:OD2  | 1:x:390:TYR:OH   | 2.32                     | 0.47              |
| 1:k:488:ALA:O    | 1:k:492:THR:HG23 | 2.14                     | 0.47              |
| 1:m:330:THR:HG21 | 1:m:395:MET:HE2  | 1.96                     | 0.47              |
| 1:o:488:ALA:O    | 1:o:492:THR:HG23 | 2.14                     | 0.47              |
| 1:p:410:GLU:OE2  | 2:iA:996:DA:N6   | 2.47                     | 0.47              |
| 1:u:380:THR:HG22 | 1:u:381:GLU:N    | 2.30                     | 0.47              |
| 1:u:619:HIS:C    | 2:nA:997:DA:H2'  | 2.38                     | 0.47              |
| 1:z:619:HIS:CA   | 2:tA:997:DA:O3'  | 2.60                     | 0.47              |
| 1:1:380:THR:HG22 | 1:1:381:GLU:N    | 2.30                     | 0.47              |
| 1:7:380:THR:HG22 | 1:7:381:GLU:N    | 2.30                     | 0.47              |
| 1:E:380:THR:HG22 | 1:E:381:GLU:N    | 2.30                     | 0.47              |
| 1:F:390:TYR:OH   | 1:R:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:I:380:THR:HG22 | 1:I:381:GLU:N    | 2.30                     | 0.47              |
| 1:O:380:THR:HG22 | 1:O:381:GLU:N    | 2.30                     | 0.47              |
| 1:O:390:TYR:OH   | 1:d:286:ASP:OD2  | 2.31                     | 0.47              |
| 1:S:488:ALA:O    | 1:S:492:THR:HG23 | 2.14                     | 0.47              |
| 1:W:410:GLU:OE2  | 2:NA:996:DA:N6   | 2.47                     | 0.47              |
| 1:Z:330:THR:HG21 | 1:Z:395:MET:HE2  | 1.96                     | 0.47              |
| 1:b:330:THR:HG21 | 1:b:395:MET:HE2  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:488:ALA:O    | 1:c:492:THR:HG23 | 2.14                     | 0.47              |
| 1:f:330:THR:HG21 | 1:f:395:MET:HE2  | 1.96                     | 0.47              |
| 1:g:678:GLU:OE2  | 1:g:680:SER:OG   | 2.24                     | 0.47              |
| 1:h:488:ALA:O    | 1:h:492:THR:HG23 | 2.14                     | 0.47              |
| 1:n:488:ALA:O    | 1:n:492:THR:HG23 | 2.14                     | 0.47              |
| 1:o:330:THR:HG21 | 1:o:395:MET:HE2  | 1.96                     | 0.47              |
| 1:p:286:ASP:OD2  | 1:q:390:TYR:OH   | 2.32                     | 0.47              |
| 1:q:372:ASN:ND2  | 1:q:376:THR:O    | 2.44                     | 0.47              |
| 1:u:488:ALA:O    | 1:u:492:THR:HG23 | 2.14                     | 0.47              |
| 1:u:681:LYS:HG3  | 1:v:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:z:332:GLN:HE21 | 1:z:395:MET:HE3  | 1.78                     | 0.47              |
| 1:3:380:THR:HG22 | 1:3:381:GLU:N    | 2.30                     | 0.47              |
| 1:5:390:TYR:OH   | 1:8:286:ASP:OD2  | 2.31                     | 0.47              |
| 1:8:332:GLN:HE21 | 1:8:395:MET:HE3  | 1.78                     | 0.47              |
| 1:A:588:GLN:HG3  | 1:G:589:GLU:OE2  | 2.14                     | 0.47              |
| 1:B:332:GLN:HE21 | 1:B:395:MET:HE3  | 1.78                     | 0.47              |
| 1:B:681:LYS:HG3  | 1:J:391:PHE:CE1  | 2.50                     | 0.47              |
| 1:C:380:THR:HG22 | 1:C:381:GLU:N    | 2.30                     | 0.47              |
| 1:C:422:ASN:HB3  | 1:C:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:D:422:ASN:HB3  | 1:D:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:E:488:ALA:O    | 1:E:492:THR:HG23 | 2.14                     | 0.47              |
| 1:F:422:ASN:HB3  | 1:F:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:G:380:THR:HG22 | 1:G:381:GLU:N    | 2.30                     | 0.47              |
| 1:G:488:ALA:O    | 1:G:492:THR:HG23 | 2.14                     | 0.47              |
| 1:G:630:LYS:HD2  | 2:0:996:DA:OP2   | 2.14                     | 0.47              |
| 1:H:391:PHE:CE1  | 1:Y:681:LYS:HG3  | 2.50                     | 0.47              |
| 1:I:286:ASP:OD2  | 1:J:390:TYR:OH   | 2.32                     | 0.47              |
| 1:K:390:TYR:OH   | 1:7:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:K:391:PHE:CE1  | 1:8:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:M:410:GLU:OE2  | 2:CA:996:DA:N6   | 2.47                     | 0.47              |
| 1:N:332:GLN:HE21 | 1:N:395:MET:HE3  | 1.78                     | 0.47              |
| 1:O:422:ASN:HB3  | 1:O:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:Q:380:THR:HG22 | 1:Q:381:GLU:N    | 2.30                     | 0.47              |
| 1:T:422:ASN:HB3  | 1:T:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:U:332:GLN:HE21 | 1:U:395:MET:HE3  | 1.78                     | 0.47              |
| 1:U:678:GLU:OE2  | 1:U:680:SER:OG   | 2.24                     | 0.47              |
| 1:W:681:LYS:HG3  | 1:Y:391:PHE:CE1  | 2.49                     | 0.47              |
| 1:X:390:TYR:OH   | 1:f:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:X:488:ALA:O    | 1:X:492:THR:HG23 | 2.14                     | 0.47              |
| 1:a:513:ASN:ND2  | 1:a:526:THR:HG22 | 2.10                     | 0.47              |
| 1:c:422:ASN:HB3  | 1:c:425:LYS:HB2  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:681:LYS:HG3  | 1:o:391:PHE:CE1  | 2.50                     | 0.47              |
| 1:e:488:ALA:O    | 1:e:492:THR:HG23 | 2.14                     | 0.47              |
| 1:g:390:TYR:OH   | 1:k:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:g:422:ASN:HB3  | 1:g:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:j:422:ASN:HB3  | 1:j:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:r:488:ALA:O    | 1:r:492:THR:HG23 | 2.14                     | 0.47              |
| 1:s:410:GLU:OE2  | 2:lA:996:DA:N6   | 2.47                     | 0.47              |
| 1:s:488:ALA:O    | 1:s:492:THR:HG23 | 2.14                     | 0.47              |
| 1:t:390:TYR:OH   | 1:y:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:t:422:ASN:HB3  | 1:t:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:v:380:THR:HG22 | 1:v:381:GLU:N    | 2.30                     | 0.47              |
| 1:w:488:ALA:O    | 1:w:492:THR:HG23 | 2.14                     | 0.47              |
| 1:x:332:GLN:HE21 | 1:x:395:MET:HE3  | 1.78                     | 0.47              |
| 1:2:422:ASN:HB3  | 1:2:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:4:410:GLU:OE2  | 2:xA:996:DA:N6   | 2.47                     | 0.47              |
| 1:6:488:ALA:O    | 1:6:492:THR:HG23 | 2.14                     | 0.47              |
| 1:E:276:ASN:O    | 1:E:606:PRO:HA   | 2.15                     | 0.47              |
| 1:N:276:ASN:O    | 1:N:606:PRO:HA   | 2.15                     | 0.47              |
| 1:N:380:THR:HG22 | 1:N:381:GLU:N    | 2.30                     | 0.47              |
| 1:S:380:THR:HG22 | 1:S:381:GLU:N    | 2.30                     | 0.47              |
| 1:T:380:THR:HG22 | 1:T:381:GLU:N    | 2.30                     | 0.47              |
| 1:X:276:ASN:O    | 1:X:606:PRO:HA   | 2.15                     | 0.47              |
| 1:Y:422:ASN:HB3  | 1:Y:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:Y:488:ALA:O    | 1:Y:492:THR:HG23 | 2.14                     | 0.47              |
| 1:b:286:ASP:OD2  | 1:o:390:TYR:OH   | 2.32                     | 0.47              |
| 1:d:619:HIS:CA   | 2:VA:997:DA:O3'  | 2.60                     | 0.47              |
| 1:j:380:THR:HG22 | 1:j:381:GLU:N    | 2.30                     | 0.47              |
| 1:u:276:ASN:O    | 1:u:606:PRO:HA   | 2.15                     | 0.47              |
| 1:w:380:THR:HG22 | 1:w:381:GLU:N    | 2.30                     | 0.47              |
| 1:1:488:ALA:O    | 1:1:492:THR:HG23 | 2.14                     | 0.47              |
| 1:2:488:ALA:O    | 1:2:492:THR:HG23 | 2.14                     | 0.47              |
| 1:3:422:ASN:HB3  | 1:3:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:6:380:THR:HG22 | 1:6:381:GLU:N    | 2.30                     | 0.47              |
| 1:8:619:HIS:CA   | 2:2A:997:DA:O3'  | 2.60                     | 0.47              |
| 1:B:619:HIS:CA   | 2:JA:997:DA:O3'  | 2.60                     | 0.47              |
| 1:H:619:HIS:C    | 2:4A:997:DA:H2'  | 2.38                     | 0.47              |
| 1:J:372:ASN:ND2  | 1:J:376:THR:O    | 2.44                     | 0.47              |
| 1:J:422:ASN:HB3  | 1:J:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:K:276:ASN:O    | 1:K:606:PRO:HA   | 2.15                     | 0.47              |
| 1:K:410:GLU:OE2  | 2:AA:996:DA:N6   | 2.47                     | 0.47              |
| 1:W:276:ASN:O    | 1:W:606:PRO:HA   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:276:ASN:O    | 1:Z:606:PRO:HA   | 2.15                     | 0.47              |
| 1:Z:451:LYS:NZ   | 1:4:350:GLU:OE2  | 2.42                     | 0.47              |
| 1:b:276:ASN:O    | 1:b:606:PRO:HA   | 2.15                     | 0.47              |
| 1:c:391:PHE:CE1  | 1:p:681:LYS:HG3  | 2.49                     | 0.47              |
| 1:e:276:ASN:O    | 1:e:606:PRO:HA   | 2.15                     | 0.47              |
| 1:g:488:ALA:O    | 1:g:492:THR:HG23 | 2.14                     | 0.47              |
| 1:j:488:ALA:O    | 1:j:492:THR:HG23 | 2.14                     | 0.47              |
| 1:k:372:ASN:ND2  | 1:k:376:THR:O    | 2.44                     | 0.47              |
| 1:k:619:HIS:CA   | 2:cA:997:DA:O3'  | 2.60                     | 0.47              |
| 1:l:276:ASN:O    | 1:l:606:PRO:HA   | 2.15                     | 0.47              |
| 1:l:380:THR:HG22 | 1:l:381:GLU:N    | 2.30                     | 0.47              |
| 1:p:276:ASN:O    | 1:p:606:PRO:HA   | 2.15                     | 0.47              |
| 1:r:276:ASN:O    | 1:r:606:PRO:HA   | 2.15                     | 0.47              |
| 1:r:619:HIS:CA   | 2:kA:997:DA:O3'  | 2.60                     | 0.47              |
| 1:z:380:THR:HG22 | 1:z:381:GLU:N    | 2.30                     | 0.47              |
| 1:3:276:ASN:O    | 1:3:606:PRO:HA   | 2.15                     | 0.47              |
| 1:5:513:ASN:ND2  | 1:5:526:THR:HG22 | 2.10                     | 0.47              |
| 1:7:422:ASN:HB3  | 1:7:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:8:380:THR:HG22 | 1:8:381:GLU:N    | 2.30                     | 0.47              |
| 1:B:380:THR:HG22 | 1:B:381:GLU:N    | 2.30                     | 0.47              |
| 1:C:276:ASN:O    | 1:C:606:PRO:HA   | 2.15                     | 0.47              |
| 1:D:488:ALA:O    | 1:D:492:THR:HG23 | 2.14                     | 0.47              |
| 1:H:286:ASP:OD2  | 1:I:390:TYR:OH   | 2.32                     | 0.47              |
| 1:H:390:TYR:OH   | 1:Z:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:H:422:ASN:HB3  | 1:H:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:I:422:ASN:HB3  | 1:I:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:J:276:ASN:O    | 1:J:606:PRO:HA   | 2.15                     | 0.47              |
| 1:P:488:ALA:O    | 1:P:492:THR:HG23 | 2.14                     | 0.47              |
| 1:R:276:ASN:O    | 1:R:606:PRO:HA   | 2.15                     | 0.47              |
| 1:R:391:PHE:CE1  | 1:U:681:LYS:HG3  | 2.50                     | 0.47              |
| 1:U:525:ASN:HD22 | 1:U:562:ALA:HB2  | 1.80                     | 0.47              |
| 1:X:619:HIS:CA   | 2:OA:997:DA:C2'  | 2.88                     | 0.47              |
| 1:Z:628:GLY:C    | 2:QA:997:DA:N1   | 2.66                     | 0.47              |
| 1:d:276:ASN:O    | 1:d:606:PRO:HA   | 2.15                     | 0.47              |
| 1:i:276:ASN:O    | 1:i:606:PRO:HA   | 2.15                     | 0.47              |
| 1:i:380:THR:HG22 | 1:i:381:GLU:N    | 2.30                     | 0.47              |
| 1:i:548:LEU:HG   | 1:i:714:PRO:HD3  | 1.97                     | 0.47              |
| 1:k:276:ASN:O    | 1:k:606:PRO:HA   | 2.15                     | 0.47              |
| 1:l:678:GLU:OE2  | 1:l:680:SER:OG   | 2.24                     | 0.47              |
| 1:n:380:THR:HG22 | 1:n:381:GLU:N    | 2.30                     | 0.47              |
| 1:n:630:LYS:HD2  | 2:eA:996:DA:OP2  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:276:ASN:O    | 1:o:606:PRO:HA   | 2.15                     | 0.47              |
| 1:o:422:ASN:HB3  | 1:o:425:LYS:HB2  | 1.97                     | 0.47              |
| 1:p:390:TYR:OH   | 1:6:286:ASP:OD2  | 2.32                     | 0.47              |
| 1:q:276:ASN:O    | 1:q:606:PRO:HA   | 2.15                     | 0.47              |
| 1:q:391:PHE:CE1  | 1:s:681:LYS:HG3  | 2.50                     | 0.47              |
| 1:s:276:ASN:O    | 1:s:606:PRO:HA   | 2.15                     | 0.47              |
| 1:x:380:THR:HG22 | 1:x:381:GLU:N    | 2.30                     | 0.47              |
| 1:x:525:ASN:HD22 | 1:x:562:ALA:HB2  | 1.80                     | 0.47              |
| 1:x:681:LYS:HG3  | 1:y:391:PHE:CE1  | 2.50                     | 0.47              |
| 1:y:276:ASN:O    | 1:y:606:PRO:HA   | 2.15                     | 0.47              |
| 1:y:372:ASN:ND2  | 1:y:376:THR:O    | 2.44                     | 0.47              |
| 1:z:276:ASN:O    | 1:z:606:PRO:HA   | 2.15                     | 0.47              |
| 1:6:548:LEU:HG   | 1:6:714:PRO:HD3  | 1.97                     | 0.47              |
| 1:G:286:ASP:OD2  | 1:W:390:TYR:OH   | 2.32                     | 0.46              |
| 1:G:548:LEU:HG   | 1:G:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:H:276:ASN:O    | 1:H:606:PRO:HA   | 2.15                     | 0.46              |
| 1:J:410:GLU:OE2  | 2:9:996:DA:N6    | 2.47                     | 0.46              |
| 1:K:422:ASN:HB3  | 1:K:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:K:525:ASN:HD22 | 1:K:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:L:276:ASN:O    | 1:L:606:PRO:HA   | 2.15                     | 0.46              |
| 1:M:391:PHE:CE1  | 1:b:681:LYS:HG3  | 2.50                     | 0.46              |
| 1:N:681:LYS:HG3  | 1:P:391:PHE:CE1  | 2.49                     | 0.46              |
| 1:O:488:ALA:O    | 1:O:492:THR:HG23 | 2.14                     | 0.46              |
| 1:O:548:LEU:HG   | 1:O:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:Q:276:ASN:O    | 1:Q:606:PRO:HA   | 2.15                     | 0.46              |
| 1:R:380:THR:HG22 | 1:R:381:GLU:N    | 2.30                     | 0.46              |
| 1:R:422:ASN:HB3  | 1:R:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:T:488:ALA:O    | 1:T:492:THR:HG23 | 2.14                     | 0.46              |
| 1:X:548:LEU:HG   | 1:X:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:Y:513:ASN:ND2  | 1:Y:526:THR:HG22 | 2.10                     | 0.46              |
| 1:d:372:ASN:ND2  | 1:d:376:THR:O    | 2.44                     | 0.46              |
| 1:d:548:LEU:HG   | 1:d:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:f:276:ASN:O    | 1:f:606:PRO:HA   | 2.15                     | 0.46              |
| 1:f:422:ASN:HB3  | 1:f:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:f:537:GLY:HA2  | 1:g:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:g:548:LEU:HG   | 1:g:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:i:537:GLY:HA2  | 1:k:453:LEU:HD22 | 1.97                     | 0.46              |
| 1:i:630:LYS:HD2  | 2:cA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:m:525:ASN:HD22 | 1:m:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:n:390:TYR:OH   | 1:r:286:ASP:OD2  | 2.32                     | 0.46              |
| 1:o:619:HIS:C    | 2:hA:997:DA:H2'  | 2.38                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:380:THR:HG22 | 1:r:381:GLU:N    | 2.30                     | 0.46              |
| 1:v:276:ASN:O    | 1:v:606:PRO:HA   | 2.15                     | 0.46              |
| 1:y:422:ASN:HB3  | 1:y:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:z:391:PHE:CE1  | 1:2:681:LYS:HG3  | 2.49                     | 0.46              |
| 1:1:330:THR:HG21 | 1:1:395:MET:HE2  | 1.96                     | 0.46              |
| 1:2:380:THR:HG22 | 1:2:381:GLU:N    | 2.30                     | 0.46              |
| 1:2:630:LYS:HD2  | 2:uA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:4:276:ASN:O    | 1:4:606:PRO:HA   | 2.15                     | 0.46              |
| 1:A:391:PHE:CE1  | 1:I:681:LYS:HG3  | 2.50                     | 0.46              |
| 1:B:630:LYS:HD2  | 2:BA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:D:380:THR:HG22 | 1:D:381:GLU:N    | 2.30                     | 0.46              |
| 1:D:537:GLY:HA2  | 1:P:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:D:630:LYS:HD2  | 2:FA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:D:681:LYS:HG3  | 1:N:391:PHE:CE1  | 2.49                     | 0.46              |
| 1:E:548:LEU:HG   | 1:E:714:PRO:HD3  | 1.97                     | 0.46              |
| 1:J:525:ASN:HD22 | 1:J:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:K:372:ASN:ND2  | 1:K:376:THR:O    | 2.44                     | 0.46              |
| 1:L:513:ASN:ND2  | 1:L:526:THR:HG22 | 2.10                     | 0.46              |
| 1:M:276:ASN:O    | 1:M:606:PRO:HA   | 2.15                     | 0.46              |
| 1:M:330:THR:HG21 | 1:M:395:MET:HE2  | 1.96                     | 0.46              |
| 1:O:453:LEU:HD22 | 1:m:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:P:330:THR:HG21 | 1:P:395:MET:HE2  | 1.96                     | 0.46              |
| 1:R:372:ASN:ND2  | 1:R:376:THR:O    | 2.44                     | 0.46              |
| 1:S:548:LEU:HG   | 1:S:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:U:380:THR:HG22 | 1:U:381:GLU:N    | 2.30                     | 0.46              |
| 1:U:548:LEU:HG   | 1:U:714:PRO:HD3  | 1.97                     | 0.46              |
| 1:Z:681:LYS:HG3  | 1:4:391:PHE:CE1  | 2.50                     | 0.46              |
| 1:a:276:ASN:O    | 1:a:606:PRO:HA   | 2.15                     | 0.46              |
| 1:b:548:LEU:HG   | 1:b:714:PRO:HD3  | 1.97                     | 0.46              |
| 1:b:628:GLY:C    | 2:SA:997:DA:N1   | 2.66                     | 0.46              |
| 1:c:619:HIS:CA   | 2:TA:997:DA:O3'  | 2.60                     | 0.46              |
| 1:d:453:LEU:HD22 | 1:l:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:d:525:ASN:HD22 | 1:d:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:f:525:ASN:HD22 | 1:f:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:h:380:THR:HG22 | 1:h:381:GLU:N    | 2.30                     | 0.46              |
| 1:h:630:LYS:HD2  | 2:XA:996:DA:OP2  | 2.15                     | 0.46              |
| 1:i:488:ALA:O    | 1:i:492:THR:HG23 | 2.14                     | 0.46              |
| 1:k:525:ASN:HD22 | 1:k:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:k:548:LEU:HG   | 1:k:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:l:488:ALA:O    | 1:l:492:THR:HG23 | 2.14                     | 0.46              |
| 1:l:548:LEU:HG   | 1:l:714:PRO:HD3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:m:276:ASN:O    | 1:m:606:PRO:HA  | 2.15                     | 0.46              |
| 1:m:422:ASN:HB3  | 1:m:425:LYS:HB2 | 1.97                     | 0.46              |
| 1:o:286:ASP:OD2  | 1:7:390:TYR:OH  | 2.32                     | 0.46              |
| 1:q:380:THR:HG22 | 1:q:381:GLU:N   | 2.30                     | 0.46              |
| 1:s:548:LEU:HG   | 1:s:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:s:619:HIS:CA   | 2:lA:997:DA:C2' | 2.88                     | 0.46              |
| 1:u:548:LEU:HG   | 1:u:714:PRO:HD3 | 1.97                     | 0.46              |
| 1:w:548:LEU:HG   | 1:w:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:x:548:LEU:HG   | 1:x:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:x:630:LYS:HD2  | 2:pA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:y:380:THR:HG22 | 1:y:381:GLU:N   | 2.30                     | 0.46              |
| 1:z:681:LYS:HG3  | 1:1:391:PHE:CE1 | 2.49                     | 0.46              |
| 1:1:453:LEU:HD22 | 1:2:537:GLY:HA2 | 1.98                     | 0.46              |
| 1:3:525:ASN:HD22 | 1:3:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:8:630:LYS:HD2  | 2:RA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:C:525:ASN:HD22 | 1:C:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:D:276:ASN:O    | 1:D:606:PRO:HA  | 2.15                     | 0.46              |
| 1:D:619:HIS:CA   | 2:fA:997:DA:C2' | 2.88                     | 0.46              |
| 1:E:453:LEU:HD22 | 1:Q:537:GLY:HA2 | 1.98                     | 0.46              |
| 1:G:525:ASN:HD22 | 1:G:562:ALA:HB2 | 1.81                     | 0.46              |
| 1:H:619:HIS:CA   | 2:4A:997:DA:O3' | 2.60                     | 0.46              |
| 1:I:525:ASN:HD22 | 1:I:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:N:548:LEU:HG   | 1:N:714:PRO:HD3 | 1.97                     | 0.46              |
| 1:N:630:LYS:HD2  | 2:fA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:R:548:LEU:HG   | 1:R:714:PRO:HD3 | 1.97                     | 0.46              |
| 1:T:410:GLU:OE2  | 2:KA:996:DA:N6  | 2.47                     | 0.46              |
| 1:U:630:LYS:HD2  | 2:IA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:V:276:ASN:O    | 1:V:606:PRO:HA  | 2.15                     | 0.46              |
| 1:V:525:ASN:HD22 | 1:V:562:ALA:HB2 | 1.81                     | 0.46              |
| 1:e:286:ASP:OD2  | 1:h:390:TYR:OH  | 2.32                     | 0.46              |
| 1:e:372:ASN:ND2  | 1:e:376:THR:O   | 2.44                     | 0.46              |
| 1:e:380:THR:HG22 | 1:e:381:GLU:N   | 2.30                     | 0.46              |
| 1:e:619:HIS:CA   | 2:WA:997:DA:O3' | 2.60                     | 0.46              |
| 1:h:286:ASP:OD2  | 1:i:390:TYR:OH  | 2.32                     | 0.46              |
| 1:h:422:ASN:HB3  | 1:h:425:LYS:HB2 | 1.97                     | 0.46              |
| 1:l:630:LYS:HD2  | 2:VA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:q:525:ASN:HD22 | 1:q:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:u:453:LEU:HD22 | 1:v:537:GLY:HA2 | 1.98                     | 0.46              |
| 1:u:525:ASN:HD22 | 1:u:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:y:548:LEU:HG   | 1:y:714:PRO:HD3 | 1.97                     | 0.46              |
| 1:z:330:THR:HG21 | 1:z:395:MET:HE2 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:525:ASN:HD22 | 1:2:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:3:391:PHE:CE1  | 1:4:681:LYS:HG3  | 2.50                     | 0.46              |
| 1:5:276:ASN:O    | 1:5:606:PRO:HA   | 2.15                     | 0.46              |
| 1:6:525:ASN:HD22 | 1:6:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:7:525:ASN:HD22 | 1:7:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:A:276:ASN:O    | 1:A:606:PRO:HA   | 2.15                     | 0.46              |
| 1:A:380:THR:HG22 | 1:A:381:GLU:N    | 2.30                     | 0.46              |
| 1:D:453:LEU:HD22 | 1:N:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:E:525:ASN:HD22 | 1:E:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:N:525:ASN:HD22 | 1:N:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:O:525:ASN:HD22 | 1:O:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:P:548:LEU:HG   | 1:P:714:PRO:HD3  | 1.97                     | 0.46              |
| 1:Q:330:THR:HG21 | 1:Q:395:MET:HE2  | 1.96                     | 0.46              |
| 1:Q:548:LEU:HG   | 1:Q:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:T:276:ASN:O    | 1:T:606:PRO:HA   | 2.15                     | 0.46              |
| 1:V:380:THR:HG22 | 1:V:381:GLU:N    | 2.30                     | 0.46              |
| 1:V:422:ASN:HB3  | 1:V:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:W:630:LYS:HD2  | 2:4A:996:DA:OP2  | 2.16                     | 0.46              |
| 1:Y:619:HIS:CA   | 2:PA:997:DA:O3'  | 2.60                     | 0.46              |
| 1:Z:548:LEU:HG   | 1:Z:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:c:380:THR:HG22 | 1:c:381:GLU:N    | 2.30                     | 0.46              |
| 1:c:410:GLU:OE2  | 2:TA:996:DA:N6   | 2.47                     | 0.46              |
| 1:g:286:ASP:OD2  | 1:1:390:TYR:OH   | 2.32                     | 0.46              |
| 1:g:332:GLN:HE21 | 1:g:395:MET:HE3  | 1.78                     | 0.46              |
| 1:j:410:GLU:OE2  | 2:bA:996:DA:N6   | 2.47                     | 0.46              |
| 1:n:422:ASN:HB3  | 1:n:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:p:630:LYS:HD2  | 2:hA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:q:422:ASN:HB3  | 1:q:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:r:372:ASN:ND2  | 1:r:376:THR:O    | 2.44                     | 0.46              |
| 1:v:548:LEU:HG   | 1:v:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:w:681:LYS:HG3  | 1:x:391:PHE:CE1  | 2.49                     | 0.46              |
| 1:z:525:ASN:HD22 | 1:z:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:z:537:GLY:HA2  | 1:2:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:z:630:LYS:HD2  | 2:vA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:1:548:LEU:HG   | 1:1:714:PRO:HD3  | 1.97                     | 0.46              |
| 1:4:330:THR:HG21 | 1:4:395:MET:HE2  | 1.96                     | 0.46              |
| 1:A:390:TYR:OH   | 1:B:286:ASP:OD2  | 2.32                     | 0.46              |
| 1:A:513:ASN:ND2  | 1:A:526:THR:HG22 | 2.10                     | 0.46              |
| 1:C:391:PHE:CE1  | 1:M:681:LYS:HG3  | 2.50                     | 0.46              |
| 1:D:525:ASN:HD22 | 1:D:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:N:422:ASN:HB3  | 1:N:425:LYS:HB2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:286:ASP:OD2  | 1:P:390:TYR:OH   | 2.32                     | 0.46              |
| 1:P:619:HIS:CA   | 2:FA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:P:630:LYS:HD2  | 2:DA:996:DA:OP2  | 2.15                     | 0.46              |
| 1:T:525:ASN:HD22 | 1:T:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:V:630:LYS:HD2  | 2:OA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:Y:410:GLU:OE2  | 2:PA:996:DA:N6   | 2.47                     | 0.46              |
| 1:Z:525:ASN:HD22 | 1:Z:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:a:380:THR:HG22 | 1:a:381:GLU:N    | 2.30                     | 0.46              |
| 1:b:525:ASN:HD22 | 1:b:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:g:525:ASN:HD22 | 1:g:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:j:525:ASN:HD22 | 1:j:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:k:422:ASN:HB3  | 1:k:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:l:390:TYR:OH   | 1:n:286:ASP:OD2  | 2.32                     | 0.46              |
| 1:n:678:GLU:OE2  | 1:n:680:SER:OG   | 2.24                     | 0.46              |
| 1:r:422:ASN:HB3  | 1:r:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:v:330:THR:HG21 | 1:v:395:MET:HE2  | 1.96                     | 0.46              |
| 1:z:422:ASN:HB3  | 1:z:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:z:548:LEU:HG   | 1:z:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:1:276:ASN:O    | 1:1:606:PRO:HA   | 2.15                     | 0.46              |
| 1:2:276:ASN:O    | 1:2:606:PRO:HA   | 2.15                     | 0.46              |
| 1:5:380:THR:HG22 | 1:5:381:GLU:N    | 2.30                     | 0.46              |
| 1:5:453:LEU:HD22 | 1:6:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:5:630:LYS:HD2  | 2:OA:996:DA:OP2  | 2.15                     | 0.46              |
| 1:A:537:GLY:HA2  | 1:I:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:681:LYS:HG3  | 1:G:391:PHE:CE1  | 2.51                     | 0.46              |
| 1:B:372:ASN:ND2  | 1:B:376:THR:O    | 2.44                     | 0.46              |
| 1:C:410:GLU:OE2  | 2:UA:996:DA:N6   | 2.47                     | 0.46              |
| 1:F:330:THR:HG21 | 1:F:395:MET:HE2  | 1.96                     | 0.46              |
| 1:G:372:ASN:ND2  | 1:G:376:THR:O    | 2.44                     | 0.46              |
| 1:K:380:THR:HG22 | 1:K:381:GLU:N    | 2.30                     | 0.46              |
| 1:L:380:THR:HG22 | 1:L:381:GLU:N    | 2.30                     | 0.46              |
| 1:N:330:THR:HG21 | 1:N:395:MET:HE2  | 1.96                     | 0.46              |
| 1:O:332:GLN:HE21 | 1:O:395:MET:HE3  | 1.78                     | 0.46              |
| 1:P:276:ASN:O    | 1:P:606:PRO:HA   | 2.15                     | 0.46              |
| 1:Q:619:HIS:CA   | 2:GA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:S:681:LYS:HG3  | 1:U:391:PHE:CE1  | 2.50                     | 0.46              |
| 1:Y:380:THR:HG22 | 1:Y:381:GLU:N    | 2.30                     | 0.46              |
| 1:a:525:ASN:HD22 | 1:a:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:d:422:ASN:HB3  | 1:d:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:e:422:ASN:HB3  | 1:e:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:e:525:ASN:HD22 | 1:e:562:ALA:HB2  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:630:LYS:HD2  | 2:YA:996:DA:OP2  | 2.15                     | 0.46              |
| 1:j:276:ASN:O    | 1:j:606:PRO:HA   | 2.15                     | 0.46              |
| 1:l:619:HIS:CA   | 2:dA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:o:619:HIS:CA   | 2:hA:997:DA:O3'  | 2.60                     | 0.46              |
| 1:r:525:ASN:HD22 | 1:r:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:t:330:THR:HG21 | 1:t:395:MET:HE2  | 1.96                     | 0.46              |
| 1:v:619:HIS:CA   | 2:oA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:w:630:LYS:HD2  | 2:sA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:x:410:GLU:OE2  | 2:rA:996:DA:N6   | 2.47                     | 0.46              |
| 1:2:619:HIS:CA   | 2:vA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:5:537:GLY:HA2  | 1:7:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:6:372:ASN:ND2  | 1:6:376:THR:O    | 2.44                     | 0.46              |
| 1:E:422:ASN:HB3  | 1:E:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:E:619:HIS:CA   | 2:qA:997:DA:O3'  | 2.60                     | 0.46              |
| 1:H:628:GLY:C    | 2:4A:997:DA:N1   | 2.66                     | 0.46              |
| 1:I:410:GLU:OE2  | 2:5A:996:DA:N6   | 2.47                     | 0.46              |
| 1:J:380:THR:HG22 | 1:J:381:GLU:N    | 2.30                     | 0.46              |
| 1:L:422:ASN:HB3  | 1:L:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:L:525:ASN:HD22 | 1:L:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:N:410:GLU:OE2  | 2:DA:996:DA:N6   | 2.47                     | 0.46              |
| 1:P:422:ASN:HB3  | 1:P:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:Q:630:LYS:HD2  | 2:qA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:S:453:LEU:HD22 | 1:U:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:X:525:ASN:HD22 | 1:X:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:Z:453:LEU:HD22 | 1:4:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:a:330:THR:HG21 | 1:a:395:MET:HE2  | 1.96                     | 0.46              |
| 1:c:513:ASN:ND2  | 1:c:526:THR:HG22 | 2.10                     | 0.46              |
| 1:f:453:LEU:HD22 | 1:h:537:GLY:HA2  | 1.97                     | 0.46              |
| 1:h:548:LEU:HG   | 1:h:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:h:678:GLU:OE2  | 1:h:680:SER:OG   | 2.24                     | 0.46              |
| 1:i:422:ASN:HB3  | 1:i:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:l:422:ASN:HB3  | 1:l:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:m:380:THR:HG22 | 1:m:381:GLU:N    | 2.30                     | 0.46              |
| 1:m:453:LEU:HD22 | 1:n:537:GLY:HA2  | 1.97                     | 0.46              |
| 1:m:630:LYS:HD2  | 2:EA:996:DA:OP2  | 2.15                     | 0.46              |
| 1:n:548:LEU:HG   | 1:n:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:o:380:THR:HG22 | 1:o:381:GLU:N    | 2.30                     | 0.46              |
| 1:p:422:ASN:HB3  | 1:p:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:s:380:THR:HG22 | 1:s:381:GLU:N    | 2.30                     | 0.46              |
| 1:s:525:ASN:HD22 | 1:s:562:ALA:HB2  | 1.81                     | 0.46              |
| 1:t:453:LEU:HD22 | 1:u:537:GLY:HA2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:422:ASN:HB3  | 1:u:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:v:422:ASN:HB3  | 1:v:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:v:630:LYS:HD2  | 2:nA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:z:410:GLU:OE2  | 2:tA:996:DA:N6   | 2.47                     | 0.46              |
| 1:1:422:ASN:HB3  | 1:1:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:3:410:GLU:OE2  | 2:wA:996:DA:N6   | 2.47                     | 0.46              |
| 1:7:410:GLU:OE2  | 2:0A:996:DA:N6   | 2.47                     | 0.46              |
| 1:B:410:GLU:OE2  | 2:JA:996:DA:N6   | 2.47                     | 0.46              |
| 1:C:537:GLY:HA2  | 1:M:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:H:380:THR:HG22 | 1:H:381:GLU:N    | 2.30                     | 0.46              |
| 1:I:630:LYS:HD2  | 2:3A:996:DA:OP2  | 2.15                     | 0.46              |
| 1:J:453:LEU:HD22 | 1:L:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:K:453:LEU:HD22 | 1:a:537:GLY:HA2  | 1.98                     | 0.46              |
| 1:K:548:LEU:HG   | 1:K:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:M:619:HIS:CA   | 2:CA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:O:410:GLU:OE2  | 2:EA:996:DA:N6   | 2.47                     | 0.46              |
| 1:Q:422:ASN:HB3  | 1:Q:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:R:619:HIS:CA   | 2:HA:997:DA:O3'  | 2.60                     | 0.46              |
| 1:S:630:LYS:HD2  | 2:HA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:a:422:ASN:HB3  | 1:a:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:a:619:HIS:CA   | 2:RA:997:DA:C2'  | 2.88                     | 0.46              |
| 1:f:380:THR:HG22 | 1:f:381:GLU:N    | 2.30                     | 0.46              |
| 1:g:372:ASN:ND2  | 1:g:376:THR:O    | 2.44                     | 0.46              |
| 1:t:525:ASN:HD22 | 1:t:562:ALA:HB2  | 1.80                     | 0.46              |
| 1:1:630:LYS:HD2  | 2:tA:996:DA:OP2  | 2.15                     | 0.46              |
| 1:3:537:GLY:HA2  | 1:4:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:4:630:LYS:HD2  | 2:QA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:8:372:ASN:ND2  | 1:8:376:THR:O    | 2.44                     | 0.46              |
| 1:B:276:ASN:O    | 1:B:606:PRO:HA   | 2.15                     | 0.46              |
| 1:B:422:ASN:HB3  | 1:B:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:C:630:LYS:HD2  | 2:CA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:E:410:GLU:OE2  | 2:qA:996:DA:N6   | 2.47                     | 0.46              |
| 1:E:537:GLY:HA2  | 1:F:453:LEU:HD22 | 1.97                     | 0.46              |
| 1:J:548:LEU:HG   | 1:J:714:PRO:HD3  | 1.98                     | 0.46              |
| 1:M:537:GLY:HA2  | 1:b:453:LEU:HD22 | 1.98                     | 0.46              |
| 1:M:630:LYS:HD2  | 2:SA:996:DA:OP2  | 2.16                     | 0.46              |
| 1:R:410:GLU:OE2  | 2:HA:996:DA:N6   | 2.47                     | 0.46              |
| 1:U:410:GLU:OE2  | 2:LA:996:DA:N6   | 2.47                     | 0.46              |
| 1:U:422:ASN:HB3  | 1:U:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:W:422:ASN:HB3  | 1:W:425:LYS:HB2  | 1.97                     | 0.46              |
| 1:X:380:THR:HG22 | 1:X:381:GLU:N    | 2.30                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:X:422:ASN:HB3  | 1:X:425:LYS:HB2 | 1.97                     | 0.46              |
| 1:X:630:LYS:HD2  | 2:WA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:Y:276:ASN:O    | 1:Y:606:PRO:HA  | 2.15                     | 0.46              |
| 1:Z:410:GLU:OE2  | 2:QA:996:DA:N6  | 2.47                     | 0.46              |
| 1:c:276:ASN:O    | 1:c:606:PRO:HA  | 2.15                     | 0.46              |
| 1:f:548:LEU:HG   | 1:f:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:h:276:ASN:O    | 1:h:606:PRO:HA  | 2.15                     | 0.46              |
| 1:k:619:HIS:CA   | 2:cA:997:DA:C2' | 2.88                     | 0.46              |
| 1:u:619:HIS:CA   | 2:nA:997:DA:O3' | 2.60                     | 0.46              |
| 1:w:453:LEU:HD22 | 1:x:537:GLY:HA2 | 1.98                     | 0.46              |
| 1:x:422:ASN:HB3  | 1:x:425:LYS:HB2 | 1.97                     | 0.46              |
| 1:7:630:LYS:HD2  | 2:zA:996:DA:OP2 | 2.15                     | 0.46              |
| 1:B:600:ASP:OD1  | 1:B:717:THR:OG1 | 2.34                     | 0.46              |
| 1:F:276:ASN:O    | 1:F:606:PRO:HA  | 2.15                     | 0.46              |
| 1:F:525:ASN:HD22 | 1:F:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:L:330:THR:HG21 | 1:L:395:MET:HE2 | 1.96                     | 0.46              |
| 1:L:619:HIS:CA   | 2:BA:997:DA:C2' | 2.88                     | 0.46              |
| 1:O:276:ASN:O    | 1:O:606:PRO:HA  | 2.15                     | 0.46              |
| 1:R:525:ASN:HD22 | 1:R:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:S:276:ASN:O    | 1:S:606:PRO:HA  | 2.15                     | 0.46              |
| 1:Y:600:ASP:OD1  | 1:Y:717:THR:OG1 | 2.34                     | 0.46              |
| 1:c:600:ASP:OD1  | 1:c:717:THR:OG1 | 2.34                     | 0.46              |
| 1:e:548:LEU:HG   | 1:e:714:PRO:HD3 | 1.97                     | 0.46              |
| 1:f:600:ASP:OD1  | 1:f:717:THR:OG1 | 2.35                     | 0.46              |
| 1:g:410:GLU:OE2  | 2:YA:996:DA:N6  | 2.47                     | 0.46              |
| 1:i:525:ASN:HD22 | 1:i:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:i:619:HIS:CA   | 2:aA:997:DA:C2' | 2.88                     | 0.46              |
| 1:i:619:HIS:CA   | 2:aA:997:DA:O3' | 2.60                     | 0.46              |
| 1:j:548:LEU:HG   | 1:j:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:k:630:LYS:HD2  | 2:bA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:l:619:HIS:CA   | 2:dA:997:DA:O3' | 2.60                     | 0.46              |
| 1:m:548:LEU:HG   | 1:m:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:r:548:LEU:HG   | 1:r:714:PRO:HD3 | 1.98                     | 0.46              |
| 1:r:600:ASP:OD1  | 1:r:717:THR:OG1 | 2.34                     | 0.46              |
| 1:w:276:ASN:O    | 1:w:606:PRO:HA  | 2.15                     | 0.46              |
| 1:y:525:ASN:HD22 | 1:y:562:ALA:HB2 | 1.80                     | 0.46              |
| 1:y:619:HIS:CA   | 2:sA:997:DA:O3' | 2.60                     | 0.46              |
| 1:3:630:LYS:HD2  | 2:xA:996:DA:OP2 | 2.16                     | 0.46              |
| 1:6:630:LYS:HD2  | 2:yA:996:DA:OP2 | 2.15                     | 0.46              |
| 1:8:410:GLU:OE2  | 2:2A:996:DA:N6  | 2.47                     | 0.46              |
| 1:8:422:ASN:HB3  | 1:8:425:LYS:HB2 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:422:ASN:HB3  | 1:A:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:A:548:LEU:HG   | 1:A:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:C:453:LEU:HD22 | 1:b:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:F:537:GLY:HA2  | 1:Q:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:G:276:ASN:O    | 1:G:606:PRO:HA   | 2.15                     | 0.45              |
| 1:K:630:LYS:HD2  | 2:2A:996:DA:OP2  | 2.16                     | 0.45              |
| 1:L:245:HIS:CD2  | 1:L:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:N:453:LEU:HD22 | 1:P:537:GLY:HA2  | 1.97                     | 0.45              |
| 1:O:372:ASN:ND2  | 1:O:376:THR:O    | 2.44                     | 0.45              |
| 1:Y:245:HIS:CD2  | 1:Y:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:Y:619:HIS:CA   | 2:PA:997:DA:C2'  | 2.88                     | 0.45              |
| 1:a:245:HIS:CD2  | 1:a:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:b:410:GLU:OE2  | 2:SA:996:DA:N6   | 2.47                     | 0.45              |
| 1:c:245:HIS:CD2  | 1:c:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:d:410:GLU:OE2  | 2:VA:996:DA:N6   | 2.47                     | 0.45              |
| 1:d:630:LYS:HD2  | 2:KA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:e:600:ASP:OD1  | 1:e:717:THR:OG1  | 2.34                     | 0.45              |
| 1:e:630:LYS:HD2  | 2:MA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:g:276:ASN:O    | 1:g:606:PRO:HA   | 2.15                     | 0.45              |
| 1:n:276:ASN:O    | 1:n:606:PRO:HA   | 2.15                     | 0.45              |
| 1:o:628:GLY:C    | 2:hA:997:DA:N1   | 2.66                     | 0.45              |
| 1:r:630:LYS:HD2  | 2:jA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:s:422:ASN:HB3  | 1:s:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:t:537:GLY:HA2  | 1:v:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:u:245:HIS:CD2  | 1:u:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:u:410:GLU:OE2  | 2:nA:996:DA:N6   | 2.47                     | 0.45              |
| 1:y:410:GLU:OE2  | 2:sA:996:DA:N6   | 2.47                     | 0.45              |
| 1:5:422:ASN:HB3  | 1:5:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:8:276:ASN:O    | 1:8:606:PRO:HA   | 2.15                     | 0.45              |
| 1:8:600:ASP:OD1  | 1:8:717:THR:OG1  | 2.34                     | 0.45              |
| 1:A:245:HIS:CD2  | 1:A:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:A:630:LYS:HD2  | 2:5A:996:DA:OP2  | 2.16                     | 0.45              |
| 1:B:525:ASN:HD22 | 1:B:562:ALA:HB2  | 1.81                     | 0.45              |
| 1:B:548:LEU:HG   | 1:B:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:E:245:HIS:CD2  | 1:E:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:F:630:LYS:HD2  | 2:GA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:I:548:LEU:HG   | 1:I:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:K:628:GLY:C    | 2:AA:997:DA:N1   | 2.66                     | 0.45              |
| 1:N:245:HIS:CD2  | 1:N:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:O:537:GLY:HA2  | 1:n:453:LEU:HD22 | 1.97                     | 0.45              |
| 1:S:525:ASN:HD22 | 1:S:562:ALA:HB2  | 1.80                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:548:LEU:HG   | 1:T:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:T:630:LYS:HD2  | 2:dA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:U:276:ASN:O    | 1:U:606:PRO:HA   | 2.15                     | 0.45              |
| 1:W:548:LEU:HG   | 1:W:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:Z:537:GLY:HA2  | 1:3:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:a:453:LEU:HD22 | 1:8:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:c:630:LYS:HD2  | 2:iA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:d:619:HIS:CA   | 2:VA:997:DA:C2'  | 2.88                     | 0.45              |
| 1:l:525:ASN:HD22 | 1:l:562:ALA:HB2  | 1.80                     | 0.45              |
| 1:n:525:ASN:HD22 | 1:n:562:ALA:HB2  | 1.80                     | 0.45              |
| 1:p:548:LEU:HG   | 1:p:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:s:630:LYS:HD2  | 2:kA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:w:525:ASN:HD22 | 1:w:562:ALA:HB2  | 1.81                     | 0.45              |
| 1:y:630:LYS:HD2  | 2:rA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:1:372:ASN:ND2  | 1:1:376:THR:O    | 2.44                     | 0.45              |
| 1:2:600:ASP:OD1  | 1:2:717:THR:OG1  | 2.34                     | 0.45              |
| 1:3:372:ASN:ND2  | 1:3:376:THR:O    | 2.44                     | 0.45              |
| 1:5:548:LEU:HG   | 1:5:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:8:548:LEU:HG   | 1:8:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:A:628:GLY:C    | 2:0:997:DA:N1    | 2.66                     | 0.45              |
| 1:B:537:GLY:HA2  | 1:L:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:245:HIS:CD2  | 1:C:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:C:335:THR:CG2  | 1:C:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:D:600:ASP:OD1  | 1:D:717:THR:OG1  | 2.34                     | 0.45              |
| 1:G:422:ASN:HB3  | 1:G:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:G:453:LEU:HD22 | 1:I:537:GLY:HA2  | 1.97                     | 0.45              |
| 1:H:548:LEU:HG   | 1:H:714:PRO:HD3  | 1.97                     | 0.45              |
| 1:J:630:LYS:HD2  | 2:JA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:T:453:LEU:HD22 | 1:d:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:W:372:ASN:ND2  | 1:W:376:THR:O    | 2.44                     | 0.45              |
| 1:Z:630:LYS:HD2  | 2:wA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:c:525:ASN:HD22 | 1:c:562:ALA:HB2  | 1.80                     | 0.45              |
| 1:c:619:HIS:CA   | 2:TA:997:DA:C2'  | 2.88                     | 0.45              |
| 1:h:245:HIS:CD2  | 1:h:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:j:453:LEU:HD22 | 1:k:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:j:630:LYS:HD2  | 2:aA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:k:410:GLU:OE2  | 2:cA:996:DA:N6   | 2.47                     | 0.45              |
| 1:o:548:LEU:HG   | 1:o:714:PRO:HD3  | 1.97                     | 0.45              |
| 1:t:276:ASN:O    | 1:t:606:PRO:HA   | 2.15                     | 0.45              |
| 1:t:548:LEU:HG   | 1:t:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:w:600:ASP:OD1  | 1:w:717:THR:OG1  | 2.34                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:z:245:HIS:CD2  | 1:z:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:4:245:HIS:CD2  | 1:4:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:4:422:ASN:HB3  | 1:4:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:4:513:ASN:ND2  | 1:4:526:THR:HG22 | 2.10                     | 0.45              |
| 1:5:245:HIS:CD2  | 1:5:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:6:276:ASN:O    | 1:6:606:PRO:HA   | 2.15                     | 0.45              |
| 1:6:422:ASN:HB3  | 1:6:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:7:548:LEU:HG   | 1:7:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:8:525:ASN:HD22 | 1:8:562:ALA:HB2  | 1.81                     | 0.45              |
| 1:C:372:ASN:ND2  | 1:C:376:THR:O    | 2.44                     | 0.45              |
| 1:E:630:LYS:HD2  | 2:1A:996:DA:OP2  | 2.15                     | 0.45              |
| 1:F:548:LEU:HG   | 1:F:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:H:335:THR:CG2  | 1:H:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:H:525:ASN:HD22 | 1:H:562:ALA:HB2  | 1.80                     | 0.45              |
| 1:K:537:GLY:HA2  | 1:8:453:LEU:HD22 | 1.97                     | 0.45              |
| 1:M:245:HIS:CD2  | 1:M:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:M:422:ASN:HB3  | 1:M:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:M:548:LEU:HG   | 1:M:714:PRO:HD3  | 1.97                     | 0.45              |
| 1:O:630:LYS:HD2  | 2:gA:996:DA:OP2  | 2.15                     | 0.45              |
| 1:P:335:THR:CG2  | 1:P:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:R:630:LYS:HD2  | 2:LA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:S:422:ASN:HB3  | 1:S:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:S:600:ASP:OD1  | 1:S:717:THR:OG1  | 2.34                     | 0.45              |
| 1:b:422:ASN:HB3  | 1:b:425:LYS:HB2  | 1.97                     | 0.45              |
| 1:b:630:LYS:HD2  | 2:UA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:f:335:THR:CG2  | 1:f:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:g:537:GLY:HA2  | 1:h:453:LEU:HD22 | 1.97                     | 0.45              |
| 1:g:600:ASP:OD1  | 1:g:717:THR:OG1  | 2.34                     | 0.45              |
| 1:h:525:ASN:HD22 | 1:h:562:ALA:HB2  | 1.81                     | 0.45              |
| 1:i:245:HIS:CD2  | 1:i:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:l:380:THR:HG22 | 1:l:381:GLU:H    | 1.82                     | 0.45              |
| 1:m:335:THR:CG2  | 1:m:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:o:335:THR:CG2  | 1:o:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:r:245:HIS:CD2  | 1:r:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:t:630:LYS:HD2  | 2:oA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:w:619:HIS:CA   | 2:pA:997:DA:O3'  | 2.60                     | 0.45              |
| 1:x:276:ASN:O    | 1:x:606:PRO:HA   | 2.15                     | 0.45              |
| 1:x:335:THR:CG2  | 1:x:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:x:633:PRO:HA   | 1:x:634:PRO:HD3  | 1.89                     | 0.45              |
| 1:z:453:LEU:HD22 | 1:1:537:GLY:HA2  | 1.97                     | 0.45              |
| 1:3:245:HIS:CD2  | 1:3:642:PRO:HB3  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:3:335:THR:CG2  | 1:3:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:4:548:LEU:HG   | 1:4:714:PRO:HD3 | 1.97                     | 0.45              |
| 1:A:525:ASN:HD22 | 1:A:562:ALA:HB2 | 1.80                     | 0.45              |
| 1:B:453:LEU:HD22 | 1:J:537:GLY:HA2 | 1.97                     | 0.45              |
| 1:G:245:HIS:CD2  | 1:G:642:PRO:HB3 | 2.51                     | 0.45              |
| 1:I:619:HIS:CA   | 2:5A:997:DA:O3' | 2.60                     | 0.45              |
| 1:J:245:HIS:CD2  | 1:J:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:K:245:HIS:CD2  | 1:K:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:L:335:THR:CG2  | 1:L:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:L:628:GLY:C    | 2:BA:997:DA:N1  | 2.66                     | 0.45              |
| 1:M:525:ASN:HD22 | 1:M:562:ALA:HB2 | 1.81                     | 0.45              |
| 1:N:633:PRO:HA   | 1:N:634:PRO:HD3 | 1.89                     | 0.45              |
| 1:O:335:THR:CG2  | 1:O:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:O:600:ASP:OD1  | 1:O:717:THR:OG1 | 2.34                     | 0.45              |
| 1:P:372:ASN:ND2  | 1:P:376:THR:O   | 2.44                     | 0.45              |
| 1:U:335:THR:CG2  | 1:U:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:V:335:THR:CG2  | 1:V:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:V:453:LEU:HD22 | 1:e:537:GLY:HA2 | 1.98                     | 0.45              |
| 1:W:525:ASN:HD22 | 1:W:562:ALA:HB2 | 1.80                     | 0.45              |
| 1:W:600:ASP:OD1  | 1:W:717:THR:OG1 | 2.34                     | 0.45              |
| 1:Y:380:THR:HG22 | 1:Y:381:GLU:H   | 1.82                     | 0.45              |
| 1:Y:525:ASN:HD22 | 1:Y:562:ALA:HB2 | 1.81                     | 0.45              |
| 1:Z:422:ASN:HB3  | 1:Z:425:LYS:HB2 | 1.97                     | 0.45              |
| 1:a:335:THR:CG2  | 1:a:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:c:380:THR:HG22 | 1:c:381:GLU:H   | 1.82                     | 0.45              |
| 1:d:628:GLY:C    | 2:VA:997:DA:N1  | 2.66                     | 0.45              |
| 1:i:380:THR:HG22 | 1:i:381:GLU:H   | 1.82                     | 0.45              |
| 1:l:245:HIS:CD2  | 1:l:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:n:245:HIS:CD2  | 1:n:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:o:525:ASN:HD22 | 1:o:562:ALA:HB2 | 1.81                     | 0.45              |
| 1:p:372:ASN:ND2  | 1:p:376:THR:O   | 2.44                     | 0.45              |
| 1:q:630:LYS:HD2  | 2:1A:996:DA:OP2 | 2.17                     | 0.45              |
| 1:u:630:LYS:HD2  | 2:mA:996:DA:OP2 | 2.15                     | 0.45              |
| 1:1:245:HIS:CD2  | 1:1:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:1:335:THR:CG2  | 1:1:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:3:628:GLY:C    | 2:wA:997:DA:N1  | 2.66                     | 0.45              |
| 1:4:525:ASN:HD22 | 1:4:562:ALA:HB2 | 1.81                     | 0.45              |
| 1:6:453:LEU:HD22 | 1:7:537:GLY:HA2 | 1.97                     | 0.45              |
| 1:B:245:HIS:CD2  | 1:B:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:C:380:THR:HG22 | 1:C:381:GLU:H   | 1.82                     | 0.45              |
| 1:E:335:THR:CG2  | 1:E:634:PRO:HB2 | 2.47                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:630:LYS:HD2  | 2:PA:996:DA:OP2 | 2.16                     | 0.45              |
| 1:J:335:THR:CG2  | 1:J:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:J:628:GLY:C    | 2:9:997:DA:N1   | 2.66                     | 0.45              |
| 1:K:335:THR:CG2  | 1:K:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:K:619:HIS:CA   | 2:AA:997:DA:O3' | 2.60                     | 0.45              |
| 1:M:633:PRO:HA   | 1:M:634:PRO:HD3 | 1.89                     | 0.45              |
| 1:O:619:HIS:CA   | 2:EA:997:DA:O3' | 2.60                     | 0.45              |
| 1:P:245:HIS:CD2  | 1:P:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:W:245:HIS:CD2  | 1:W:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:W:335:THR:CG2  | 1:W:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:Y:630:LYS:HD2  | 2:NA:996:DA:OP2 | 2.16                     | 0.45              |
| 1:b:633:PRO:HA   | 1:b:634:PRO:HD3 | 1.89                     | 0.45              |
| 1:f:380:THR:HG22 | 1:f:381:GLU:H   | 1.82                     | 0.45              |
| 1:g:335:THR:CG2  | 1:g:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:g:619:HIS:CA   | 2:YA:997:DA:O3' | 2.60                     | 0.45              |
| 1:g:630:LYS:HD2  | 2:ZA:996:DA:OP2 | 2.15                     | 0.45              |
| 1:m:380:THR:HG22 | 1:m:381:GLU:H   | 1.82                     | 0.45              |
| 1:p:335:THR:CG2  | 1:p:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:p:600:ASP:OD1  | 1:p:717:THR:OG1 | 2.34                     | 0.45              |
| 1:q:335:THR:CG2  | 1:q:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:q:453:LEU:HD22 | 1:r:537:GLY:HA2 | 1.98                     | 0.45              |
| 1:u:335:THR:CG2  | 1:u:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:v:525:ASN:HD22 | 1:v:562:ALA:HB2 | 1.80                     | 0.45              |
| 1:w:422:ASN:HB3  | 1:w:425:LYS:HB2 | 1.97                     | 0.45              |
| 1:y:245:HIS:CD2  | 1:y:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:y:619:HIS:CA   | 2:sA:997:DA:C2' | 2.88                     | 0.45              |
| 1:3:380:THR:HG22 | 1:3:381:GLU:H   | 1.82                     | 0.45              |
| 1:5:525:ASN:HD22 | 1:5:562:ALA:HB2 | 1.81                     | 0.45              |
| 1:5:628:GLY:C    | 2:yA:997:DA:N1  | 2.66                     | 0.45              |
| 1:C:628:GLY:C    | 2:UA:997:DA:N1  | 2.66                     | 0.45              |
| 1:D:548:LEU:HG   | 1:D:714:PRO:HD3 | 1.98                     | 0.45              |
| 1:F:245:HIS:CD2  | 1:F:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:H:380:THR:HG22 | 1:H:381:GLU:H   | 1.82                     | 0.45              |
| 1:O:633:PRO:HA   | 1:O:634:PRO:HD3 | 1.89                     | 0.45              |
| 1:Q:525:ASN:HD22 | 1:Q:562:ALA:HB2 | 1.80                     | 0.45              |
| 1:R:245:HIS:CD2  | 1:R:642:PRO:HB3 | 2.52                     | 0.45              |
| 1:S:335:THR:CG2  | 1:S:634:PRO:HB2 | 2.47                     | 0.45              |
| 1:S:619:HIS:CA   | 2:IA:997:DA:O3' | 2.60                     | 0.45              |
| 1:U:245:HIS:CD2  | 1:U:642:PRO:HB3 | 2.51                     | 0.45              |
| 1:V:548:LEU:HG   | 1:V:714:PRO:HD3 | 1.98                     | 0.45              |
| 1:W:380:THR:HG22 | 1:W:381:GLU:H   | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:537:GLY:HA2  | 1:e:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:Y:548:LEU:HG   | 1:Y:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:d:335:THR:CG2  | 1:d:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:e:245:HIS:CD2  | 1:e:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:k:335:THR:CG2  | 1:k:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:o:380:THR:HG22 | 1:o:381:GLU:H    | 1.82                     | 0.45              |
| 1:o:513:ASN:ND2  | 1:o:526:THR:HG22 | 2.10                     | 0.45              |
| 1:o:630:LYS:HD2  | 2:TA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:q:548:LEU:HG   | 1:q:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:r:453:LEU:HD22 | 1:s:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:t:600:ASP:OD1  | 1:t:717:THR:OG1  | 2.34                     | 0.45              |
| 1:x:453:LEU:HD22 | 1:y:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:7:276:ASN:O    | 1:7:606:PRO:HA   | 2.15                     | 0.45              |
| 1:H:245:HIS:CD2  | 1:H:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:H:537:GLY:HA2  | 1:Y:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:J:619:HIS:CA   | 2:9:997:DA:O3'   | 2.60                     | 0.45              |
| 1:P:525:ASN:HD22 | 1:P:562:ALA:HB2  | 1.80                     | 0.45              |
| 1:Q:600:ASP:OD1  | 1:Q:717:THR:OG1  | 2.34                     | 0.45              |
| 1:R:380:THR:HG22 | 1:R:381:GLU:H    | 1.82                     | 0.45              |
| 1:R:537:GLY:HA2  | 1:U:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:S:245:HIS:CD2  | 1:S:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:T:600:ASP:OD1  | 1:T:717:THR:OG1  | 2.34                     | 0.45              |
| 1:W:453:LEU:HD22 | 1:Y:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:X:335:THR:CG2  | 1:X:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:X:380:THR:HG22 | 1:X:381:GLU:H    | 1.82                     | 0.45              |
| 1:c:537:GLY:HA2  | 1:p:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:c:548:LEU:HG   | 1:c:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:d:439:VAL:HG21 | 1:d:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:g:245:HIS:CD2  | 1:g:642:PRO:HB3  | 2.51                     | 0.45              |
| 1:i:453:LEU:HD22 | 1:j:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:j:600:ASP:OD1  | 1:j:717:THR:OG1  | 2.34                     | 0.45              |
| 1:k:439:VAL:HG21 | 1:k:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:k:628:GLY:C    | 2:cA:997:DA:N1   | 2.66                     | 0.45              |
| 1:p:245:HIS:CD2  | 1:p:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:p:380:THR:HG22 | 1:p:381:GLU:H    | 1.82                     | 0.45              |
| 1:p:525:ASN:HD22 | 1:p:562:ALA:HB2  | 1.81                     | 0.45              |
| 1:r:380:THR:HG22 | 1:r:381:GLU:H    | 1.82                     | 0.45              |
| 1:s:335:THR:CG2  | 1:s:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:t:245:HIS:CD2  | 1:t:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:v:245:HIS:CD2  | 1:v:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:w:335:THR:CG2  | 1:w:634:PRO:HB2  | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:628:GLY:C    | 2:pA:997:DA:N1   | 2.66                     | 0.45              |
| 1:x:245:HIS:CD2  | 1:x:642:PRO:HB3  | 2.51                     | 0.45              |
| 1:x:380:THR:HG22 | 1:x:381:GLU:H    | 1.82                     | 0.45              |
| 1:z:372:ASN:ND2  | 1:z:376:THR:O    | 2.44                     | 0.45              |
| 1:2:335:THR:CG2  | 1:2:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:2:548:LEU:HG   | 1:2:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:3:548:LEU:HG   | 1:3:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:6:245:HIS:CD2  | 1:6:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:7:619:HIS:CA   | 2:0A:997:DA:O3'  | 2.60                     | 0.45              |
| 1:8:245:HIS:CD2  | 1:8:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:C:439:VAL:HG21 | 1:C:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:C:548:LEU:HG   | 1:C:714:PRO:HD3  | 1.98                     | 0.45              |
| 1:D:335:THR:CG2  | 1:D:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:F:600:ASP:OD1  | 1:F:717:THR:OG1  | 2.34                     | 0.45              |
| 1:I:276:ASN:O    | 1:I:606:PRO:HA   | 2.15                     | 0.45              |
| 1:J:380:THR:HG22 | 1:J:381:GLU:H    | 1.82                     | 0.45              |
| 1:Q:245:HIS:CD2  | 1:Q:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:Q:335:THR:CG2  | 1:Q:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:T:537:GLY:HA2  | 1:l:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:U:380:THR:HG22 | 1:U:381:GLU:H    | 1.82                     | 0.45              |
| 1:U:633:PRO:HA   | 1:U:634:PRO:HD3  | 1.89                     | 0.45              |
| 1:X:245:HIS:CD2  | 1:X:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:a:628:GLY:C    | 2:RA:997:DA:N1   | 2.66                     | 0.45              |
| 1:a:630:LYS:HD2  | 2:AA:996:DA:OP2  | 2.16                     | 0.45              |
| 1:e:380:THR:HG22 | 1:e:381:GLU:H    | 1.82                     | 0.45              |
| 1:f:245:HIS:CD2  | 1:f:642:PRO:HB3  | 2.51                     | 0.45              |
| 1:f:410:GLU:OE2  | 2:XA:996:DA:N6   | 2.47                     | 0.45              |
| 1:j:245:HIS:CD2  | 1:j:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:j:619:HIS:CA   | 2:bA:997:DA:C2'  | 2.88                     | 0.45              |
| 1:m:245:HIS:CD2  | 1:m:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:m:410:GLU:OE2  | 2:eA:996:DA:N6   | 2.47                     | 0.45              |
| 1:o:245:HIS:CD2  | 1:o:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:u:339:TYR:OH   | 1:u:632:PRO:O    | 2.34                     | 0.45              |
| 1:v:335:THR:CG2  | 1:v:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:v:600:ASP:OD1  | 1:v:717:THR:OG1  | 2.34                     | 0.45              |
| 1:w:245:HIS:CD2  | 1:w:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:y:380:THR:HG22 | 1:y:381:GLU:H    | 1.82                     | 0.45              |
| 1:3:439:VAL:HG21 | 1:3:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:5:380:THR:HG22 | 1:5:381:GLU:H    | 1.82                     | 0.45              |
| 1:A:619:HIS:CA   | 2:0:997:DA:O3'   | 2.60                     | 0.45              |
| 1:D:245:HIS:CD2  | 1:D:642:PRO:HB3  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:380:THR:HG22 | 1:E:381:GLU:H    | 1.82                     | 0.45              |
| 1:H:513:ASN:ND2  | 1:H:526:THR:HG22 | 2.10                     | 0.45              |
| 1:I:245:HIS:CD2  | 1:I:642:PRO:HB3  | 2.51                     | 0.45              |
| 1:I:439:VAL:HG21 | 1:I:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:I:600:ASP:OD1  | 1:I:717:THR:OG1  | 2.34                     | 0.45              |
| 1:K:380:THR:HG22 | 1:K:381:GLU:H    | 1.82                     | 0.45              |
| 1:N:372:ASN:ND2  | 1:N:376:THR:O    | 2.44                     | 0.45              |
| 1:O:245:HIS:CD2  | 1:O:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:Q:633:PRO:HA   | 1:Q:634:PRO:HD3  | 1.89                     | 0.45              |
| 1:R:335:THR:CG2  | 1:R:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:R:619:HIS:CA   | 2:HA:997:DA:C2'  | 2.88                     | 0.45              |
| 1:T:245:HIS:CD2  | 1:T:642:PRO:HB3  | 2.52                     | 0.45              |
| 1:V:537:GLY:HA2  | 1:X:453:LEU:HD22 | 1.98                     | 0.45              |
| 1:X:439:VAL:HG21 | 1:X:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:Z:439:VAL:HG21 | 1:Z:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:b:439:VAL:HG21 | 1:b:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:c:453:LEU:HD22 | 1:o:537:GLY:HA2  | 1.98                     | 0.45              |
| 1:e:439:VAL:HG21 | 1:e:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:g:633:PRO:HA   | 1:g:634:PRO:HD3  | 1.89                     | 0.45              |
| 1:i:335:THR:CG2  | 1:i:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:j:335:THR:CG2  | 1:j:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:l:381:GLU:OE2  | 1:n:696:PRO:HG3  | 2.17                     | 0.45              |
| 1:m:696:PRO:HG3  | 1:s:381:GLU:OE2  | 2.17                     | 0.45              |
| 1:s:380:THR:HG22 | 1:s:381:GLU:H    | 1.82                     | 0.45              |
| 1:t:335:THR:CG2  | 1:t:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:u:380:THR:HG22 | 1:u:381:GLU:H    | 1.82                     | 0.45              |
| 1:u:619:HIS:CA   | 2:nA:997:DA:C2'  | 2.88                     | 0.45              |
| 1:y:335:THR:CG2  | 1:y:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:5:335:THR:CG2  | 1:5:634:PRO:HB2  | 2.47                     | 0.45              |
| 1:7:245:HIS:CD2  | 1:7:642:PRO:HB3  | 2.51                     | 0.45              |
| 1:7:439:VAL:HG21 | 1:7:450:ASN:HB2  | 1.99                     | 0.45              |
| 1:A:335:THR:CG2  | 1:A:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:A:380:THR:HG22 | 1:A:381:GLU:H    | 1.82                     | 0.44              |
| 1:D:410:GLU:OE2  | 2:fA:996:DA:N6   | 2.47                     | 0.44              |
| 1:E:339:TYR:OH   | 1:E:632:PRO:O    | 2.34                     | 0.44              |
| 1:G:439:VAL:HG21 | 1:G:450:ASN:HB2  | 1.99                     | 0.44              |
| 1:G:600:ASP:OD1  | 1:G:717:THR:OG1  | 2.34                     | 0.44              |
| 1:I:380:THR:HG22 | 1:I:381:GLU:H    | 1.82                     | 0.44              |
| 1:L:439:VAL:HG21 | 1:L:450:ASN:HB2  | 1.99                     | 0.44              |
| 1:M:513:ASN:ND2  | 1:M:526:THR:HG22 | 2.10                     | 0.44              |
| 1:N:335:THR:CG2  | 1:N:634:PRO:HB2  | 2.47                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:Q:439:VAL:HG21 | 1:Q:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:S:628:GLY:C    | 2:IA:997:DA:N1  | 2.66                     | 0.44              |
| 1:T:335:THR:CG2  | 1:T:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:T:439:VAL:HG21 | 1:T:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:W:339:TYR:OH   | 1:W:632:PRO:O   | 2.34                     | 0.44              |
| 1:Y:439:VAL:HG21 | 1:Y:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:Z:245:HIS:CD2  | 1:Z:642:PRO:HB3 | 2.52                     | 0.44              |
| 1:f:628:GLY:C    | 2:XA:997:DA:N1  | 2.66                     | 0.44              |
| 1:l:335:THR:CG2  | 1:l:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:n:335:THR:CG2  | 1:n:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:p:339:TYR:OH   | 1:p:632:PRO:O   | 2.34                     | 0.44              |
| 1:r:439:VAL:HG21 | 1:r:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:s:245:HIS:CD2  | 1:s:642:PRO:HB3 | 2.52                     | 0.44              |
| 1:s:439:VAL:HG21 | 1:s:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:v:439:VAL:HG21 | 1:v:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:1:525:ASN:HD22 | 1:1:562:ALA:HB2 | 1.81                     | 0.44              |
| 1:2:410:GLU:OE2  | 2:vA:996:DA:N6  | 2.47                     | 0.44              |
| 1:4:633:PRO:HA   | 1:4:634:PRO:HD3 | 1.89                     | 0.44              |
| 1:6:439:VAL:HG21 | 1:6:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:7:380:THR:HG22 | 1:7:381:GLU:H   | 1.82                     | 0.44              |
| 1:7:600:ASP:OD1  | 1:7:717:THR:OG1 | 2.34                     | 0.44              |
| 1:C:600:ASP:OD1  | 1:C:717:THR:OG1 | 2.34                     | 0.44              |
| 1:E:619:HIS:CA   | 2:qA:997:DA:C2' | 2.88                     | 0.44              |
| 1:F:335:THR:CG2  | 1:F:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:F:439:VAL:HG21 | 1:F:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:F:619:HIS:CA   | 2:1A:997:DA:O3' | 2.60                     | 0.44              |
| 1:L:548:LEU:HG   | 1:L:714:PRO:HD3 | 1.98                     | 0.44              |
| 1:L:630:LYS:HD2  | 2:9:996:DA:OP2  | 2.16                     | 0.44              |
| 1:N:380:THR:HG22 | 1:N:381:GLU:H   | 1.82                     | 0.44              |
| 1:U:439:VAL:HG21 | 1:U:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:V:245:HIS:CD2  | 1:V:642:PRO:HB3 | 2.52                     | 0.44              |
| 1:Z:335:THR:CG2  | 1:Z:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:a:439:VAL:HG21 | 1:a:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:b:245:HIS:CD2  | 1:b:642:PRO:HB3 | 2.52                     | 0.44              |
| 1:b:335:THR:CG2  | 1:b:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:c:439:VAL:HG21 | 1:c:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:d:245:HIS:CD2  | 1:d:642:PRO:HB3 | 2.52                     | 0.44              |
| 1:h:335:THR:CG2  | 1:h:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:h:696:PRO:HG3  | 1:i:381:GLU:OE2 | 2.18                     | 0.44              |
| 1:j:439:VAL:HG21 | 1:j:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:k:245:HIS:CD2  | 1:k:642:PRO:HB3 | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:537:GLY:HA2  | 1:s:453:LEU:HD22 | 1.98                     | 0.44              |
| 1:t:372:ASN:ND2  | 1:t:376:THR:O    | 2.44                     | 0.44              |
| 1:t:619:HIS:CA   | 2:mA:997:DA:O3'  | 2.60                     | 0.44              |
| 1:t:633:PRO:HA   | 1:t:634:PRO:HD3  | 1.89                     | 0.44              |
| 1:v:633:PRO:HA   | 1:v:634:PRO:HD3  | 1.89                     | 0.44              |
| 1:z:335:THR:CG2  | 1:z:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:2:245:HIS:CD2  | 1:2:642:PRO:HB3  | 2.52                     | 0.44              |
| 1:4:335:THR:CG2  | 1:4:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:6:600:ASP:OD1  | 1:6:717:THR:OG1  | 2.34                     | 0.44              |
| 1:7:619:HIS:CA   | 2:0A:997:DA:C2'  | 2.88                     | 0.44              |
| 1:F:633:PRO:HA   | 1:F:634:PRO:HD3  | 1.89                     | 0.44              |
| 1:I:619:HIS:CA   | 2:5A:997:DA:C2'  | 2.88                     | 0.44              |
| 1:L:600:ASP:OD1  | 1:L:717:THR:OG1  | 2.34                     | 0.44              |
| 1:Q:628:GLY:C    | 2:GA:997:DA:N1   | 2.66                     | 0.44              |
| 1:T:619:HIS:CA   | 2:KA:997:DA:C2'  | 2.88                     | 0.44              |
| 1:V:380:THR:HG22 | 1:V:381:GLU:H    | 1.82                     | 0.44              |
| 1:Z:600:ASP:OD1  | 1:Z:717:THR:OG1  | 2.34                     | 0.44              |
| 1:a:600:ASP:OD1  | 1:a:717:THR:OG1  | 2.34                     | 0.44              |
| 1:d:633:PRO:HA   | 1:d:634:PRO:HD3  | 1.89                     | 0.44              |
| 1:k:633:PRO:HA   | 1:k:634:PRO:HD3  | 1.89                     | 0.44              |
| 1:q:380:THR:HG22 | 1:q:381:GLU:H    | 1.82                     | 0.44              |
| 1:t:439:VAL:HG21 | 1:t:450:ASN:HB2  | 1.99                     | 0.44              |
| 1:x:439:VAL:HG21 | 1:x:450:ASN:HB2  | 1.99                     | 0.44              |
| 1:x:600:ASP:OD1  | 1:x:717:THR:OG1  | 2.34                     | 0.44              |
| 1:z:380:THR:HG22 | 1:z:381:GLU:H    | 1.82                     | 0.44              |
| 1:4:600:ASP:OD1  | 1:4:717:THR:OG1  | 2.34                     | 0.44              |
| 1:5:619:HIS:CA   | 2:yA:997:DA:C2'  | 2.88                     | 0.44              |
| 1:6:335:THR:CG2  | 1:6:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:M:335:THR:CG2  | 1:M:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:M:439:VAL:HG21 | 1:M:450:ASN:HB2  | 2.00                     | 0.44              |
| 1:M:482:ASN:HB3  | 1:M:483:ARG:H    | 1.62                     | 0.44              |
| 1:O:370:THR:HG21 | 1:O:384:SER:O    | 2.18                     | 0.44              |
| 1:O:696:PRO:HG3  | 1:P:381:GLU:OE2  | 2.18                     | 0.44              |
| 1:R:453:LEU:HD22 | 1:S:537:GLY:HA2  | 1.98                     | 0.44              |
| 1:U:600:ASP:OD1  | 1:U:717:THR:OG1  | 2.34                     | 0.44              |
| 1:a:548:LEU:HG   | 1:a:714:PRO:HD3  | 1.98                     | 0.44              |
| 1:g:370:THR:HG21 | 1:g:384:SER:O    | 2.18                     | 0.44              |
| 1:g:696:PRO:HG3  | 1:l:381:GLU:OE2  | 2.18                     | 0.44              |
| 1:h:370:THR:HG21 | 1:h:384:SER:O    | 2.18                     | 0.44              |
| 1:m:628:GLY:C    | 2:eA:997:DA:N1   | 2.66                     | 0.44              |
| 1:p:370:THR:HG21 | 1:p:384:SER:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:p:619:HIS:CA   | 2:iA:997:DA:O3'  | 2.60                     | 0.44              |
| 1:q:245:HIS:CD2  | 1:q:642:PRO:HB3  | 2.52                     | 0.44              |
| 1:v:628:GLY:C    | 2:oA:997:DA:N1   | 2.66                     | 0.44              |
| 1:3:600:ASP:OD1  | 1:3:717:THR:OG1  | 2.34                     | 0.44              |
| 1:5:619:HIS:CA   | 2:yA:997:DA:O3'  | 2.60                     | 0.44              |
| 1:B:439:VAL:HG21 | 1:B:450:ASN:HB2  | 1.99                     | 0.44              |
| 1:F:372:ASN:ND2  | 1:F:376:THR:O    | 2.44                     | 0.44              |
| 1:G:335:THR:CG2  | 1:G:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:I:335:THR:CG2  | 1:I:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:I:628:GLY:C    | 2:5A:997:DA:N1   | 2.66                     | 0.44              |
| 1:L:380:THR:HG22 | 1:L:381:GLU:H    | 1.82                     | 0.44              |
| 1:M:600:ASP:OD1  | 1:M:717:THR:OG1  | 2.34                     | 0.44              |
| 1:M:628:GLY:C    | 2:CA:997:DA:N1   | 2.66                     | 0.44              |
| 1:W:370:THR:HG21 | 1:W:384:SER:O    | 2.18                     | 0.44              |
| 1:X:381:GLU:OE2  | 1:f:696:PRO:HG3  | 2.18                     | 0.44              |
| 1:b:370:THR:HG21 | 1:b:384:SER:O    | 2.18                     | 0.44              |
| 1:b:600:ASP:OD1  | 1:b:717:THR:OG1  | 2.34                     | 0.44              |
| 1:c:482:ASN:HB3  | 1:c:483:ARG:H    | 1.62                     | 0.44              |
| 1:d:380:THR:HG22 | 1:d:381:GLU:H    | 1.82                     | 0.44              |
| 1:k:370:THR:HG21 | 1:k:384:SER:O    | 2.18                     | 0.44              |
| 1:n:370:THR:HG21 | 1:n:384:SER:O    | 2.18                     | 0.44              |
| 1:n:380:THR:HG22 | 1:n:381:GLU:H    | 1.82                     | 0.44              |
| 1:o:453:LEU:HD22 | 1:p:537:GLY:HA2  | 1.98                     | 0.44              |
| 1:q:619:HIS:CA   | 2:jA:997:DA:C2'  | 2.88                     | 0.44              |
| 1:w:537:GLY:HA2  | 1:y:453:LEU:HD22 | 1.98                     | 0.44              |
| 1:1:370:THR:HG21 | 1:1:384:SER:O    | 2.18                     | 0.44              |
| 1:4:439:VAL:HG21 | 1:4:450:ASN:HB2  | 2.00                     | 0.44              |
| 1:4:482:ASN:HB3  | 1:4:483:ARG:H    | 1.62                     | 0.44              |
| 1:7:335:THR:CG2  | 1:7:634:PRO:HB2  | 2.47                     | 0.44              |
| 1:H:370:THR:HG21 | 1:H:384:SER:O    | 2.18                     | 0.44              |
| 1:H:453:LEU:HD22 | 1:W:537:GLY:HA2  | 1.98                     | 0.44              |
| 1:J:696:PRO:HG3  | 1:a:381:GLU:OE2  | 2.18                     | 0.44              |
| 1:K:696:PRO:HG3  | 1:L:381:GLU:OE2  | 2.18                     | 0.44              |
| 1:M:370:THR:HG21 | 1:M:384:SER:O    | 2.18                     | 0.44              |
| 1:P:370:THR:HG21 | 1:P:384:SER:O    | 2.18                     | 0.44              |
| 1:T:380:THR:HG22 | 1:T:381:GLU:H    | 1.82                     | 0.44              |
| 1:V:370:THR:HG21 | 1:V:384:SER:O    | 2.18                     | 0.44              |
| 1:V:619:HIS:CA   | 2:MA:997:DA:C2'  | 2.88                     | 0.44              |
| 1:Z:370:THR:HG21 | 1:Z:384:SER:O    | 2.18                     | 0.44              |
| 1:a:380:THR:HG22 | 1:a:381:GLU:H    | 1.82                     | 0.44              |
| 1:d:370:THR:HG21 | 1:d:384:SER:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:k:380:THR:HG22 | 1:k:381:GLU:H   | 1.82                     | 0.44              |
| 1:r:339:TYR:OH   | 1:r:632:PRO:O   | 2.34                     | 0.44              |
| 1:w:380:THR:HG22 | 1:w:381:GLU:H   | 1.82                     | 0.44              |
| 1:z:370:THR:HG21 | 1:z:384:SER:O   | 2.18                     | 0.44              |
| 1:4:380:THR:HG22 | 1:4:381:GLU:H   | 1.82                     | 0.44              |
| 1:7:628:GLY:C    | 2:0A:997:DA:N1  | 2.66                     | 0.44              |
| 1:8:335:THR:CG2  | 1:8:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:8:380:THR:HG22 | 1:8:381:GLU:H   | 1.82                     | 0.44              |
| 1:8:439:VAL:HG21 | 1:8:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:A:619:HIS:CA   | 2:0:997:DA:C2'  | 2.88                     | 0.44              |
| 1:B:335:THR:CG2  | 1:B:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:G:696:PRO:HG3  | 1:W:381:GLU:OE2 | 2.18                     | 0.44              |
| 1:I:696:PRO:HG3  | 1:J:381:GLU:OE2 | 2.17                     | 0.44              |
| 1:W:619:HIS:CA   | 2:NA:997:DA:O3' | 2.60                     | 0.44              |
| 1:a:372:ASN:ND2  | 1:a:376:THR:O   | 2.44                     | 0.44              |
| 1:f:339:TYR:OH   | 1:f:632:PRO:O   | 2.34                     | 0.44              |
| 1:h:380:THR:HG22 | 1:h:381:GLU:H   | 1.82                     | 0.44              |
| 1:j:380:THR:HG22 | 1:j:381:GLU:H   | 1.82                     | 0.44              |
| 1:p:628:GLY:C    | 2:iA:997:DA:N1  | 2.66                     | 0.44              |
| 1:y:339:TYR:OH   | 1:y:632:PRO:O   | 2.34                     | 0.44              |
| 1:z:339:TYR:OH   | 1:z:632:PRO:O   | 2.34                     | 0.44              |
| 1:4:370:THR:HG21 | 1:4:384:SER:O   | 2.18                     | 0.44              |
| 1:6:380:THR:HG22 | 1:6:381:GLU:H   | 1.82                     | 0.44              |
| 1:B:370:THR:HG21 | 1:B:384:SER:O   | 2.18                     | 0.44              |
| 1:B:380:THR:HG22 | 1:B:381:GLU:H   | 1.82                     | 0.44              |
| 1:K:381:GLU:OE2  | 1:7:696:PRO:HG3 | 2.17                     | 0.44              |
| 1:M:380:THR:HG22 | 1:M:381:GLU:H   | 1.82                     | 0.44              |
| 1:N:370:THR:HG21 | 1:N:384:SER:O   | 2.18                     | 0.44              |
| 1:P:439:VAL:HG21 | 1:P:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:e:335:THR:CG2  | 1:e:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:e:339:TYR:OH   | 1:e:632:PRO:O   | 2.34                     | 0.44              |
| 1:g:619:HIS:CA   | 2:YA:997:DA:C2' | 2.88                     | 0.44              |
| 1:n:619:HIS:CA   | 2:gA:997:DA:O3' | 2.60                     | 0.44              |
| 1:o:370:THR:HG21 | 1:o:384:SER:O   | 2.18                     | 0.44              |
| 1:q:439:VAL:HG21 | 1:q:450:ASN:HB2 | 1.99                     | 0.44              |
| 1:r:335:THR:CG2  | 1:r:634:PRO:HB2 | 2.47                     | 0.44              |
| 1:s:633:PRO:HA   | 1:s:634:PRO:HD3 | 1.89                     | 0.44              |
| 1:8:370:THR:HG21 | 1:8:384:SER:O   | 2.18                     | 0.44              |
| 1:A:370:THR:HG21 | 1:A:384:SER:O   | 2.18                     | 0.44              |
| 1:C:370:THR:HG21 | 1:C:384:SER:O   | 2.18                     | 0.44              |
| 1:Q:696:PRO:HG3  | 1:S:381:GLU:OE2 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:339:TYR:OH   | 1:R:632:PRO:O    | 2.34                     | 0.44              |
| 1:R:633:PRO:HA   | 1:R:634:PRO:HD3  | 1.89                     | 0.44              |
| 1:S:380:THR:HG22 | 1:S:381:GLU:H    | 1.82                     | 0.44              |
| 1:T:370:THR:HG21 | 1:T:384:SER:O    | 2.18                     | 0.44              |
| 1:Y:370:THR:HG21 | 1:Y:384:SER:O    | 2.18                     | 0.44              |
| 1:f:370:THR:HG21 | 1:f:384:SER:O    | 2.18                     | 0.44              |
| 1:k:381:GLU:OE2  | 1:w:696:PRO:HG3  | 2.18                     | 0.44              |
| 1:p:381:GLU:OE2  | 1:6:696:PRO:HG3  | 2.18                     | 0.44              |
| 1:q:370:THR:HG21 | 1:q:384:SER:O    | 2.18                     | 0.44              |
| 1:r:370:THR:HG21 | 1:r:384:SER:O    | 2.18                     | 0.44              |
| 1:v:696:PRO:HG3  | 1:w:381:GLU:OE2  | 2.18                     | 0.44              |
| 1:1:439:VAL:HG21 | 1:1:450:ASN:HB2  | 1.99                     | 0.44              |
| 1:3:370:THR:HG21 | 1:3:384:SER:O    | 2.18                     | 0.44              |
| 1:4:628:GLY:C    | 2:xA:997:DA:N1   | 2.66                     | 0.44              |
| 1:5:370:THR:HG21 | 1:5:384:SER:O    | 2.18                     | 0.44              |
| 1:E:370:THR:HG21 | 1:E:384:SER:O    | 2.18                     | 0.43              |
| 1:F:696:PRO:HG3  | 1:G:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:H:696:PRO:HG3  | 1:I:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:S:696:PRO:HG3  | 1:d:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:U:370:THR:HG21 | 1:U:384:SER:O    | 2.18                     | 0.43              |
| 1:V:439:VAL:HG21 | 1:V:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:W:628:GLY:C    | 2:NA:997:DA:N1   | 2.67                     | 0.43              |
| 1:X:633:PRO:HA   | 1:X:634:PRO:HD3  | 1.89                     | 0.43              |
| 1:Y:482:ASN:HB3  | 1:Y:483:ARG:H    | 1.62                     | 0.43              |
| 1:e:370:THR:HG21 | 1:e:384:SER:O    | 2.18                     | 0.43              |
| 1:j:370:THR:HG21 | 1:j:384:SER:O    | 2.18                     | 0.43              |
| 1:j:696:PRO:HG3  | 1:x:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:m:339:TYR:OH   | 1:m:632:PRO:O    | 2.34                     | 0.43              |
| 1:m:370:THR:HG21 | 1:m:384:SER:O    | 2.18                     | 0.43              |
| 1:n:513:ASN:ND2  | 1:n:526:THR:HG22 | 2.10                     | 0.43              |
| 1:q:600:ASP:OD1  | 1:q:717:THR:OG1  | 2.34                     | 0.43              |
| 1:t:696:PRO:HG3  | 1:6:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:u:370:THR:HG21 | 1:u:384:SER:O    | 2.18                     | 0.43              |
| 1:x:370:THR:HG21 | 1:x:384:SER:O    | 2.18                     | 0.43              |
| 1:2:370:THR:HG21 | 1:2:384:SER:O    | 2.18                     | 0.43              |
| 1:2:696:PRO:HG3  | 1:3:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:3:482:ASN:HB3  | 1:3:483:ARG:H    | 1.62                     | 0.43              |
| 1:7:372:ASN:ND2  | 1:7:376:THR:O    | 2.44                     | 0.43              |
| 1:C:381:GLU:OE2  | 1:D:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:D:370:THR:HG21 | 1:D:384:SER:O    | 2.18                     | 0.43              |
| 1:G:370:THR:HG21 | 1:G:384:SER:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:380:THR:HG22 | 1:G:381:GLU:H   | 1.82                     | 0.43              |
| 1:I:235:ARG:HG3  | 1:I:353:LEU:HB3 | 2.00                     | 0.43              |
| 1:I:370:THR:HG21 | 1:I:384:SER:O   | 2.18                     | 0.43              |
| 1:J:235:ARG:HG3  | 1:J:353:LEU:HB3 | 2.00                     | 0.43              |
| 1:K:235:ARG:HG3  | 1:K:353:LEU:HB3 | 2.00                     | 0.43              |
| 1:K:370:THR:HG21 | 1:K:384:SER:O   | 2.18                     | 0.43              |
| 1:L:372:ASN:ND2  | 1:L:376:THR:O   | 2.44                     | 0.43              |
| 1:N:235:ARG:HG3  | 1:N:353:LEU:HB3 | 2.01                     | 0.43              |
| 1:P:696:PRO:HG3  | 1:Q:381:GLU:OE2 | 2.18                     | 0.43              |
| 1:Q:235:ARG:HG3  | 1:Q:353:LEU:HB3 | 2.01                     | 0.43              |
| 1:S:410:GLU:OE2  | 2:IA:996:DA:N6  | 2.47                     | 0.43              |
| 1:T:381:GLU:OE2  | 1:i:696:PRO:HG3 | 2.18                     | 0.43              |
| 1:T:696:PRO:HG3  | 1:U:381:GLU:OE2 | 2.18                     | 0.43              |
| 1:V:235:ARG:HG3  | 1:V:353:LEU:HB3 | 2.01                     | 0.43              |
| 1:V:381:GLU:OE2  | 1:W:696:PRO:HG3 | 2.18                     | 0.43              |
| 1:X:235:ARG:HG3  | 1:X:353:LEU:HB3 | 2.00                     | 0.43              |
| 1:X:600:ASP:OD1  | 1:X:717:THR:OG1 | 2.34                     | 0.43              |
| 1:Z:235:ARG:HG3  | 1:Z:353:LEU:HB3 | 2.00                     | 0.43              |
| 1:b:235:ARG:HG3  | 1:b:353:LEU:HB3 | 2.00                     | 0.43              |
| 1:c:335:THR:CG2  | 1:c:634:PRO:HB2 | 2.47                     | 0.43              |
| 1:c:370:THR:HG21 | 1:c:384:SER:O   | 2.18                     | 0.43              |
| 1:g:381:GLU:OE2  | 1:k:696:PRO:HG3 | 2.18                     | 0.43              |
| 1:h:619:HIS:CA   | 2:ZA:997:DA:O3' | 2.60                     | 0.43              |
| 1:i:370:THR:HG21 | 1:i:384:SER:O   | 2.18                     | 0.43              |
| 1:l:370:THR:HG21 | 1:l:384:SER:O   | 2.18                     | 0.43              |
| 1:o:600:ASP:OD1  | 1:o:717:THR:OG1 | 2.34                     | 0.43              |
| 1:o:696:PRO:HG3  | 1:7:381:GLU:OE2 | 2.18                     | 0.43              |
| 1:p:696:PRO:HG3  | 1:q:381:GLU:OE2 | 2.18                     | 0.43              |
| 1:q:235:ARG:HG3  | 1:q:353:LEU:HB3 | 2.01                     | 0.43              |
| 1:t:380:THR:HG22 | 1:t:381:GLU:H   | 1.82                     | 0.43              |
| 1:u:381:GLU:OE2  | 1:5:696:PRO:HG3 | 2.18                     | 0.43              |
| 1:v:235:ARG:HG3  | 1:v:353:LEU:HB3 | 2.01                     | 0.43              |
| 1:w:372:ASN:ND2  | 1:w:376:THR:O   | 2.44                     | 0.43              |
| 1:w:678:GLU:OE2  | 1:w:680:SER:OG  | 2.24                     | 0.43              |
| 1:z:235:ARG:HG3  | 1:z:353:LEU:HB3 | 2.01                     | 0.43              |
| 1:B:381:GLU:OE2  | 1:C:696:PRO:HG3 | 2.18                     | 0.43              |
| 1:J:370:THR:HG21 | 1:J:384:SER:O   | 2.18                     | 0.43              |
| 1:O:619:HIS:CA   | 2:EA:997:DA:C2' | 2.88                     | 0.43              |
| 1:V:600:ASP:OD1  | 1:V:717:THR:OG1 | 2.34                     | 0.43              |
| 1:X:696:PRO:HG3  | 1:Y:381:GLU:OE2 | 2.18                     | 0.43              |
| 1:Y:335:THR:CG2  | 1:Y:634:PRO:HB2 | 2.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:439:VAL:HG21 | 1:g:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:i:372:ASN:ND2  | 1:i:376:THR:O    | 2.44                     | 0.43              |
| 1:i:439:VAL:HG21 | 1:i:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:j:381:GLU:OE2  | 1:l:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:l:439:VAL:HG21 | 1:l:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:v:381:GLU:OE2  | 1:l:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:w:370:THR:HG21 | 1:w:384:SER:O    | 2.18                     | 0.43              |
| 1:y:633:PRO:HA   | 1:y:634:PRO:HD3  | 1.89                     | 0.43              |
| 1:3:696:PRO:HG3  | 1:8:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:6:370:THR:HG21 | 1:6:384:SER:O    | 2.18                     | 0.43              |
| 1:7:235:ARG:HG3  | 1:7:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:7:370:THR:HG21 | 1:7:384:SER:O    | 2.18                     | 0.43              |
| 1:C:619:HIS:CA   | 2:UA:997:DA:C2'  | 2.88                     | 0.43              |
| 1:F:380:THR:HG22 | 1:F:381:GLU:H    | 1.82                     | 0.43              |
| 1:H:600:ASP:OD1  | 1:H:717:THR:OG1  | 2.34                     | 0.43              |
| 1:O:381:GLU:OE2  | 1:d:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:O:439:VAL:HG21 | 1:O:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:R:495:MET:SD   | 1:U:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:S:372:ASN:ND2  | 1:S:376:THR:O    | 2.44                     | 0.43              |
| 1:U:619:HIS:CA   | 2:LA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:X:619:HIS:CA   | 2:OA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:Z:339:TYR:OH   | 1:Z:632:PRO:O    | 2.34                     | 0.43              |
| 1:Z:633:PRO:HA   | 1:Z:634:PRO:HD3  | 1.89                     | 0.43              |
| 1:k:235:ARG:HG3  | 1:k:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:l:372:ASN:ND2  | 1:l:376:THR:O    | 2.44                     | 0.43              |
| 1:n:600:ASP:OD1  | 1:n:717:THR:OG1  | 2.34                     | 0.43              |
| 1:r:466:PRO:HD2  | 1:s:495:MET:SD   | 2.59                     | 0.43              |
| 1:s:235:ARG:HG3  | 1:s:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:s:600:ASP:OD1  | 1:s:717:THR:OG1  | 2.34                     | 0.43              |
| 1:v:370:THR:HG21 | 1:v:384:SER:O    | 2.18                     | 0.43              |
| 1:v:372:ASN:ND2  | 1:v:376:THR:O    | 2.44                     | 0.43              |
| 1:w:410:GLU:OE2  | 2:pA:996:DA:N6   | 2.47                     | 0.43              |
| 1:x:466:PRO:HD2  | 1:y:495:MET:SD   | 2.59                     | 0.43              |
| 1:x:619:HIS:CA   | 2:rA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:5:314:VAL:HG13 | 1:5:660:THR:HG23 | 2.01                     | 0.43              |
| 1:5:466:PRO:HD2  | 1:6:495:MET:SD   | 2.59                     | 0.43              |
| 1:6:235:ARG:HG3  | 1:6:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:314:VAL:HG13 | 1:A:660:THR:HG23 | 2.01                     | 0.43              |
| 1:C:314:VAL:HG13 | 1:C:660:THR:HG23 | 2.01                     | 0.43              |
| 1:G:235:ARG:HG3  | 1:G:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:G:482:ASN:HB3  | 1:G:483:ARG:H    | 1.62                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:372:ASN:ND2  | 1:I:376:THR:O    | 2.44                     | 0.43              |
| 1:M:235:ARG:HG3  | 1:M:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:M:381:GLU:OE2  | 1:c:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:M:696:PRO:HG3  | 1:N:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:N:439:VAL:HG21 | 1:N:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:O:380:THR:HG22 | 1:O:381:GLU:H    | 1.82                     | 0.43              |
| 1:R:235:ARG:HG3  | 1:R:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:S:370:THR:HG21 | 1:S:384:SER:O    | 2.18                     | 0.43              |
| 1:S:619:HIS:CA   | 2:IA:997:DA:C2'  | 2.88                     | 0.43              |
| 1:W:439:VAL:HG21 | 1:W:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:W:466:PRO:HD2  | 1:Y:495:MET:SD   | 2.59                     | 0.43              |
| 1:Z:380:THR:HG22 | 1:Z:381:GLU:H    | 1.82                     | 0.43              |
| 1:b:339:TYR:OH   | 1:b:632:PRO:O    | 2.34                     | 0.43              |
| 1:d:235:ARG:HG3  | 1:d:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:e:696:PRO:HG3  | 1:h:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:r:381:GLU:OE2  | 1:x:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:r:628:GLY:C    | 2:kA:997:DA:N1   | 2.66                     | 0.43              |
| 1:s:619:HIS:CA   | 2:IA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:w:439:VAL:HG21 | 1:w:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:3:314:VAL:HG13 | 1:3:660:THR:HG23 | 2.01                     | 0.43              |
| 1:4:235:ARG:HG3  | 1:4:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:6:482:ASN:HB3  | 1:6:483:ARG:H    | 1.62                     | 0.43              |
| 1:B:235:ARG:HG3  | 1:B:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:C:495:MET:SD   | 1:M:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:H:439:VAL:HG21 | 1:H:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:H:495:MET:SD   | 1:Y:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:I:482:ASN:HB3  | 1:I:483:ARG:H    | 1.62                     | 0.43              |
| 1:N:314:VAL:HG13 | 1:N:660:THR:HG23 | 2.01                     | 0.43              |
| 1:O:314:VAL:HG13 | 1:O:660:THR:HG23 | 2.01                     | 0.43              |
| 1:Q:370:THR:HG21 | 1:Q:384:SER:O    | 2.18                     | 0.43              |
| 1:S:235:ARG:HG3  | 1:S:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:S:439:VAL:HG21 | 1:S:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:S:466:PRO:HD2  | 1:U:495:MET:SD   | 2.59                     | 0.43              |
| 1:T:466:PRO:HD2  | 1:d:495:MET:SD   | 2.59                     | 0.43              |
| 1:V:619:HIS:CA   | 2:MA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:X:495:MET:SD   | 1:e:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:Y:696:PRO:HG3  | 1:4:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:b:380:THR:HG22 | 1:b:381:GLU:H    | 1.82                     | 0.43              |
| 1:c:466:PRO:HD2  | 1:o:495:MET:SD   | 2.59                     | 0.43              |
| 1:c:495:MET:SD   | 1:p:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:f:235:ARG:HG3  | 1:f:353:LEU:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:380:THR:HG22 | 1:g:381:GLU:H    | 1.82                     | 0.43              |
| 1:h:600:ASP:OD1  | 1:h:717:THR:OG1  | 2.35                     | 0.43              |
| 1:i:356:PHE:HA   | 1:i:357:PRO:HD3  | 1.92                     | 0.43              |
| 1:i:466:PRO:HD2  | 1:j:495:MET:SD   | 2.59                     | 0.43              |
| 1:j:466:PRO:HD2  | 1:k:495:MET:SD   | 2.59                     | 0.43              |
| 1:m:235:ARG:HG3  | 1:m:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:p:439:VAL:HG21 | 1:p:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:q:619:HIS:CA   | 2:jA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:u:314:VAL:HG13 | 1:u:660:THR:HG23 | 2.01                     | 0.43              |
| 1:w:235:ARG:HG3  | 1:w:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:w:619:HIS:CA   | 2:pA:997:DA:C2'  | 2.88                     | 0.43              |
| 1:y:235:ARG:HG3  | 1:y:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:y:314:VAL:HG13 | 1:y:660:THR:HG23 | 2.01                     | 0.43              |
| 1:2:380:THR:HG22 | 1:2:381:GLU:H    | 1.82                     | 0.43              |
| 1:5:439:VAL:HG21 | 1:5:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:8:235:ARG:HG3  | 1:8:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:439:VAL:HG21 | 1:A:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:B:422:ASN:OD1  | 1:B:423:LEU:N    | 2.52                     | 0.43              |
| 1:D:235:ARG:HG3  | 1:D:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:D:314:VAL:HG13 | 1:D:660:THR:HG23 | 2.01                     | 0.43              |
| 1:H:410:GLU:OE2  | 2:4A:996:DA:N6   | 2.47                     | 0.43              |
| 1:M:619:HIS:CA   | 2:CA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:Q:422:ASN:OD1  | 1:Q:423:LEU:N    | 2.52                     | 0.43              |
| 1:R:314:VAL:HG13 | 1:R:660:THR:HG23 | 2.01                     | 0.43              |
| 1:T:495:MET:SD   | 1:l:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:U:696:PRO:HG3  | 1:e:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:W:235:ARG:HG3  | 1:W:353:LEU:HB3  | 2.00                     | 0.43              |
| 1:X:422:ASN:OD1  | 1:X:423:LEU:N    | 2.52                     | 0.43              |
| 1:f:439:VAL:HG21 | 1:f:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:k:600:ASP:OD1  | 1:k:717:THR:OG1  | 2.34                     | 0.43              |
| 1:m:439:VAL:HG21 | 1:m:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:n:381:GLU:OE2  | 1:r:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:n:410:GLU:OE2  | 2:gA:996:DA:N6   | 2.47                     | 0.43              |
| 1:n:439:VAL:HG21 | 1:n:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:u:235:ARG:HG3  | 1:u:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:w:466:PRO:HD2  | 1:x:495:MET:SD   | 2.59                     | 0.43              |
| 1:z:314:VAL:HG13 | 1:z:660:THR:HG23 | 2.01                     | 0.43              |
| 1:z:439:VAL:HG21 | 1:z:450:ASN:HB2  | 2.00                     | 0.43              |
| 1:2:314:VAL:HG13 | 1:2:660:THR:HG23 | 2.01                     | 0.43              |
| 1:3:495:MET:SD   | 1:4:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:3:619:HIS:CA   | 2:wA:997:DA:C2'  | 2.88                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:7:422:ASN:OD1  | 1:7:423:LEU:N    | 2.52                     | 0.43              |
| 1:8:422:ASN:OD1  | 1:8:423:LEU:N    | 2.52                     | 0.43              |
| 1:B:495:MET:SD   | 1:L:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:C:238:VAL:HG13 | 1:C:362:THR:HG22 | 2.01                     | 0.43              |
| 1:D:380:THR:HG22 | 1:D:381:GLU:H    | 1.82                     | 0.43              |
| 1:D:439:VAL:HG21 | 1:D:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:E:235:ARG:HG3  | 1:E:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:E:314:VAL:HG13 | 1:E:660:THR:HG23 | 2.01                     | 0.43              |
| 1:E:422:ASN:OD1  | 1:E:423:LEU:N    | 2.52                     | 0.43              |
| 1:F:314:VAL:HG13 | 1:F:660:THR:HG23 | 2.01                     | 0.43              |
| 1:I:422:ASN:OD1  | 1:I:423:LEU:N    | 2.52                     | 0.43              |
| 1:J:466:PRO:HD2  | 1:L:495:MET:SD   | 2.59                     | 0.43              |
| 1:J:600:ASP:OD1  | 1:J:717:THR:OG1  | 2.34                     | 0.43              |
| 1:K:466:PRO:HD2  | 1:a:495:MET:SD   | 2.59                     | 0.43              |
| 1:T:314:VAL:HG13 | 1:T:660:THR:HG23 | 2.01                     | 0.43              |
| 1:X:238:VAL:HG13 | 1:X:362:THR:HG22 | 2.01                     | 0.43              |
| 1:a:370:THR:HG21 | 1:a:384:SER:O    | 2.18                     | 0.43              |
| 1:a:466:PRO:HD2  | 1:8:495:MET:SD   | 2.59                     | 0.43              |
| 1:g:314:VAL:HG13 | 1:g:660:THR:HG23 | 2.01                     | 0.43              |
| 1:j:314:VAL:HG13 | 1:j:660:THR:HG23 | 2.01                     | 0.43              |
| 1:k:314:VAL:HG13 | 1:k:660:THR:HG23 | 2.01                     | 0.43              |
| 1:o:439:VAL:HG21 | 1:o:450:ASN:HB2  | 2.00                     | 0.43              |
| 1:r:314:VAL:HG13 | 1:r:660:THR:HG23 | 2.01                     | 0.43              |
| 1:t:370:THR:HG21 | 1:t:384:SER:O    | 2.18                     | 0.43              |
| 1:u:422:ASN:OD1  | 1:u:423:LEU:N    | 2.52                     | 0.43              |
| 1:v:422:ASN:OD1  | 1:v:423:LEU:N    | 2.52                     | 0.43              |
| 1:2:235:ARG:HG3  | 1:2:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:2:439:VAL:HG21 | 1:2:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:3:238:VAL:HG13 | 1:3:362:THR:HG22 | 2.01                     | 0.43              |
| 1:B:238:VAL:HG13 | 1:B:362:THR:HG22 | 2.01                     | 0.43              |
| 1:B:633:PRO:HA   | 1:B:634:PRO:HD3  | 1.89                     | 0.43              |
| 1:D:238:VAL:HG13 | 1:D:362:THR:HG22 | 2.01                     | 0.43              |
| 1:D:381:GLU:OE2  | 1:E:696:PRO:HG3  | 2.18                     | 0.43              |
| 1:D:466:PRO:HD2  | 1:N:495:MET:SD   | 2.59                     | 0.43              |
| 1:E:428:ASN:HB3  | 1:E:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:F:422:ASN:OD1  | 1:F:423:LEU:N    | 2.52                     | 0.43              |
| 1:G:422:ASN:OD1  | 1:G:423:LEU:N    | 2.52                     | 0.43              |
| 1:I:238:VAL:HG13 | 1:I:362:THR:HG22 | 2.01                     | 0.43              |
| 1:K:600:ASP:OD1  | 1:K:717:THR:OG1  | 2.34                     | 0.43              |
| 1:L:370:THR:HG21 | 1:L:384:SER:O    | 2.18                     | 0.43              |
| 1:M:422:ASN:OD1  | 1:M:423:LEU:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:422:ASN:OD1  | 1:N:423:LEU:N    | 2.52                     | 0.43              |
| 1:N:696:PRO:HG3  | 1:m:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:O:628:GLY:C    | 2:EA:997:DA:N1   | 2.66                     | 0.43              |
| 1:P:428:ASN:HB3  | 1:P:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:Q:372:ASN:ND2  | 1:Q:376:THR:O    | 2.44                     | 0.43              |
| 1:R:439:VAL:HG21 | 1:R:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:S:314:VAL:HG13 | 1:S:660:THR:HG23 | 2.01                     | 0.43              |
| 1:U:314:VAL:HG13 | 1:U:660:THR:HG23 | 2.01                     | 0.43              |
| 1:U:422:ASN:OD1  | 1:U:423:LEU:N    | 2.52                     | 0.43              |
| 1:Z:619:HIS:CA   | 2:QA:997:DA:C2'  | 2.88                     | 0.43              |
| 1:b:619:HIS:CA   | 2:SA:997:DA:C2'  | 2.88                     | 0.43              |
| 1:d:238:VAL:HG13 | 1:d:362:THR:HG22 | 2.01                     | 0.43              |
| 1:d:314:VAL:HG13 | 1:d:660:THR:HG23 | 2.01                     | 0.43              |
| 1:d:428:ASN:HB3  | 1:d:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:d:600:ASP:OD1  | 1:d:717:THR:OG1  | 2.34                     | 0.43              |
| 1:e:628:GLY:C    | 2:WA:997:DA:N1   | 2.66                     | 0.43              |
| 1:f:495:MET:SD   | 1:g:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:h:314:VAL:HG13 | 1:h:660:THR:HG23 | 2.01                     | 0.43              |
| 1:h:439:VAL:HG21 | 1:h:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:k:238:VAL:HG13 | 1:k:362:THR:HG22 | 2.01                     | 0.43              |
| 1:l:422:ASN:OD1  | 1:l:423:LEU:N    | 2.52                     | 0.43              |
| 1:l:600:ASP:OD1  | 1:l:717:THR:OG1  | 2.34                     | 0.43              |
| 1:m:398:THR:HG22 | 1:s:397:ARG:HH12 | 1.84                     | 0.43              |
| 1:m:422:ASN:OD1  | 1:m:423:LEU:N    | 2.52                     | 0.43              |
| 1:n:314:VAL:HG13 | 1:n:660:THR:HG23 | 2.01                     | 0.43              |
| 1:o:410:GLU:OE2  | 2:hA:996:DA:N6   | 2.47                     | 0.43              |
| 1:p:235:ARG:HG3  | 1:p:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:s:238:VAL:HG13 | 1:s:362:THR:HG22 | 2.01                     | 0.43              |
| 1:s:422:ASN:OD1  | 1:s:423:LEU:N    | 2.52                     | 0.43              |
| 1:t:314:VAL:HG13 | 1:t:660:THR:HG23 | 2.01                     | 0.43              |
| 1:u:428:ASN:HB3  | 1:u:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:u:696:PRO:HG3  | 1:2:381:GLU:OE2  | 2.18                     | 0.43              |
| 1:x:422:ASN:OD1  | 1:x:423:LEU:N    | 2.52                     | 0.43              |
| 1:z:422:ASN:OD1  | 1:z:423:LEU:N    | 2.52                     | 0.43              |
| 1:z:495:MET:SD   | 1:2:466:PRO:HD2  | 2.59                     | 0.43              |
| 1:1:428:ASN:HB3  | 1:1:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:3:422:ASN:OD1  | 1:3:423:LEU:N    | 2.52                     | 0.43              |
| 1:4:422:ASN:OD1  | 1:4:423:LEU:N    | 2.52                     | 0.43              |
| 1:4:619:HIS:CA   | 2:xA:997:DA:O3'  | 2.60                     | 0.43              |
| 1:5:235:ARG:HG3  | 1:5:353:LEU:HB3  | 2.00                     | 0.43              |
| 1:5:600:ASP:OD1  | 1:5:717:THR:OG1  | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6:339:TYR:OH   | 1:6:632:PRO:O    | 2.34                     | 0.43              |
| 1:6:422:ASN:OD1  | 1:6:423:LEU:N    | 2.52                     | 0.43              |
| 1:7:238:VAL:HG13 | 1:7:362:THR:HG22 | 2.01                     | 0.43              |
| 1:8:238:VAL:HG13 | 1:8:362:THR:HG22 | 2.01                     | 0.43              |
| 1:C:235:ARG:HG3  | 1:C:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:C:422:ASN:OD1  | 1:C:423:LEU:N    | 2.52                     | 0.43              |
| 1:D:422:ASN:OD1  | 1:D:423:LEU:N    | 2.52                     | 0.43              |
| 1:F:370:THR:HG21 | 1:F:384:SER:O    | 2.18                     | 0.43              |
| 1:G:238:VAL:HG13 | 1:G:362:THR:HG22 | 2.01                     | 0.43              |
| 1:H:422:ASN:OD1  | 1:H:423:LEU:N    | 2.52                     | 0.43              |
| 1:J:422:ASN:OD1  | 1:J:423:LEU:N    | 2.52                     | 0.43              |
| 1:O:422:ASN:OD1  | 1:O:423:LEU:N    | 2.52                     | 0.43              |
| 1:O:466:PRO:HD2  | 1:m:495:MET:SD   | 2.59                     | 0.43              |
| 1:R:370:THR:HG21 | 1:R:384:SER:O    | 2.18                     | 0.43              |
| 1:R:428:ASN:HB3  | 1:R:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:T:238:VAL:HG13 | 1:T:362:THR:HG22 | 2.01                     | 0.43              |
| 1:W:428:ASN:HB3  | 1:W:431:VAL:HG22 | 2.01                     | 0.43              |
| 1:e:314:VAL:HG13 | 1:e:660:THR:HG23 | 2.01                     | 0.43              |
| 1:e:422:ASN:OD1  | 1:e:423:LEU:N    | 2.52                     | 0.43              |
| 1:f:381:GLU:OE2  | 1:z:696:PRO:HG3  | 2.19                     | 0.43              |
| 1:f:422:ASN:OD1  | 1:f:423:LEU:N    | 2.52                     | 0.43              |
| 1:f:466:PRO:HD2  | 1:h:495:MET:SD   | 2.59                     | 0.43              |
| 1:g:422:ASN:OD1  | 1:g:423:LEU:N    | 2.52                     | 0.43              |
| 1:h:410:GLU:OE2  | 2:ZA:996:DA:N6   | 2.47                     | 0.43              |
| 1:i:422:ASN:OD1  | 1:i:423:LEU:N    | 2.52                     | 0.43              |
| 1:j:238:VAL:HG13 | 1:j:362:THR:HG22 | 2.01                     | 0.43              |
| 1:m:466:PRO:HD2  | 1:n:495:MET:SD   | 2.59                     | 0.43              |
| 1:o:422:ASN:OD1  | 1:o:423:LEU:N    | 2.52                     | 0.43              |
| 1:s:370:THR:HG21 | 1:s:384:SER:O    | 2.18                     | 0.43              |
| 1:t:422:ASN:OD1  | 1:t:423:LEU:N    | 2.52                     | 0.43              |
| 1:t:619:HIS:CA   | 2:mA:997:DA:C2'  | 2.88                     | 0.43              |
| 1:u:439:VAL:HG21 | 1:u:450:ASN:HB2  | 1.99                     | 0.43              |
| 1:w:314:VAL:HG13 | 1:w:660:THR:HG23 | 2.01                     | 0.43              |
| 1:x:314:VAL:HG13 | 1:x:660:THR:HG23 | 2.01                     | 0.43              |
| 1:1:380:THR:HG22 | 1:1:381:GLU:H    | 1.82                     | 0.43              |
| 1:3:235:ARG:HG3  | 1:3:353:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:235:ARG:HG3  | 1:A:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:F:619:HIS:CA   | 2:1A:997:DA:C2'  | 2.88                     | 0.42              |
| 1:J:619:HIS:CA   | 2:9:997:DA:C2'   | 2.88                     | 0.42              |
| 1:K:422:ASN:OD1  | 1:K:423:LEU:N    | 2.52                     | 0.42              |
| 1:L:235:ARG:HG3  | 1:L:353:LEU:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:422:ASN:OD1  | 1:L:423:LEU:N    | 2.52                     | 0.42              |
| 1:P:380:THR:HG22 | 1:P:381:GLU:H    | 1.82                     | 0.42              |
| 1:Q:380:THR:HG22 | 1:Q:381:GLU:H    | 1.82                     | 0.42              |
| 1:Q:428:ASN:HB3  | 1:Q:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:S:428:ASN:HB3  | 1:S:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:T:339:TYR:OH   | 1:T:632:PRO:O    | 2.34                     | 0.42              |
| 1:V:422:ASN:OD1  | 1:V:423:LEU:N    | 2.52                     | 0.42              |
| 1:W:314:VAL:HG13 | 1:W:660:THR:HG23 | 2.01                     | 0.42              |
| 1:W:482:ASN:HB3  | 1:W:483:ARG:H    | 1.62                     | 0.42              |
| 1:Y:422:ASN:OD1  | 1:Y:423:LEU:N    | 2.52                     | 0.42              |
| 1:Z:495:MET:SD   | 1:3:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:a:422:ASN:OD1  | 1:a:423:LEU:N    | 2.52                     | 0.42              |
| 1:f:314:VAL:HG13 | 1:f:660:THR:HG23 | 2.01                     | 0.42              |
| 1:i:600:ASP:OD1  | 1:i:717:THR:OG1  | 2.34                     | 0.42              |
| 1:k:428:ASN:HB3  | 1:k:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:n:422:ASN:OD1  | 1:n:423:LEU:N    | 2.52                     | 0.42              |
| 1:p:314:VAL:HG13 | 1:p:660:THR:HG23 | 2.01                     | 0.42              |
| 1:p:428:ASN:HB3  | 1:p:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:q:422:ASN:OD1  | 1:q:423:LEU:N    | 2.52                     | 0.42              |
| 1:q:696:PRO:HG3  | 1:y:381:GLU:OE2  | 2.18                     | 0.42              |
| 1:r:422:ASN:OD1  | 1:r:423:LEU:N    | 2.52                     | 0.42              |
| 1:v:380:THR:HG22 | 1:v:381:GLU:H    | 1.82                     | 0.42              |
| 1:v:428:ASN:HB3  | 1:v:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:w:428:ASN:HB3  | 1:w:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:y:428:ASN:HB3  | 1:y:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:y:439:VAL:HG21 | 1:y:450:ASN:HB2  | 2.00                     | 0.42              |
| 1:z:381:GLU:OE2  | 1:4:696:PRO:HG3  | 2.19                     | 0.42              |
| 1:2:238:VAL:HG13 | 1:2:362:THR:HG22 | 2.01                     | 0.42              |
| 1:2:422:ASN:OD1  | 1:2:423:LEU:N    | 2.52                     | 0.42              |
| 1:5:381:GLU:OE2  | 1:8:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:6:238:VAL:HG13 | 1:6:362:THR:HG22 | 2.01                     | 0.42              |
| 1:A:600:ASP:OD1  | 1:A:717:THR:OG1  | 2.34                     | 0.42              |
| 1:C:466:PRO:HD2  | 1:b:495:MET:SD   | 2.59                     | 0.42              |
| 1:E:439:VAL:HG21 | 1:E:450:ASN:HB2  | 1.99                     | 0.42              |
| 1:G:339:TYR:OH   | 1:G:632:PRO:O    | 2.34                     | 0.42              |
| 1:H:238:VAL:HG13 | 1:H:362:THR:HG22 | 2.01                     | 0.42              |
| 1:J:439:VAL:HG21 | 1:J:450:ASN:HB2  | 1.99                     | 0.42              |
| 1:N:238:VAL:HG13 | 1:N:362:THR:HG22 | 2.01                     | 0.42              |
| 1:T:428:ASN:HB3  | 1:T:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:V:238:VAL:HG13 | 1:V:362:THR:HG22 | 2.01                     | 0.42              |
| 1:V:495:MET:SD   | 1:X:466:PRO:HD2  | 2.59                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:619:HIS:CD2  | 2:OA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:Z:381:GLU:OE2  | 1:a:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:b:696:PRO:HG3  | 1:o:381:GLU:OE2  | 2.18                     | 0.42              |
| 1:c:381:GLU:OE2  | 1:s:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:c:422:ASN:OD1  | 1:c:423:LEU:N    | 2.52                     | 0.42              |
| 1:d:422:ASN:OD1  | 1:d:423:LEU:N    | 2.52                     | 0.42              |
| 1:g:495:MET:SD   | 1:h:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:g:628:GLY:C    | 2:YA:997:DA:N1   | 2.66                     | 0.42              |
| 1:h:422:ASN:OD1  | 1:h:423:LEU:N    | 2.52                     | 0.42              |
| 1:j:428:ASN:HB3  | 1:j:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:l:356:PHE:HA   | 1:l:357:PRO:HD3  | 1.92                     | 0.42              |
| 1:m:314:VAL:HG13 | 1:m:660:THR:HG23 | 2.01                     | 0.42              |
| 1:o:466:PRO:HD2  | 1:p:495:MET:SD   | 2.59                     | 0.42              |
| 1:q:238:VAL:HG13 | 1:q:362:THR:HG22 | 2.01                     | 0.42              |
| 1:t:466:PRO:HD2  | 1:u:495:MET:SD   | 2.59                     | 0.42              |
| 1:y:370:THR:HG21 | 1:y:384:SER:O    | 2.18                     | 0.42              |
| 1:y:422:ASN:OD1  | 1:y:423:LEU:N    | 2.52                     | 0.42              |
| 1:z:238:VAL:HG13 | 1:z:362:THR:HG22 | 2.01                     | 0.42              |
| 1:1:339:TYR:OH   | 1:1:632:PRO:O    | 2.34                     | 0.42              |
| 1:1:600:ASP:OD1  | 1:1:717:THR:OG1  | 2.34                     | 0.42              |
| 1:1:628:GLY:C    | 2:uA:997:DA:N1   | 2.66                     | 0.42              |
| 1:5:238:VAL:HG13 | 1:5:362:THR:HG22 | 2.01                     | 0.42              |
| 1:A:238:VAL:HG13 | 1:A:362:THR:HG22 | 2.01                     | 0.42              |
| 1:B:466:PRO:HD2  | 1:J:495:MET:SD   | 2.59                     | 0.42              |
| 1:E:495:MET:SD   | 1:F:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:H:381:GLU:OE2  | 1:Z:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:H:428:ASN:HB3  | 1:H:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:H:466:PRO:HD2  | 1:W:495:MET:SD   | 2.59                     | 0.42              |
| 1:I:619:HIS:CD2  | 2:5A:997:DA:H3'  | 2.55                     | 0.42              |
| 1:L:696:PRO:HG3  | 1:b:381:GLU:OE2  | 2.18                     | 0.42              |
| 1:N:428:ASN:HB3  | 1:N:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:O:428:ASN:HB3  | 1:O:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:O:495:MET:SD   | 1:n:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:P:422:ASN:OD1  | 1:P:423:LEU:N    | 2.52                     | 0.42              |
| 1:P:600:ASP:OD1  | 1:P:717:THR:OG1  | 2.34                     | 0.42              |
| 1:P:619:HIS:CD2  | 2:FA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:R:381:GLU:OE2  | 1:V:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:R:422:ASN:OD1  | 1:R:423:LEU:N    | 2.52                     | 0.42              |
| 1:X:370:THR:HG21 | 1:X:384:SER:O    | 2.18                     | 0.42              |
| 1:a:235:ARG:HG3  | 1:a:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:c:314:VAL:HG13 | 1:c:660:THR:HG23 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:422:ASN:OD1  | 1:j:423:LEU:N    | 2.52                     | 0.42              |
| 1:k:356:PHE:HA   | 1:k:357:PRO:HD3  | 1.92                     | 0.42              |
| 1:o:238:VAL:HG13 | 1:o:362:THR:HG22 | 2.01                     | 0.42              |
| 1:s:619:HIS:CD2  | 2:lA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:t:235:ARG:HG3  | 1:t:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:y:600:ASP:OD1  | 1:y:717:THR:OG1  | 2.34                     | 0.42              |
| 1:z:428:ASN:HB3  | 1:z:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:z:466:PRO:HD2  | 1:1:495:MET:SD   | 2.59                     | 0.42              |
| 1:1:466:PRO:HD2  | 1:2:495:MET:SD   | 2.59                     | 0.42              |
| 1:1:619:HIS:CD2  | 2:uA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:7:619:HIS:CD2  | 2:0A:997:DA:H3'  | 2.55                     | 0.42              |
| 1:D:495:MET:SD   | 1:P:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:K:428:ASN:HB3  | 1:K:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:K:439:VAL:HG21 | 1:K:450:ASN:HB2  | 1.99                     | 0.42              |
| 1:K:495:MET:SD   | 1:8:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:P:628:GLY:C    | 2:FA:997:DA:N1   | 2.66                     | 0.42              |
| 1:T:422:ASN:OD1  | 1:T:423:LEU:N    | 2.52                     | 0.42              |
| 1:V:619:HIS:CD2  | 2:MA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:a:428:ASN:HB3  | 1:a:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:d:619:HIS:CD2  | 2:VA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:g:428:ASN:HB3  | 1:g:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:h:356:PHE:HA   | 1:h:357:PRO:HD3  | 1.92                     | 0.42              |
| 1:j:339:TYR:OH   | 1:j:632:PRO:O    | 2.34                     | 0.42              |
| 1:k:422:ASN:OD1  | 1:k:423:LEU:N    | 2.52                     | 0.42              |
| 1:k:619:HIS:CD2  | 2:cA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:o:428:ASN:HB3  | 1:o:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:q:619:HIS:CD2  | 2:jA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:u:372:ASN:ND2  | 1:u:376:THR:O    | 2.44                     | 0.42              |
| 1:w:619:HIS:CD2  | 2:pA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:1:422:ASN:OD1  | 1:1:423:LEU:N    | 2.52                     | 0.42              |
| 1:2:619:HIS:CD2  | 2:vA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:8:633:PRO:HA   | 1:8:634:PRO:HD3  | 1.89                     | 0.42              |
| 1:A:422:ASN:OD1  | 1:A:423:LEU:N    | 2.52                     | 0.42              |
| 1:A:466:PRO:HD2  | 1:G:495:MET:SD   | 2.60                     | 0.42              |
| 1:D:619:HIS:CD2  | 2:fA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:F:235:ARG:HG3  | 1:F:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:F:381:GLU:OE2  | 1:R:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:G:466:PRO:HD2  | 1:I:495:MET:SD   | 2.59                     | 0.42              |
| 1:H:235:ARG:HG3  | 1:H:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:J:428:ASN:HB3  | 1:J:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:J:619:HIS:CD2  | 2:9:997:DA:H3'   | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:397:ARG:HH12 | 1:7:398:THR:HG22 | 1.85                     | 0.42              |
| 1:K:619:HIS:CA   | 2:AA:997:DA:C2'  | 2.88                     | 0.42              |
| 1:K:619:HIS:CD2  | 2:AA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:L:428:ASN:HB3  | 1:L:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:N:466:PRO:HD2  | 1:P:495:MET:SD   | 2.59                     | 0.42              |
| 1:O:356:PHE:HA   | 1:O:357:PRO:HD3  | 1.92                     | 0.42              |
| 1:P:339:TYR:OH   | 1:P:632:PRO:O    | 2.34                     | 0.42              |
| 1:Q:482:ASN:HB3  | 1:Q:483:ARG:H    | 1.62                     | 0.42              |
| 1:R:600:ASP:OD1  | 1:R:717:THR:OG1  | 2.34                     | 0.42              |
| 1:S:238:VAL:HG13 | 1:S:362:THR:HG22 | 2.01                     | 0.42              |
| 1:S:422:ASN:OD1  | 1:S:423:LEU:N    | 2.52                     | 0.42              |
| 1:S:619:HIS:CD2  | 2:IA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:Y:235:ARG:HG3  | 1:Y:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:Y:314:VAL:HG13 | 1:Y:660:THR:HG23 | 2.01                     | 0.42              |
| 1:Y:428:ASN:HB3  | 1:Y:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:Y:619:HIS:CD2  | 2:PA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:Z:238:VAL:HG13 | 1:Z:362:THR:HG22 | 2.01                     | 0.42              |
| 1:c:235:ARG:HG3  | 1:c:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:c:372:ASN:ND2  | 1:c:376:THR:O    | 2.44                     | 0.42              |
| 1:c:428:ASN:HB3  | 1:c:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:c:619:HIS:CD2  | 2:TA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:d:466:PRO:HD2  | 1:l:495:MET:SD   | 2.59                     | 0.42              |
| 1:g:235:ARG:HG3  | 1:g:353:LEU:HB3  | 2.00                     | 0.42              |
| 1:i:495:MET:SD   | 1:k:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:n:619:HIS:CD2  | 2:gA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:t:381:GLU:OE2  | 1:y:696:PRO:HG3  | 2.18                     | 0.42              |
| 1:w:238:VAL:HG13 | 1:w:362:THR:HG22 | 2.01                     | 0.42              |
| 1:w:422:ASN:OD1  | 1:w:423:LEU:N    | 2.52                     | 0.42              |
| 1:w:495:MET:SD   | 1:y:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:5:422:ASN:OD1  | 1:5:423:LEU:N    | 2.52                     | 0.42              |
| 1:5:495:MET:SD   | 1:7:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:8:339:TYR:OH   | 1:8:632:PRO:O    | 2.34                     | 0.42              |
| 1:E:238:VAL:HG13 | 1:E:362:THR:HG22 | 2.01                     | 0.42              |
| 1:E:466:PRO:HD2  | 1:Q:495:MET:SD   | 2.59                     | 0.42              |
| 1:G:619:HIS:CD2  | 2:3A:997:DA:H3'  | 2.55                     | 0.42              |
| 1:I:398:THR:HG22 | 1:J:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:J:292:ASN:O    | 1:J:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:L:238:VAL:HG13 | 1:L:362:THR:HG22 | 2.01                     | 0.42              |
| 1:L:398:THR:HG22 | 1:b:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:M:495:MET:SD   | 1:b:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:N:619:HIS:CD2  | 2:DA:997:DA:H3'  | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:238:VAL:HG13 | 1:Q:362:THR:HG22 | 2.01                     | 0.42              |
| 1:T:619:HIS:CD2  | 2:KA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:V:397:ARG:HH12 | 1:W:398:THR:HG22 | 1.84                     | 0.42              |
| 1:X:398:THR:HG22 | 1:Y:397:ARG:HH12 | 1.84                     | 0.42              |
| 1:Y:372:ASN:ND2  | 1:Y:376:THR:O    | 2.44                     | 0.42              |
| 1:Z:397:ARG:HH12 | 1:a:398:THR:HG22 | 1.85                     | 0.42              |
| 1:a:619:HIS:CD2  | 2:RA:997:DA:H3'  | 2.54                     | 0.42              |
| 1:b:238:VAL:HG13 | 1:b:362:THR:HG22 | 2.01                     | 0.42              |
| 1:e:238:VAL:HG13 | 1:e:362:THR:HG22 | 2.01                     | 0.42              |
| 1:h:619:HIS:CD2  | 2:ZA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:o:292:ASN:O    | 1:o:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:p:238:VAL:HG13 | 1:p:362:THR:HG22 | 2.01                     | 0.42              |
| 1:p:398:THR:HG22 | 1:q:397:ARG:HH12 | 1.84                     | 0.42              |
| 1:p:482:ASN:HB3  | 1:p:483:ARG:H    | 1.62                     | 0.42              |
| 1:r:238:VAL:HG13 | 1:r:362:THR:HG22 | 2.01                     | 0.42              |
| 1:u:238:VAL:HG13 | 1:u:362:THR:HG22 | 2.01                     | 0.42              |
| 1:u:466:PRO:HD2  | 1:v:495:MET:SD   | 2.59                     | 0.42              |
| 1:z:619:HIS:CD2  | 2:tA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:1:235:ARG:HG3  | 1:1:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:6:466:PRO:HD2  | 1:7:495:MET:SD   | 2.59                     | 0.42              |
| 1:6:619:HIS:CD2  | 2:zA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:A:495:MET:SD   | 1:I:466:PRO:HD2  | 2.59                     | 0.42              |
| 1:A:560:ARG:HG2  | 1:G:496:GLU:O    | 2.20                     | 0.42              |
| 1:G:560:ARG:HG2  | 1:I:496:GLU:O    | 2.20                     | 0.42              |
| 1:H:292:ASN:O    | 1:H:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:H:314:VAL:HG13 | 1:H:660:THR:HG23 | 2.01                     | 0.42              |
| 1:K:292:ASN:O    | 1:K:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:L:619:HIS:CD2  | 2:BA:997:DA:H3'  | 2.54                     | 0.42              |
| 1:M:292:ASN:O    | 1:M:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:M:428:ASN:HB3  | 1:M:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:O:235:ARG:HG3  | 1:O:353:LEU:HB3  | 2.00                     | 0.42              |
| 1:P:235:ARG:HG3  | 1:P:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:R:292:ASN:O    | 1:R:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:V:466:PRO:HD2  | 1:e:495:MET:SD   | 2.59                     | 0.42              |
| 1:W:238:VAL:HG13 | 1:W:362:THR:HG22 | 2.01                     | 0.42              |
| 1:W:422:ASN:OD1  | 1:W:423:LEU:N    | 2.52                     | 0.42              |
| 1:X:397:ARG:HH12 | 1:f:398:THR:HG22 | 1.85                     | 0.42              |
| 1:X:433:GLN:O    | 1:X:451:LYS:NZ   | 2.48                     | 0.42              |
| 1:Z:422:ASN:OD1  | 1:Z:423:LEU:N    | 2.52                     | 0.42              |
| 1:a:238:VAL:HG13 | 1:a:362:THR:HG22 | 2.01                     | 0.42              |
| 1:a:314:VAL:HG13 | 1:a:660:THR:HG23 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:422:ASN:OD1  | 1:b:423:LEU:N    | 2.52                     | 0.42              |
| 1:e:619:HIS:CD2  | 2:WA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:f:238:VAL:HG13 | 1:f:362:THR:HG22 | 2.01                     | 0.42              |
| 1:f:619:HIS:CA   | 2:XA:997:DA:O3'  | 2.60                     | 0.42              |
| 1:g:339:TYR:OH   | 1:g:632:PRO:O    | 2.34                     | 0.42              |
| 1:m:238:VAL:HG13 | 1:m:362:THR:HG22 | 2.01                     | 0.42              |
| 1:o:372:ASN:ND2  | 1:o:376:THR:O    | 2.44                     | 0.42              |
| 1:s:372:ASN:ND2  | 1:s:376:THR:O    | 2.44                     | 0.42              |
| 1:v:398:THR:HG22 | 1:w:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:v:619:HIS:CD2  | 2:oA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:x:619:HIS:CD2  | 2:rA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:1:292:ASN:O    | 1:1:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:8:292:ASN:O    | 1:8:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:B:292:ASN:O    | 1:B:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:E:372:ASN:ND2  | 1:E:376:THR:O    | 2.44                     | 0.42              |
| 1:K:398:THR:HG22 | 1:L:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:L:314:VAL:HG13 | 1:L:660:THR:HG23 | 2.01                     | 0.42              |
| 1:L:611:ILE:HD11 | 2:BA:997:DA:C2   | 2.55                     | 0.42              |
| 1:M:397:ARG:HH12 | 1:c:398:THR:HG22 | 1.85                     | 0.42              |
| 1:N:398:THR:HG22 | 1:m:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:Q:398:THR:HG22 | 1:S:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:Q:619:HIS:CD2  | 2:GA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:R:466:PRO:HD2  | 1:S:495:MET:SD   | 2.59                     | 0.42              |
| 1:U:235:ARG:HG3  | 1:U:353:LEU:HB3  | 2.00                     | 0.42              |
| 1:U:619:HIS:CD2  | 2:LA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:W:292:ASN:O    | 1:W:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:X:372:ASN:ND2  | 1:X:376:THR:O    | 2.44                     | 0.42              |
| 1:Y:398:THR:HG22 | 1:4:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:Z:619:HIS:CD2  | 2:QA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:a:611:ILE:HD11 | 2:RA:997:DA:C2   | 2.55                     | 0.42              |
| 1:b:292:ASN:O    | 1:b:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:b:611:ILE:HD11 | 2:SA:997:DA:C2   | 2.55                     | 0.42              |
| 1:b:619:HIS:CD2  | 2:SA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:d:292:ASN:O    | 1:d:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:h:611:ILE:HD11 | 2:ZA:997:DA:C2   | 2.55                     | 0.42              |
| 1:j:619:HIS:CD2  | 2:bA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:k:292:ASN:O    | 1:k:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:n:356:PHE:HA   | 1:n:357:PRO:HD3  | 1.92                     | 0.42              |
| 1:n:428:ASN:HB3  | 1:n:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:o:235:ARG:HG3  | 1:o:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:o:314:VAL:HG13 | 1:o:660:THR:HG23 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:p:422:ASN:OD1  | 1:p:423:LEU:N    | 2.52                     | 0.42              |
| 1:r:619:HIS:CD2  | 2:kA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:v:238:VAL:HG13 | 1:v:362:THR:HG22 | 2.01                     | 0.42              |
| 1:x:235:ARG:HG3  | 1:x:353:LEU:HB3  | 2.00                     | 0.42              |
| 1:y:292:ASN:O    | 1:y:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:4:292:ASN:O    | 1:4:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:4:339:TYR:OH   | 1:4:632:PRO:O    | 2.34                     | 0.42              |
| 1:4:428:ASN:HB3  | 1:4:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:6:560:ARG:HG2  | 1:7:496:GLU:O    | 2.20                     | 0.42              |
| 1:C:560:ARG:HG2  | 1:b:496:GLU:O    | 2.20                     | 0.42              |
| 1:G:314:VAL:HG13 | 1:G:660:THR:HG23 | 2.01                     | 0.42              |
| 1:H:372:ASN:ND2  | 1:H:376:THR:O    | 2.44                     | 0.42              |
| 1:H:619:HIS:CD2  | 2:4A:997:DA:H3'  | 2.55                     | 0.42              |
| 1:I:611:ILE:HD11 | 2:5A:997:DA:C2   | 2.55                     | 0.42              |
| 1:J:314:VAL:HG13 | 1:J:660:THR:HG23 | 2.01                     | 0.42              |
| 1:J:398:THR:HG22 | 1:a:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:M:339:TYR:OH   | 1:M:632:PRO:O    | 2.34                     | 0.42              |
| 1:N:600:ASP:OD1  | 1:N:717:THR:OG1  | 2.34                     | 0.42              |
| 1:O:496:GLU:O    | 1:n:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:P:292:ASN:O    | 1:P:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:T:292:ASN:O    | 1:T:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:V:611:ILE:HD11 | 2:MA:997:DA:C2   | 2.55                     | 0.42              |
| 1:Z:292:ASN:O    | 1:Z:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:Z:482:ASN:HB3  | 1:Z:483:ARG:H    | 1.62                     | 0.42              |
| 1:Z:611:ILE:HD11 | 2:QA:997:DA:C2   | 2.55                     | 0.42              |
| 1:b:398:THR:HG22 | 1:o:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:e:398:THR:HG22 | 1:h:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:f:397:ARG:HH12 | 1:z:398:THR:HG22 | 1.85                     | 0.42              |
| 1:h:292:ASN:O    | 1:h:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:i:235:ARG:HG3  | 1:i:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:i:428:ASN:HB3  | 1:i:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:i:496:GLU:O    | 1:k:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:i:560:ARG:HG2  | 1:j:496:GLU:O    | 2.20                     | 0.42              |
| 1:j:292:ASN:O    | 1:j:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:l:235:ARG:HG3  | 1:l:353:LEU:HB3  | 2.00                     | 0.42              |
| 1:l:428:ASN:HB3  | 1:l:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:l:611:ILE:HD11 | 2:dA:997:DA:C2   | 2.55                     | 0.42              |
| 1:n:235:ARG:HG3  | 1:n:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:n:292:ASN:O    | 1:n:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:n:611:ILE:HD11 | 2:gA:997:DA:C2   | 2.55                     | 0.42              |
| 1:p:292:ASN:O    | 1:p:720:LEU:HD21 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:466:PRO:HD2  | 1:r:495:MET:SD   | 2.59                     | 0.42              |
| 1:q:611:ILE:HD11 | 2:jA:997:DA:C2   | 2.55                     | 0.42              |
| 1:v:482:ASN:HB3  | 1:v:483:ARG:H    | 1.62                     | 0.42              |
| 1:z:496:GLU:O    | 1:2:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:z:600:ASP:OD1  | 1:z:717:THR:OG1  | 2.34                     | 0.42              |
| 1:2:619:HIS:CA   | 2:vA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:5:372:ASN:ND2  | 1:5:376:THR:O    | 2.44                     | 0.42              |
| 1:6:314:VAL:HG13 | 1:6:660:THR:HG23 | 2.01                     | 0.42              |
| 1:7:292:ASN:O    | 1:7:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:7:611:ILE:HD11 | 2:0A:997:DA:C2   | 2.55                     | 0.42              |
| 2:aA:996:DA:C2'  | 2:aA:997:DA:H5'  | 2.49                     | 0.42              |
| 1:B:560:ARG:HG2  | 1:J:496:GLU:O    | 2.20                     | 0.42              |
| 1:C:496:GLU:O    | 1:M:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:D:496:GLU:O    | 1:P:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:D:619:HIS:CA   | 2:fA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:H:339:TYR:OH   | 1:H:632:PRO:O    | 2.34                     | 0.42              |
| 1:I:292:ASN:O    | 1:I:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:K:314:VAL:HG13 | 1:K:660:THR:HG23 | 2.01                     | 0.42              |
| 1:M:496:GLU:O    | 1:b:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:M:611:ILE:HD11 | 2:CA:997:DA:C2   | 2.55                     | 0.42              |
| 1:N:292:ASN:O    | 1:N:720:LEU:HD21 | 2.20                     | 0.42              |
| 1:O:339:TYR:OH   | 1:O:632:PRO:O    | 2.34                     | 0.42              |
| 1:P:611:ILE:HD11 | 2:FA:997:DA:C2   | 2.55                     | 0.42              |
| 1:R:560:ARG:HG2  | 1:S:496:GLU:O    | 2.20                     | 0.42              |
| 1:S:560:ARG:HG2  | 1:U:496:GLU:O    | 2.20                     | 0.42              |
| 1:T:496:GLU:O    | 1:l:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:T:611:ILE:HD11 | 2:KA:997:DA:C2   | 2.55                     | 0.42              |
| 1:U:619:HIS:CA   | 2:LA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:V:313:GLU:N    | 1:V:324:ALA:O    | 2.53                     | 0.42              |
| 1:X:496:GLU:O    | 1:e:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:Y:619:HIS:CA   | 2:PA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:Z:466:PRO:HD2  | 1:4:495:MET:SD   | 2.59                     | 0.42              |
| 1:Z:496:GLU:O    | 1:3:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:Z:560:ARG:HG2  | 1:4:496:GLU:O    | 2.20                     | 0.42              |
| 1:c:496:GLU:O    | 1:p:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:c:619:HIS:CA   | 2:TA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:d:560:ARG:HG2  | 1:l:496:GLU:O    | 2.20                     | 0.42              |
| 1:g:356:PHE:HA   | 1:g:357:PRO:HD3  | 1.92                     | 0.42              |
| 1:g:496:GLU:O    | 1:h:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:h:235:ARG:HG3  | 1:h:353:LEU:HB3  | 2.01                     | 0.42              |
| 1:h:428:ASN:HB3  | 1:h:431:VAL:HG22 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:619:HIS:CA   | 2:ZA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:i:314:VAL:HG13 | 1:i:660:THR:HG23 | 2.01                     | 0.42              |
| 1:i:611:ILE:HD11 | 2:aA:997:DA:C2   | 2.55                     | 0.42              |
| 1:j:611:ILE:HD11 | 2:bA:997:DA:C2   | 2.55                     | 0.42              |
| 1:m:619:HIS:CA   | 2:eA:997:DA:O3'  | 2.60                     | 0.42              |
| 1:n:238:VAL:HG13 | 1:n:362:THR:HG22 | 2.01                     | 0.42              |
| 1:n:619:HIS:CA   | 2:gA:997:DA:H2'  | 2.50                     | 0.42              |
| 1:o:619:HIS:CD2  | 2:hA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:q:313:GLU:N    | 1:q:324:ALA:O    | 2.53                     | 0.42              |
| 1:u:619:HIS:CD2  | 2:nA:997:DA:H3'  | 2.55                     | 0.42              |
| 1:w:560:ARG:HG2  | 1:x:496:GLU:O    | 2.20                     | 0.42              |
| 1:1:314:VAL:HG13 | 1:1:660:THR:HG23 | 2.01                     | 0.42              |
| 1:1:560:ARG:HG2  | 1:2:496:GLU:O    | 2.20                     | 0.42              |
| 1:2:611:ILE:HD11 | 2:vA:997:DA:C2   | 2.55                     | 0.42              |
| 1:3:496:GLU:O    | 1:4:560:ARG:HG2  | 2.20                     | 0.42              |
| 1:4:611:ILE:HD11 | 2:xA:997:DA:C2   | 2.55                     | 0.42              |
| 1:5:560:ARG:HG2  | 1:6:496:GLU:O    | 2.20                     | 0.42              |
| 1:8:428:ASN:HB3  | 1:8:431:VAL:HG22 | 2.01                     | 0.42              |
| 1:8:619:HIS:CA   | 2:2A:997:DA:C2'  | 2.88                     | 0.42              |
| 1:A:696:PRO:HG3  | 1:E:381:GLU:OE2  | 2.20                     | 0.41              |
| 1:B:227:ASP:O    | 1:B:675:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:356:PHE:HA   | 1:B:357:PRO:HD3  | 1.92                     | 0.41              |
| 1:B:428:ASN:HB3  | 1:B:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:C:292:ASN:O    | 1:C:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:D:560:ARG:HG2  | 1:N:496:GLU:O    | 2.20                     | 0.41              |
| 1:D:611:ILE:HD11 | 2:fA:997:DA:C2   | 2.55                     | 0.41              |
| 1:E:619:HIS:CD2  | 2:qA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:F:313:GLU:N    | 1:F:324:ALA:O    | 2.53                     | 0.41              |
| 1:H:397:ARG:HH12 | 1:Z:398:THR:HG22 | 1.85                     | 0.41              |
| 1:J:611:ILE:HD11 | 2:9:997:DA:C2    | 2.55                     | 0.41              |
| 1:K:496:GLU:O    | 1:8:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:K:611:ILE:HD11 | 2:AA:997:DA:C2   | 2.55                     | 0.41              |
| 1:O:560:ARG:HG2  | 1:m:496:GLU:O    | 2.20                     | 0.41              |
| 1:P:238:VAL:HG13 | 1:P:362:THR:HG22 | 2.01                     | 0.41              |
| 1:P:314:VAL:HG13 | 1:P:660:THR:HG23 | 2.01                     | 0.41              |
| 1:Q:314:VAL:HG13 | 1:Q:660:THR:HG23 | 2.01                     | 0.41              |
| 1:R:619:HIS:CD2  | 2:HA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:T:398:THR:HG22 | 1:U:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:V:428:ASN:HB3  | 1:V:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:Z:313:GLU:N    | 1:Z:324:ALA:O    | 2.53                     | 0.41              |
| 1:b:313:GLU:N    | 1:b:324:ALA:O    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:496:GLU:O    | 1:g:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:g:292:ASN:O    | 1:g:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:h:238:VAL:HG13 | 1:h:362:THR:HG22 | 2.01                     | 0.41              |
| 1:i:292:ASN:O    | 1:i:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:j:398:THR:HG22 | 1:x:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:l:292:ASN:O    | 1:l:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:l:313:GLU:N    | 1:l:324:ALA:O    | 2.53                     | 0.41              |
| 1:p:397:ARG:HH12 | 1:6:398:THR:HG22 | 1.85                     | 0.41              |
| 1:q:314:VAL:HG13 | 1:q:660:THR:HG23 | 2.01                     | 0.41              |
| 1:q:428:ASN:HB3  | 1:q:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:t:313:GLU:N    | 1:t:324:ALA:O    | 2.53                     | 0.41              |
| 1:t:619:HIS:CD2  | 2:mA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:v:227:ASP:O    | 1:v:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:v:611:ILE:HD11 | 2:oA:997:DA:C2   | 2.55                     | 0.41              |
| 1:w:496:GLU:O    | 1:y:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:x:560:ARG:HG2  | 1:y:496:GLU:O    | 2.20                     | 0.41              |
| 1:z:292:ASN:O    | 1:z:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:1:611:ILE:HD11 | 2:uA:997:DA:C2   | 2.55                     | 0.41              |
| 1:2:398:THR:HG22 | 1:3:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:8:227:ASP:O    | 1:8:675:LEU:HB2  | 2.20                     | 0.41              |
| 2:1A:996:DA:C2'  | 2:1A:997:DA:H5'  | 2.49                     | 0.41              |
| 2:3A:996:DA:C2'  | 2:3A:997:DA:H5'  | 2.49                     | 0.41              |
| 1:A:313:GLU:N    | 1:A:324:ALA:O    | 2.53                     | 0.41              |
| 1:A:428:ASN:HB3  | 1:A:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:B:313:GLU:N    | 1:B:324:ALA:O    | 2.53                     | 0.41              |
| 1:B:619:HIS:CD2  | 2:JA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:C:397:ARG:HH12 | 1:D:398:THR:HG22 | 1.85                     | 0.41              |
| 1:C:619:HIS:CD2  | 2:UA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:E:560:ARG:HG2  | 1:Q:496:GLU:O    | 2.20                     | 0.41              |
| 1:E:611:ILE:HD11 | 2:qA:997:DA:C2   | 2.55                     | 0.41              |
| 1:F:398:THR:HG22 | 1:G:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:F:619:HIS:CD2  | 2:1A:997:DA:H3'  | 2.55                     | 0.41              |
| 1:H:560:ARG:HG2  | 1:W:496:GLU:O    | 2.20                     | 0.41              |
| 1:J:619:HIS:CA   | 2:9:997:DA:H2'   | 2.50                     | 0.41              |
| 1:O:292:ASN:O    | 1:O:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:Q:227:ASP:O    | 1:Q:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:Q:611:ILE:HD11 | 2:GA:997:DA:C2   | 2.55                     | 0.41              |
| 1:T:619:HIS:CA   | 2:KA:997:DA:O3'  | 2.60                     | 0.41              |
| 1:V:314:VAL:HG13 | 1:V:660:THR:HG23 | 2.01                     | 0.41              |
| 1:W:560:ARG:HG2  | 1:Y:496:GLU:O    | 2.20                     | 0.41              |
| 1:a:292:ASN:O    | 1:a:720:LEU:HD21 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:611:ILE:HD11 | 2:VA:997:DA:C2   | 2.55                     | 0.41              |
| 1:e:227:ASP:O    | 1:e:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:e:619:HIS:CA   | 2:WA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:e:619:HIS:CA   | 2:WA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:g:397:ARG:HH12 | 1:k:398:THR:HG22 | 1.85                     | 0.41              |
| 1:h:313:GLU:N    | 1:h:324:ALA:O    | 2.53                     | 0.41              |
| 1:m:619:HIS:CA   | 2:eA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:o:560:ARG:HG2  | 1:p:496:GLU:O    | 2.20                     | 0.41              |
| 1:p:619:HIS:CD2  | 2:iA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:q:495:MET:SD   | 1:s:466:PRO:HD2  | 2.60                     | 0.41              |
| 1:r:227:ASP:O    | 1:r:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:r:619:HIS:CA   | 2:kA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:u:292:ASN:O    | 1:u:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:v:314:VAL:HG13 | 1:v:660:THR:HG23 | 2.01                     | 0.41              |
| 1:w:292:ASN:O    | 1:w:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:y:619:HIS:CD2  | 2:sA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:z:397:ARG:HH12 | 1:4:398:THR:HG22 | 1.85                     | 0.41              |
| 1:z:619:HIS:CA   | 2:tA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:3:292:ASN:O    | 1:3:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:4:372:ASN:ND2  | 1:4:376:THR:O    | 2.44                     | 0.41              |
| 1:5:313:GLU:N    | 1:5:324:ALA:O    | 2.53                     | 0.41              |
| 1:8:313:GLU:N    | 1:8:324:ALA:O    | 2.53                     | 0.41              |
| 1:8:314:VAL:HG13 | 1:8:660:THR:HG23 | 2.01                     | 0.41              |
| 2:mA:996:DA:C2'  | 2:mA:997:DA:H5'  | 2.49                     | 0.41              |
| 1:A:381:GLU:OE2  | 1:B:696:PRO:HG3  | 2.19                     | 0.41              |
| 1:B:314:VAL:HG13 | 1:B:660:THR:HG23 | 2.01                     | 0.41              |
| 1:B:619:HIS:CA   | 2:JA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:D:428:ASN:HB3  | 1:D:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:D:678:GLU:OE2  | 1:D:680:SER:OG   | 2.24                     | 0.41              |
| 1:E:292:ASN:O    | 1:E:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:F:227:ASP:O    | 1:F:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:F:495:MET:SD   | 1:Q:466:PRO:HD2  | 2.59                     | 0.41              |
| 1:G:428:ASN:HB3  | 1:G:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:K:619:HIS:CA   | 2:AA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:L:227:ASP:O    | 1:L:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:L:292:ASN:O    | 1:L:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:M:372:ASN:ND2  | 1:M:376:THR:O    | 2.44                     | 0.41              |
| 1:N:619:HIS:CA   | 2:DA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:R:496:GLU:O    | 1:U:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:S:292:ASN:O    | 1:S:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:T:227:ASP:O    | 1:T:675:LEU:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:235:ARG:HG3  | 1:T:353:LEU:HB3  | 2.01                     | 0.41              |
| 1:U:619:HIS:CA   | 2:LA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:V:560:ARG:HG2  | 1:e:496:GLU:O    | 2.20                     | 0.41              |
| 1:W:619:HIS:CD2  | 2:NA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:a:227:ASP:O    | 1:a:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:a:560:ARG:HG2  | 1:8:496:GLU:O    | 2.20                     | 0.41              |
| 1:a:619:HIS:CA   | 2:RA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:e:235:ARG:HG3  | 1:e:353:LEU:HB3  | 2.01                     | 0.41              |
| 1:f:619:HIS:CA   | 2:XA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:g:619:HIS:CA   | 2:YA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:i:313:GLU:N    | 1:i:324:ALA:O    | 2.54                     | 0.41              |
| 1:l:314:VAL:HG13 | 1:l:660:THR:HG23 | 2.01                     | 0.41              |
| 1:n:313:GLU:N    | 1:n:324:ALA:O    | 2.53                     | 0.41              |
| 1:n:397:ARG:HH12 | 1:r:398:THR:HG22 | 1.85                     | 0.41              |
| 1:q:560:ARG:HG2  | 1:r:496:GLU:O    | 2.20                     | 0.41              |
| 1:t:227:ASP:O    | 1:t:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:t:398:THR:HG22 | 1:6:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:u:560:ARG:HG2  | 1:v:496:GLU:O    | 2.20                     | 0.41              |
| 1:u:611:ILE:HD11 | 2:nA:997:DA:C2   | 2.55                     | 0.41              |
| 1:w:339:TYR:OH   | 1:w:632:PRO:O    | 2.34                     | 0.41              |
| 1:x:238:VAL:HG13 | 1:x:362:THR:HG22 | 2.01                     | 0.41              |
| 1:x:428:ASN:HB3  | 1:x:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:y:619:HIS:CA   | 2:sA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:1:238:VAL:HG13 | 1:1:362:THR:HG22 | 2.01                     | 0.41              |
| 1:2:428:ASN:HB3  | 1:2:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:3:619:HIS:CD2  | 2:wA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:4:238:VAL:HG13 | 1:4:362:THR:HG22 | 2.01                     | 0.41              |
| 1:5:428:ASN:HB3  | 1:5:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:5:619:HIS:CD2  | 2:yA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:6:428:ASN:HB3  | 1:6:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:8:619:HIS:CD2  | 2:2A:997:DA:H3'  | 2.55                     | 0.41              |
| 2:gA:996:DA:C2'  | 2:gA:997:DA:H5'  | 2.49                     | 0.41              |
| 1:A:372:ASN:ND2  | 1:A:376:THR:O    | 2.44                     | 0.41              |
| 1:A:398:THR:HG22 | 1:E:397:ARG:HH12 | 1.84                     | 0.41              |
| 1:A:458:ALA:H    | 1:G:261:ASN:ND2  | 2.19                     | 0.41              |
| 1:A:619:HIS:CD2  | 2:0:997:DA:H3'   | 2.55                     | 0.41              |
| 1:B:496:GLU:O    | 1:L:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:D:292:ASN:O    | 1:D:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:F:238:VAL:HG13 | 1:F:362:THR:HG22 | 2.01                     | 0.41              |
| 1:G:398:THR:HG22 | 1:W:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:L:619:HIS:CA   | 2:BA:997:DA:H2'  | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:238:VAL:HG13 | 1:M:362:THR:HG22 | 2.01                     | 0.41              |
| 1:M:314:VAL:HG13 | 1:M:660:THR:HG23 | 2.01                     | 0.41              |
| 1:M:398:THR:HG22 | 1:N:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:O:238:VAL:HG13 | 1:O:362:THR:HG22 | 2.01                     | 0.41              |
| 1:O:397:ARG:HH12 | 1:d:398:THR:HG22 | 1.85                     | 0.41              |
| 1:O:619:HIS:CA   | 2:EA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:R:619:HIS:CA   | 2:HA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:U:428:ASN:HB3  | 1:U:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:W:227:ASP:O    | 1:W:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:X:314:VAL:HG13 | 1:X:660:THR:HG23 | 2.01                     | 0.41              |
| 1:Y:292:ASN:O    | 1:Y:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:b:619:HIS:CA   | 2:SA:997:DA:O3'  | 2.60                     | 0.41              |
| 1:c:644:PRO:HG3  | 1:s:360:VAL:HG11 | 2.02                     | 0.41              |
| 1:j:227:ASP:O    | 1:j:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:j:235:ARG:HG3  | 1:j:353:LEU:HB3  | 2.01                     | 0.41              |
| 1:k:611:ILE:HD11 | 2:cA:997:DA:C2   | 2.55                     | 0.41              |
| 1:l:619:HIS:CA   | 2:dA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:m:313:GLU:N    | 1:m:324:ALA:O    | 2.53                     | 0.41              |
| 1:m:428:ASN:HB3  | 1:m:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:o:339:TYR:OH   | 1:o:632:PRO:O    | 2.34                     | 0.41              |
| 1:p:227:ASP:O    | 1:p:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:t:560:ARG:HG2  | 1:u:496:GLU:O    | 2.20                     | 0.41              |
| 1:x:227:ASP:O    | 1:x:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:2:292:ASN:O    | 1:2:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:4:314:VAL:HG13 | 1:4:660:THR:HG23 | 2.01                     | 0.41              |
| 1:8:356:PHE:HA   | 1:8:357:PRO:HD3  | 1.92                     | 0.41              |
| 2:ZA:996:DA:C2'  | 2:ZA:997:DA:H5'  | 2.49                     | 0.41              |
| 1:E:496:GLU:O    | 1:F:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:I:428:ASN:HB3  | 1:I:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:N:611:ILE:HD11 | 2:DA:997:DA:C2   | 2.55                     | 0.41              |
| 1:O:619:HIS:CD2  | 2:EA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:R:227:ASP:O    | 1:R:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:U:227:ASP:O    | 1:U:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:U:238:VAL:HG13 | 1:U:362:THR:HG22 | 2.01                     | 0.41              |
| 1:V:227:ASP:O    | 1:V:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:V:496:GLU:O    | 1:X:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:b:482:ASN:HB3  | 1:b:483:ARG:H    | 1.62                     | 0.41              |
| 1:f:313:GLU:N    | 1:f:324:ALA:O    | 2.53                     | 0.41              |
| 1:g:227:ASP:O    | 1:g:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:i:238:VAL:HG13 | 1:i:362:THR:HG22 | 2.01                     | 0.41              |
| 1:i:619:HIS:CA   | 2:aA:997:DA:H2'  | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:619:HIS:CD2  | 2:aA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:j:372:ASN:ND2  | 1:j:376:THR:O    | 2.44                     | 0.41              |
| 1:j:560:ARG:HG2  | 1:k:496:GLU:O    | 2.20                     | 0.41              |
| 1:j:619:HIS:CA   | 2:bA:997:DA:O3'  | 2.61                     | 0.41              |
| 1:l:238:VAL:HG13 | 1:l:362:THR:HG22 | 2.01                     | 0.41              |
| 1:l:619:HIS:CD2  | 2:dA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:r:235:ARG:HG3  | 1:r:353:LEU:HB3  | 2.01                     | 0.41              |
| 1:r:560:ARG:HG2  | 1:s:496:GLU:O    | 2.21                     | 0.41              |
| 1:r:619:HIS:CA   | 2:kA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:s:314:VAL:HG13 | 1:s:660:THR:HG23 | 2.01                     | 0.41              |
| 1:t:238:VAL:HG13 | 1:t:362:THR:HG22 | 2.01                     | 0.41              |
| 1:t:495:MET:SD   | 1:v:466:PRO:HD2  | 2.59                     | 0.41              |
| 1:t:611:ILE:HD11 | 2:mA:997:DA:C2   | 2.55                     | 0.41              |
| 1:w:227:ASP:O    | 1:w:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:2:678:GLU:OE2  | 1:2:680:SER:OG   | 2.24                     | 0.41              |
| 1:3:481:VAL:O    | 1:4:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:7:314:VAL:HG13 | 1:7:660:THR:HG23 | 2.01                     | 0.41              |
| 1:A:292:ASN:O    | 1:A:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:C:481:VAL:O    | 1:M:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:D:397:ARG:HH12 | 1:E:398:THR:HG22 | 1.85                     | 0.41              |
| 1:F:611:ILE:HD11 | 2:1A:997:DA:C2   | 2.55                     | 0.41              |
| 1:O:227:ASP:O    | 1:O:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:S:227:ASP:O    | 1:S:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:S:339:TYR:OH   | 1:S:632:PRO:O    | 2.34                     | 0.41              |
| 1:S:611:ILE:HD11 | 2:1A:997:DA:C2   | 2.55                     | 0.41              |
| 1:T:560:ARG:HG2  | 1:d:496:GLU:O    | 2.20                     | 0.41              |
| 1:W:611:ILE:HD11 | 2:NA:997:DA:C2   | 2.55                     | 0.41              |
| 1:X:428:ASN:HB3  | 1:X:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:Z:619:HIS:CA   | 2:QA:997:DA:O3'  | 2.60                     | 0.41              |
| 1:b:314:VAL:HG13 | 1:b:660:THR:HG23 | 2.01                     | 0.41              |
| 1:c:292:ASN:O    | 1:c:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:d:227:ASP:O    | 1:d:675:LEU:HB2  | 2.20                     | 0.41              |
| 1:e:428:ASN:HB3  | 1:e:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:f:428:ASN:HB3  | 1:f:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:f:560:ARG:HG2  | 1:h:496:GLU:O    | 2.20                     | 0.41              |
| 1:f:644:PRO:HG3  | 1:z:360:VAL:HG11 | 2.03                     | 0.41              |
| 1:g:238:VAL:HG13 | 1:g:362:THR:HG22 | 2.01                     | 0.41              |
| 1:g:619:HIS:CD2  | 2:YA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:h:227:ASP:O    | 1:h:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:k:227:ASP:O    | 1:k:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:m:611:ILE:HD11 | 2:eA:997:DA:C2   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:619:HIS:CA   | 2:eA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:q:227:ASP:O    | 1:q:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:r:428:ASN:HB3  | 1:r:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:u:482:ASN:HB3  | 1:u:483:ARG:H    | 1.62                     | 0.41              |
| 1:w:611:ILE:HD11 | 2:pA:997:DA:C2   | 2.55                     | 0.41              |
| 1:y:227:ASP:O    | 1:y:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:z:611:ILE:HD11 | 2:tA:997:DA:C2   | 2.55                     | 0.41              |
| 1:1:619:HIS:CA   | 2:uA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:4:619:HIS:CA   | 2:xA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:5:292:ASN:O    | 1:5:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:6:611:ILE:HD11 | 2:zA:997:DA:C2   | 2.55                     | 0.41              |
| 1:7:428:ASN:HB3  | 1:7:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:7:633:PRO:HA   | 1:7:634:PRO:HD3  | 1.89                     | 0.41              |
| 1:A:472:THR:HG23 | 1:A:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:A:565:VAL:O    | 1:G:496:GLU:HG3  | 2.21                     | 0.41              |
| 1:C:611:ILE:HD11 | 2:UA:997:DA:C2   | 2.55                     | 0.41              |
| 1:G:611:ILE:HD11 | 2:3A:997:DA:C2   | 2.55                     | 0.41              |
| 1:H:611:ILE:HD11 | 2:4A:997:DA:C2   | 2.55                     | 0.41              |
| 1:I:314:VAL:HG13 | 1:I:660:THR:HG23 | 2.01                     | 0.41              |
| 1:M:619:HIS:CA   | 2:CA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:N:360:VAL:HG11 | 1:m:644:PRO:HG3  | 2.03                     | 0.41              |
| 1:P:398:THR:HG22 | 1:Q:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:U:398:THR:HG22 | 1:e:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:U:611:ILE:HD11 | 2:LA:997:DA:C2   | 2.55                     | 0.41              |
| 1:W:619:HIS:CA   | 2:NA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:X:227:ASP:O    | 1:X:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:Y:611:ILE:HD11 | 2:PA:997:DA:C2   | 2.55                     | 0.41              |
| 1:f:611:ILE:HD11 | 2:XA:997:DA:C2   | 2.55                     | 0.41              |
| 1:n:227:ASP:O    | 1:n:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:o:611:ILE:HD11 | 2:hA:997:DA:C2   | 2.55                     | 0.41              |
| 1:q:433:GLN:O    | 1:q:451:LYS:NZ   | 2.48                     | 0.41              |
| 1:s:611:ILE:HD11 | 2:lA:997:DA:C2   | 2.55                     | 0.41              |
| 1:t:397:ARG:HH12 | 1:y:398:THR:HG22 | 1.85                     | 0.41              |
| 1:t:428:ASN:HB3  | 1:t:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:u:397:ARG:HH12 | 1:5:398:THR:HG22 | 1.85                     | 0.41              |
| 1:v:397:ARG:HH12 | 1:1:398:THR:HG22 | 1.85                     | 0.41              |
| 1:x:292:ASN:O    | 1:x:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:x:619:HIS:CA   | 2:rA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:3:339:TYR:OH   | 1:3:632:PRO:O    | 2.34                     | 0.41              |
| 1:3:611:ILE:HD11 | 2:wA:997:DA:C2   | 2.55                     | 0.41              |
| 1:5:472:THR:HG23 | 1:5:522:ALA:HB1  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6:313:GLU:N    | 1:6:324:ALA:O    | 2.53                     | 0.41              |
| 1:A:481:VAL:O    | 1:I:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:A:611:ILE:HD11 | 2:0:997:DA:C2    | 2.55                     | 0.41              |
| 1:A:644:PRO:HG3  | 1:B:360:VAL:HG11 | 2.03                     | 0.41              |
| 1:B:397:ARG:HH12 | 1:C:398:THR:HG22 | 1.85                     | 0.41              |
| 1:D:651:SER:OG   | 1:D:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:E:482:ASN:HB3  | 1:E:483:ARG:H    | 1.62                     | 0.41              |
| 1:E:651:SER:OG   | 1:E:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:F:397:ARG:HH12 | 1:R:398:THR:HG22 | 1.85                     | 0.41              |
| 1:H:398:THR:HG22 | 1:I:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:H:496:GLU:O    | 1:Y:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:I:227:ASP:O    | 1:I:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:O:651:SER:OG   | 1:O:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:R:238:VAL:HG13 | 1:R:362:THR:HG22 | 2.01                     | 0.41              |
| 1:R:445:GLY:HA3  | 1:S:481:VAL:O    | 2.21                     | 0.41              |
| 1:U:292:ASN:O    | 1:U:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:W:445:GLY:HA3  | 1:Y:481:VAL:O    | 2.21                     | 0.41              |
| 1:Y:472:THR:HG23 | 1:Y:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:Z:314:VAL:HG13 | 1:Z:660:THR:HG23 | 2.01                     | 0.41              |
| 1:b:428:ASN:HB3  | 1:b:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:c:472:THR:HG23 | 1:c:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:c:611:ILE:HD11 | 2:TA:997:DA:C2   | 2.55                     | 0.41              |
| 1:d:472:THR:HG23 | 1:d:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:d:482:ASN:HB3  | 1:d:483:ARG:H    | 1.62                     | 0.41              |
| 1:f:292:ASN:O    | 1:f:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:g:651:SER:OG   | 1:g:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:h:398:THR:HG22 | 1:i:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:j:397:ARG:HH12 | 1:l:398:THR:HG22 | 1.85                     | 0.41              |
| 1:m:292:ASN:O    | 1:m:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:m:560:ARG:HG2  | 1:n:496:GLU:O    | 2.20                     | 0.41              |
| 1:p:611:ILE:HD11 | 2:iA:997:DA:C2   | 2.55                     | 0.41              |
| 1:r:611:ILE:HD11 | 2:kA:997:DA:C2   | 2.55                     | 0.41              |
| 1:u:651:SER:OG   | 1:u:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:w:445:GLY:HA3  | 1:x:481:VAL:O    | 2.21                     | 0.41              |
| 1:w:481:VAL:O    | 1:y:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:x:611:ILE:HD11 | 2:rA:997:DA:C2   | 2.55                     | 0.41              |
| 1:z:678:GLU:OE2  | 1:z:680:SER:OG   | 2.24                     | 0.41              |
| 1:2:651:SER:OG   | 1:2:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:3:398:THR:HG22 | 1:8:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:3:428:ASN:HB3  | 1:3:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:7:227:ASP:O    | 1:7:675:LEU:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:8:611:ILE:HD11 | 2:2A:997:DA:C2   | 2.55                     | 0.41              |
| 2:iA:996:DA:C2'  | 2:iA:997:DA:H5'  | 2.49                     | 0.41              |
| 1:A:397:ARG:HH12 | 1:B:398:THR:HG22 | 1.85                     | 0.41              |
| 1:A:496:GLU:O    | 1:I:560:ARG:HG2  | 2.20                     | 0.41              |
| 1:B:339:TYR:OH   | 1:B:632:PRO:O    | 2.34                     | 0.41              |
| 1:B:472:THR:HG23 | 1:B:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:B:611:ILE:HD11 | 2:JA:997:DA:C2   | 2.55                     | 0.41              |
| 1:C:227:ASP:O    | 1:C:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:C:339:TYR:OH   | 1:C:632:PRO:O    | 2.34                     | 0.41              |
| 1:C:428:ASN:HB3  | 1:C:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:D:482:ASN:HB3  | 1:D:483:ARG:H    | 1.62                     | 0.41              |
| 1:E:313:GLU:N    | 1:E:324:ALA:O    | 2.53                     | 0.41              |
| 1:F:292:ASN:O    | 1:F:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:F:428:ASN:HB3  | 1:F:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:G:651:SER:OG   | 1:G:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:J:238:VAL:HG13 | 1:J:362:THR:HG22 | 2.01                     | 0.41              |
| 1:J:560:ARG:HG2  | 1:L:496:GLU:O    | 2.20                     | 0.41              |
| 1:K:238:VAL:HG13 | 1:K:362:THR:HG22 | 2.01                     | 0.41              |
| 1:K:560:ARG:HG2  | 1:a:496:GLU:O    | 2.20                     | 0.41              |
| 1:M:651:SER:OG   | 1:M:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:N:560:ARG:HG2  | 1:P:496:GLU:O    | 2.20                     | 0.41              |
| 1:P:227:ASP:O    | 1:P:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:S:445:GLY:HA3  | 1:U:481:VAL:O    | 2.21                     | 0.41              |
| 1:S:678:GLU:OE2  | 1:S:680:SER:OG   | 2.24                     | 0.41              |
| 1:T:313:GLU:N    | 1:T:324:ALA:O    | 2.53                     | 0.41              |
| 1:T:372:ASN:ND2  | 1:T:376:THR:O    | 2.44                     | 0.41              |
| 1:T:397:ARG:HH12 | 1:i:398:THR:HG22 | 1.85                     | 0.41              |
| 1:T:619:HIS:CA   | 2:KA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:V:292:ASN:O    | 1:V:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:X:292:ASN:O    | 1:X:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:X:472:THR:HG23 | 1:X:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:X:611:ILE:HD11 | 2:OA:997:DA:C2   | 2.55                     | 0.41              |
| 1:Z:428:ASN:HB3  | 1:Z:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:c:238:VAL:HG13 | 1:c:362:THR:HG22 | 2.01                     | 0.41              |
| 1:c:389:GLU:HG3  | 1:s:358:PRO:HG3  | 2.03                     | 0.41              |
| 1:c:481:VAL:O    | 1:p:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:c:560:ARG:HG2  | 1:o:496:GLU:O    | 2.20                     | 0.41              |
| 1:d:651:SER:OG   | 1:d:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:e:611:ILE:HD11 | 2:WA:997:DA:C2   | 2.55                     | 0.41              |
| 1:f:619:HIS:CA   | 2:XA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:f:619:HIS:CD2  | 2:XA:997:DA:H3'  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:372:ASN:ND2  | 1:h:376:THR:O    | 2.44                     | 0.41              |
| 1:j:313:GLU:N    | 1:j:324:ALA:O    | 2.53                     | 0.41              |
| 1:j:360:VAL:HG11 | 1:x:644:PRO:HG3  | 2.03                     | 0.41              |
| 1:j:619:HIS:CA   | 2:bA:997:DA:H2'  | 2.50                     | 0.41              |
| 1:k:397:ARG:HH12 | 1:w:398:THR:HG22 | 1.85                     | 0.41              |
| 1:k:472:THR:HG23 | 1:k:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:m:600:ASP:OD1  | 1:m:717:THR:OG1  | 2.34                     | 0.41              |
| 1:o:313:GLU:N    | 1:o:324:ALA:O    | 2.53                     | 0.41              |
| 1:p:619:HIS:CA   | 2:iA:997:DA:C2'  | 2.88                     | 0.41              |
| 1:q:292:ASN:O    | 1:q:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:r:397:ARG:HH12 | 1:x:398:THR:HG22 | 1.85                     | 0.41              |
| 1:r:431:VAL:HG23 | 1:s:349:THR:HB   | 2.03                     | 0.41              |
| 1:s:227:ASP:O    | 1:s:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:s:388:LEU:HD13 | 1:s:637:LEU:HD13 | 2.03                     | 0.41              |
| 1:s:428:ASN:HB3  | 1:s:431:VAL:HG22 | 2.01                     | 0.41              |
| 1:s:678:GLU:OE2  | 1:s:680:SER:OG   | 2.24                     | 0.41              |
| 1:u:313:GLU:N    | 1:u:324:ALA:O    | 2.53                     | 0.41              |
| 1:u:398:THR:HG22 | 1:2:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:u:472:THR:HG23 | 1:u:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:w:472:THR:HG23 | 1:w:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:y:238:VAL:HG13 | 1:y:362:THR:HG22 | 2.01                     | 0.41              |
| 1:1:227:ASP:O    | 1:1:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:2:339:TYR:OH   | 1:2:632:PRO:O    | 2.34                     | 0.41              |
| 1:3:227:ASP:O    | 1:3:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:4:651:SER:OG   | 1:4:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:5:565:VAL:O    | 1:6:496:GLU:HG3  | 2.21                     | 0.41              |
| 1:5:611:ILE:HD11 | 2:yA:997:DA:C2   | 2.55                     | 0.41              |
| 1:5:644:PRO:HG3  | 1:8:360:VAL:HG11 | 2.03                     | 0.41              |
| 1:6:619:HIS:CA   | 2:zA:997:DA:O3'  | 2.60                     | 0.41              |
| 1:6:633:PRO:HA   | 1:6:634:PRO:HD3  | 1.89                     | 0.41              |
| 1:8:472:THR:HG23 | 1:8:522:ALA:HB1  | 2.03                     | 0.41              |
| 2:BA:996:DA:C2'  | 2:BA:997:DA:H5'  | 2.49                     | 0.41              |
| 1:A:227:ASP:O    | 1:A:675:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:388:LEU:HD13 | 1:A:637:LEU:HD13 | 2.03                     | 0.41              |
| 1:C:445:GLY:HA3  | 1:b:481:VAL:O    | 2.21                     | 0.41              |
| 1:E:472:THR:HG23 | 1:E:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:F:239:LEU:HD13 | 1:F:363:LEU:HD12 | 2.03                     | 0.41              |
| 1:G:633:PRO:HA   | 1:G:634:PRO:HD3  | 1.89                     | 0.41              |
| 1:I:633:PRO:HA   | 1:I:634:PRO:HD3  | 1.89                     | 0.41              |
| 1:I:651:SER:OG   | 1:I:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:K:227:ASP:O    | 1:K:675:LEU:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:678:GLU:OE2  | 1:N:680:SER:OG   | 2.24                     | 0.41              |
| 1:O:398:THR:HG22 | 1:P:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:O:611:ILE:HD11 | 2:EA:997:DA:C2   | 2.55                     | 0.41              |
| 1:P:619:HIS:CA   | 2:FA:997:DA:O3'  | 2.60                     | 0.41              |
| 1:Q:292:ASN:O    | 1:Q:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:S:398:THR:HG22 | 1:d:397:ARG:HH12 | 1.85                     | 0.41              |
| 1:S:472:THR:HG23 | 1:S:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:T:360:VAL:HG11 | 1:U:644:PRO:HG3  | 2.03                     | 0.41              |
| 1:T:651:SER:OG   | 1:T:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:U:651:SER:OG   | 1:U:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:Y:238:VAL:HG13 | 1:Y:362:THR:HG22 | 2.01                     | 0.41              |
| 1:Z:481:VAL:O    | 1:3:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:e:388:LEU:HD13 | 1:e:637:LEU:HD13 | 2.03                     | 0.41              |
| 1:f:565:VAL:O    | 1:h:496:GLU:HG3  | 2.21                     | 0.41              |
| 1:f:651:SER:OG   | 1:f:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:h:633:PRO:HA   | 1:h:634:PRO:HD3  | 1.89                     | 0.41              |
| 1:i:388:LEU:HD13 | 1:i:637:LEU:HD13 | 2.03                     | 0.41              |
| 1:j:651:SER:OG   | 1:j:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:k:651:SER:OG   | 1:k:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:l:397:ARG:HH12 | 1:n:398:THR:HG22 | 1.85                     | 0.41              |
| 1:m:565:VAL:O    | 1:n:496:GLU:HG3  | 2.21                     | 0.41              |
| 1:m:619:HIS:CD2  | 2:eA:997:DA:H3'  | 2.55                     | 0.41              |
| 1:n:239:LEU:HD13 | 1:n:363:LEU:HD12 | 2.04                     | 0.41              |
| 1:s:292:ASN:O    | 1:s:720:LEU:HD21 | 2.20                     | 0.41              |
| 1:s:472:THR:HG23 | 1:s:522:ALA:HB1  | 2.03                     | 0.41              |
| 1:t:239:LEU:HD13 | 1:t:363:LEU:HD12 | 2.03                     | 0.41              |
| 1:v:356:PHE:HA   | 1:v:357:PRO:HD3  | 1.92                     | 0.41              |
| 1:x:651:SER:OG   | 1:x:653:VAL:HG22 | 2.21                     | 0.41              |
| 1:z:481:VAL:O    | 1:2:445:GLY:HA3  | 2.21                     | 0.41              |
| 1:6:651:SER:OG   | 1:6:653:VAL:HG22 | 2.21                     | 0.41              |
| 2:LA:996:DA:C2'  | 2:LA:997:DA:H5'  | 2.49                     | 0.41              |
| 2:NA:996:DA:C2'  | 2:NA:997:DA:H5'  | 2.49                     | 0.41              |
| 1:A:360:VAL:HG11 | 1:E:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:D:339:TYR:OH   | 1:D:632:PRO:O    | 2.34                     | 0.40              |
| 1:D:445:GLY:HA3  | 1:N:481:VAL:O    | 2.21                     | 0.40              |
| 1:G:356:PHE:HA   | 1:G:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:G:619:HIS:CA   | 2:3A:997:DA:O3'  | 2.60                     | 0.40              |
| 1:H:313:GLU:N    | 1:H:324:ALA:O    | 2.53                     | 0.40              |
| 1:H:388:LEU:HD13 | 1:H:637:LEU:HD13 | 2.03                     | 0.40              |
| 1:J:227:ASP:O    | 1:J:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:J:565:VAL:O    | 1:L:496:GLU:HG3  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:313:GLU:N    | 1:K:324:ALA:O    | 2.53                     | 0.40              |
| 1:K:565:VAL:O    | 1:a:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:L:239:LEU:HD13 | 1:L:363:LEU:HD12 | 2.04                     | 0.40              |
| 1:L:619:HIS:CA   | 2:BA:997:DA:O3'  | 2.60                     | 0.40              |
| 1:M:472:THR:HG23 | 1:M:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:M:644:PRO:HG3  | 1:c:360:VAL:HG11 | 2.03                     | 0.40              |
| 1:O:358:PRO:HG3  | 1:P:389:GLU:HG3  | 2.04                     | 0.40              |
| 1:O:388:LEU:HD13 | 1:O:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:P:356:PHE:HA   | 1:P:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:Q:305:LYS:HB3  | 1:Q:668:THR:HG22 | 2.04                     | 0.40              |
| 1:Q:356:PHE:HA   | 1:Q:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:R:481:VAL:O    | 1:U:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:S:651:SER:OG   | 1:S:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:T:678:GLU:OE2  | 1:T:680:SER:OG   | 2.24                     | 0.40              |
| 1:V:496:GLU:HG3  | 1:X:565:VAL:O    | 2.22                     | 0.40              |
| 1:V:565:VAL:O    | 1:e:496:GLU:HG3  | 2.21                     | 0.40              |
| 1:X:239:LEU:HD13 | 1:X:363:LEU:HD12 | 2.04                     | 0.40              |
| 1:X:313:GLU:N    | 1:X:324:ALA:O    | 2.53                     | 0.40              |
| 1:X:388:LEU:HD13 | 1:X:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:X:678:GLU:OE2  | 1:X:680:SER:OG   | 2.24                     | 0.40              |
| 1:Y:313:GLU:N    | 1:Y:324:ALA:O    | 2.53                     | 0.40              |
| 1:Y:651:SER:OG   | 1:Y:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:Z:239:LEU:HD13 | 1:Z:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:Z:349:THR:HB   | 1:3:431:VAL:HG23 | 2.04                     | 0.40              |
| 1:b:239:LEU:HD13 | 1:b:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:b:298:ARG:HH12 | 2:SA:996:DA:N6   | 2.20                     | 0.40              |
| 1:b:388:LEU:HD13 | 1:b:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:c:227:ASP:O    | 1:c:675:LEU:HB2  | 2.20                     | 0.40              |
| 1:c:397:ARG:HH12 | 1:s:398:THR:HG22 | 1.86                     | 0.40              |
| 1:d:239:LEU:HD13 | 1:d:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:f:633:PRO:HA   | 1:f:634:PRO:HD3  | 1.89                     | 0.40              |
| 1:g:358:PRO:HG3  | 1:l:389:GLU:HG3  | 2.04                     | 0.40              |
| 1:g:388:LEU:HD13 | 1:g:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:g:398:THR:HG22 | 1:l:397:ARG:HH12 | 1.85                     | 0.40              |
| 1:g:611:ILE:HD11 | 2:YA:997:DA:C2   | 2.55                     | 0.40              |
| 1:h:239:LEU:HD13 | 1:h:363:LEU:HD12 | 2.04                     | 0.40              |
| 1:h:472:THR:HG23 | 1:h:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:j:472:THR:HG23 | 1:j:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:k:239:LEU:HD13 | 1:k:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:l:388:LEU:HD13 | 1:l:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:m:298:ARG:HH12 | 2:eA:996:DA:N6   | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:651:SER:OG   | 1:m:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:n:472:THR:HG23 | 1:n:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:o:388:LEU:HD13 | 1:o:637:LEU:HD13 | 2.03                     | 0.40              |
| 1:o:398:THR:HG22 | 1:7:397:ARG:HH12 | 1.85                     | 0.40              |
| 1:o:619:HIS:CA   | 2:hA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:p:388:LEU:HD13 | 1:p:637:LEU:HD13 | 2.03                     | 0.40              |
| 1:q:349:THR:HB   | 1:s:431:VAL:HG23 | 2.03                     | 0.40              |
| 1:r:388:LEU:HD13 | 1:r:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:s:313:GLU:N    | 1:s:324:ALA:O    | 2.53                     | 0.40              |
| 1:t:292:ASN:O    | 1:t:720:LEU:HD21 | 2.20                     | 0.40              |
| 1:t:619:HIS:CA   | 2:mA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:t:628:GLY:C    | 2:mA:997:DA:N1   | 2.66                     | 0.40              |
| 1:u:227:ASP:O    | 1:u:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:v:513:ASN:ND2  | 1:v:526:THR:HG22 | 2.10                     | 0.40              |
| 1:x:388:LEU:HD13 | 1:x:637:LEU:HD13 | 2.03                     | 0.40              |
| 1:y:611:ILE:HD11 | 2:sA:997:DA:C2   | 2.55                     | 0.40              |
| 1:z:349:THR:HB   | 1:2:431:VAL:HG23 | 2.04                     | 0.40              |
| 1:2:482:ASN:HB3  | 1:2:483:ARG:H    | 1.62                     | 0.40              |
| 1:5:227:ASP:O    | 1:5:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:5:388:LEU:HD13 | 1:5:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:6:227:ASP:O    | 1:6:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:6:356:PHE:HA   | 1:6:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:6:619:HIS:CA   | 2:zA:997:DA:C2'  | 2.88                     | 0.40              |
| 1:7:651:SER:OG   | 1:7:653:VAL:HG22 | 2.21                     | 0.40              |
| 2:OA:996:DA:C2'  | 2:OA:997:DA:H5'  | 2.49                     | 0.40              |
| 2:RA:996:DA:C2'  | 2:RA:997:DA:H5'  | 2.49                     | 0.40              |
| 1:B:298:ARG:HH12 | 2:JA:996:DA:N6   | 2.20                     | 0.40              |
| 1:B:481:VAL:O    | 1:L:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:C:431:VAL:HG23 | 1:b:349:THR:HB   | 2.04                     | 0.40              |
| 1:E:227:ASP:O    | 1:E:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:F:481:VAL:O    | 1:Q:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:F:628:GLY:C    | 2:1A:997:DA:N1   | 2.66                     | 0.40              |
| 1:G:305:LYS:HB3  | 1:G:668:THR:HG22 | 2.04                     | 0.40              |
| 1:G:619:HIS:CA   | 2:3A:997:DA:H2'  | 2.50                     | 0.40              |
| 1:H:360:VAL:HG11 | 1:I:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:H:496:GLU:HG3  | 1:Y:565:VAL:O    | 2.21                     | 0.40              |
| 1:H:619:HIS:CA   | 2:4A:997:DA:H2'  | 2.50                     | 0.40              |
| 1:M:619:HIS:CD2  | 2:CA:997:DA:H3'  | 2.55                     | 0.40              |
| 1:O:472:THR:HG23 | 1:O:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:O:496:GLU:HG3  | 1:n:565:VAL:O    | 2.21                     | 0.40              |
| 1:P:305:LYS:HB3  | 1:P:668:THR:HG22 | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:513:ASN:ND2  | 1:Q:526:THR:HG22 | 2.10                     | 0.40              |
| 1:T:472:THR:HG23 | 1:T:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:U:388:LEU:HD13 | 1:U:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:W:388:LEU:HD13 | 1:W:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:X:339:TYR:OH   | 1:X:632:PRO:O    | 2.34                     | 0.40              |
| 1:Y:339:TYR:OH   | 1:Y:632:PRO:O    | 2.34                     | 0.40              |
| 1:Y:360:VAL:HG11 | 1:4:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:Z:298:ARG:HH12 | 2:QA:996:DA:N6   | 2.20                     | 0.40              |
| 1:Z:388:LEU:HD13 | 1:Z:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:Z:445:GLY:HA3  | 1:4:481:VAL:O    | 2.21                     | 0.40              |
| 1:a:239:LEU:HD13 | 1:a:363:LEU:HD12 | 2.04                     | 0.40              |
| 1:a:445:GLY:HA3  | 1:8:481:VAL:O    | 2.21                     | 0.40              |
| 1:a:619:HIS:CA   | 2:RA:997:DA:O3'  | 2.60                     | 0.40              |
| 1:b:227:ASP:O    | 1:b:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:c:313:GLU:N    | 1:c:324:ALA:O    | 2.53                     | 0.40              |
| 1:c:339:TYR:OH   | 1:c:632:PRO:O    | 2.34                     | 0.40              |
| 1:d:305:LYS:HB3  | 1:d:668:THR:HG22 | 2.04                     | 0.40              |
| 1:d:565:VAL:O    | 1:l:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:e:472:THR:HG23 | 1:e:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:f:298:ARG:HH12 | 2:XA:996:DA:N6   | 2.20                     | 0.40              |
| 1:h:298:ARG:HH12 | 2:ZA:996:DA:N6   | 2.20                     | 0.40              |
| 1:h:651:SER:OG   | 1:h:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:i:496:GLU:HG3  | 1:k:565:VAL:O    | 2.22                     | 0.40              |
| 1:i:633:PRO:HA   | 1:i:634:PRO:HD3  | 1.89                     | 0.40              |
| 1:k:305:LYS:HB3  | 1:k:668:THR:HG22 | 2.04                     | 0.40              |
| 1:m:358:PRO:HG3  | 1:s:389:GLU:HG3  | 2.03                     | 0.40              |
| 1:n:372:ASN:ND2  | 1:n:376:THR:O    | 2.44                     | 0.40              |
| 1:n:651:SER:OG   | 1:n:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:o:651:SER:OG   | 1:o:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:q:239:LEU:HD13 | 1:q:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:q:496:GLU:O    | 1:s:560:ARG:HG2  | 2.21                     | 0.40              |
| 1:r:292:ASN:O    | 1:r:720:LEU:HD21 | 2.20                     | 0.40              |
| 1:r:305:LYS:HB3  | 1:r:668:THR:HG22 | 2.04                     | 0.40              |
| 1:r:472:THR:HG23 | 1:r:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:s:239:LEU:HD13 | 1:s:363:LEU:HD12 | 2.04                     | 0.40              |
| 1:t:481:VAL:O    | 1:v:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:v:292:ASN:O    | 1:v:720:LEU:HD21 | 2.20                     | 0.40              |
| 1:v:305:LYS:HB3  | 1:v:668:THR:HG22 | 2.04                     | 0.40              |
| 1:w:651:SER:OG   | 1:w:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:x:445:GLY:HA3  | 1:y:481:VAL:O    | 2.21                     | 0.40              |
| 1:x:565:VAL:O    | 1:y:496:GLU:HG3  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:z:388:LEU:HD13 | 1:z:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:z:560:ARG:HG2  | 1:1:496:GLU:O    | 2.20                     | 0.40              |
| 1:1:356:PHE:HA   | 1:1:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:4:619:HIS:CD2  | 2:xA:997:DA:H3'  | 2.55                     | 0.40              |
| 1:5:397:ARG:HH12 | 1:8:398:THR:HG22 | 1.85                     | 0.40              |
| 1:6:305:LYS:HB3  | 1:6:668:THR:HG22 | 2.04                     | 0.40              |
| 1:8:298:ARG:HH12 | 2:2A:996:DA:N6   | 2.20                     | 0.40              |
| 2:DA:996:DA:C2'  | 2:DA:997:DA:H5'  | 2.49                     | 0.40              |
| 2:KA:996:DA:C2'  | 2:KA:997:DA:H5'  | 2.49                     | 0.40              |
| 2:rA:996:DA:C2'  | 2:rA:997:DA:H5'  | 2.49                     | 0.40              |
| 1:A:496:GLU:HG3  | 1:I:565:VAL:O    | 2.21                     | 0.40              |
| 1:B:388:LEU:HD13 | 1:B:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:F:298:ARG:HH12 | 2:1A:996:DA:N6   | 2.20                     | 0.40              |
| 1:G:227:ASP:O    | 1:G:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:G:292:ASN:O    | 1:G:720:LEU:HD21 | 2.20                     | 0.40              |
| 1:G:619:HIS:CA   | 2:3A:997:DA:C2'  | 2.88                     | 0.40              |
| 1:J:298:ARG:HH12 | 2:9:996:DA:N6    | 2.20                     | 0.40              |
| 1:K:298:ARG:HH12 | 2:AA:996:DA:N6   | 2.20                     | 0.40              |
| 1:K:445:GLY:HA3  | 1:a:481:VAL:O    | 2.21                     | 0.40              |
| 1:L:476:ASN:CB   | 1:L:480:GLY:HA3  | 2.47                     | 0.40              |
| 1:M:239:LEU:HD13 | 1:M:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:M:481:VAL:O    | 1:b:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:N:228:ARG:HA   | 1:N:228:ARG:HD3  | 1.95                     | 0.40              |
| 1:N:388:LEU:HD13 | 1:N:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:N:651:SER:OG   | 1:N:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:P:388:LEU:HD13 | 1:P:637:LEU:HD13 | 2.03                     | 0.40              |
| 1:Q:360:VAL:HG11 | 1:S:644:PRO:HG3  | 2.04                     | 0.40              |
| 1:R:496:GLU:HG3  | 1:U:565:VAL:O    | 2.22                     | 0.40              |
| 1:R:611:ILE:HD11 | 2:HA:997:DA:C2   | 2.55                     | 0.40              |
| 1:T:298:ARG:HH12 | 2:KA:996:DA:N6   | 2.20                     | 0.40              |
| 1:T:305:LYS:HB3  | 1:T:668:THR:HG22 | 2.04                     | 0.40              |
| 1:T:445:GLY:HA3  | 1:d:481:VAL:O    | 2.21                     | 0.40              |
| 1:T:481:VAL:O    | 1:l:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:T:565:VAL:O    | 1:d:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:T:644:PRO:HG3  | 1:i:360:VAL:HG11 | 2.04                     | 0.40              |
| 1:V:239:LEU:HD13 | 1:V:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:V:651:SER:OG   | 1:V:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:X:349:THR:HB   | 1:e:431:VAL:HG23 | 2.04                     | 0.40              |
| 1:X:360:VAL:HG11 | 1:Y:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:Y:227:ASP:O    | 1:Y:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:c:565:VAL:O    | 1:o:496:GLU:HG3  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:651:SER:OG   | 1:c:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:g:305:LYS:HB3  | 1:g:668:THR:HG22 | 2.04                     | 0.40              |
| 1:g:472:THR:HG23 | 1:g:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:g:496:GLU:HG3  | 1:h:565:VAL:O    | 2.21                     | 0.40              |
| 1:i:445:GLY:HA3  | 1:j:481:VAL:O    | 2.21                     | 0.40              |
| 1:j:565:VAL:O    | 1:k:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:j:644:PRO:HG3  | 1:l:360:VAL:HG11 | 2.03                     | 0.40              |
| 1:j:678:GLU:OE2  | 1:j:680:SER:OG   | 2.24                     | 0.40              |
| 1:k:482:ASN:HB3  | 1:k:483:ARG:H    | 1.62                     | 0.40              |
| 1:n:298:ARG:HH12 | 2:gA:996:DA:N6   | 2.20                     | 0.40              |
| 1:o:360:VAL:HG11 | 1:7:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:p:298:ARG:HH12 | 2:iA:996:DA:N6   | 2.20                     | 0.40              |
| 1:p:472:THR:HG23 | 1:p:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:q:565:VAL:O    | 1:r:496:GLU:HG3  | 2.21                     | 0.40              |
| 1:q:651:SER:OG   | 1:q:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:r:644:PRO:HG3  | 1:x:360:VAL:HG11 | 2.03                     | 0.40              |
| 1:s:339:TYR:OH   | 1:s:632:PRO:O    | 2.34                     | 0.40              |
| 1:s:356:PHE:HA   | 1:s:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:t:298:ARG:HH12 | 2:mA:996:DA:N6   | 2.20                     | 0.40              |
| 1:v:239:LEU:HD13 | 1:v:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:w:388:LEU:HD13 | 1:w:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:w:619:HIS:CA   | 2:pA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:x:356:PHE:HA   | 1:x:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:z:651:SER:OG   | 1:z:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:1:228:ARG:HA   | 1:1:228:ARG:HD3  | 1.95                     | 0.40              |
| 1:1:239:LEU:HD13 | 1:1:363:LEU:HD12 | 2.04                     | 0.40              |
| 1:1:305:LYS:HB3  | 1:1:668:THR:HG22 | 2.04                     | 0.40              |
| 1:1:619:HIS:CA   | 2:uA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:4:472:THR:HG23 | 1:4:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:5:481:VAL:O    | 1:7:445:GLY:HA3  | 2.21                     | 0.40              |
| 1:8:388:LEU:HD13 | 1:8:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:A:356:PHE:HA   | 1:A:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:A:619:HIS:CA   | 2:0:997:DA:H2'   | 2.50                     | 0.40              |
| 1:B:433:GLN:O    | 1:B:451:LYS:NZ   | 2.48                     | 0.40              |
| 1:C:356:PHE:HA   | 1:C:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:D:431:VAL:HG23 | 1:N:349:THR:HB   | 2.04                     | 0.40              |
| 1:F:619:HIS:CA   | 2:1A:997:DA:H2'  | 2.50                     | 0.40              |
| 1:F:644:PRO:HG3  | 1:R:360:VAL:HG11 | 2.03                     | 0.40              |
| 1:H:644:PRO:HG3  | 1:Z:360:VAL:HG11 | 2.03                     | 0.40              |
| 1:H:651:SER:OG   | 1:H:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:M:496:GLU:HG3  | 1:b:565:VAL:O    | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:227:ASP:O    | 1:N:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:O:305:LYS:HB3  | 1:O:668:THR:HG22 | 2.04                     | 0.40              |
| 1:P:239:LEU:HD13 | 1:P:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:Q:239:LEU:HD13 | 1:Q:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:S:619:HIS:CA   | 2:IA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:V:349:THR:HB   | 1:X:431:VAL:HG23 | 2.03                     | 0.40              |
| 1:V:633:PRO:HA   | 1:V:634:PRO:HD3  | 1.89                     | 0.40              |
| 1:W:298:ARG:HH12 | 2:NA:996:DA:N6   | 2.20                     | 0.40              |
| 1:W:431:VAL:HG23 | 1:Y:349:THR:HB   | 2.03                     | 0.40              |
| 1:X:305:LYS:HB3  | 1:X:668:THR:HG22 | 2.04                     | 0.40              |
| 1:X:356:PHE:HA   | 1:X:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:X:651:SER:OG   | 1:X:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:Z:372:ASN:ND2  | 1:Z:376:THR:O    | 2.44                     | 0.40              |
| 1:Z:565:VAL:O    | 1:4:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:Z:651:SER:OG   | 1:Z:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:b:372:ASN:ND2  | 1:b:376:THR:O    | 2.44                     | 0.40              |
| 1:b:651:SER:OG   | 1:b:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:c:349:THR:HB   | 1:p:431:VAL:HG23 | 2.03                     | 0.40              |
| 1:e:292:ASN:O    | 1:e:720:LEU:HD21 | 2.20                     | 0.40              |
| 1:e:305:LYS:HB3  | 1:e:668:THR:HG22 | 2.04                     | 0.40              |
| 1:j:298:ARG:HH12 | 2:bA:996:DA:N6   | 2.20                     | 0.40              |
| 1:j:305:LYS:HB3  | 1:j:668:THR:HG22 | 2.04                     | 0.40              |
| 1:j:445:GLY:HA3  | 1:k:481:VAL:O    | 2.21                     | 0.40              |
| 1:o:565:VAL:O    | 1:p:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:s:305:LYS:HB3  | 1:s:668:THR:HG22 | 2.04                     | 0.40              |
| 1:s:651:SER:OG   | 1:s:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:t:644:PRO:HG3  | 1:y:360:VAL:HG11 | 2.03                     | 0.40              |
| 1:y:651:SER:OG   | 1:y:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:1:445:GLY:HA3  | 1:2:481:VAL:O    | 2.22                     | 0.40              |
| 1:4:239:LEU:HD13 | 1:4:363:LEU:HD12 | 2.03                     | 0.40              |
| 1:4:619:HIS:CA   | 2:xA:997:DA:C2'  | 2.88                     | 0.40              |
| 1:5:619:HIS:CA   | 2:yA:997:DA:H2'  | 2.50                     | 0.40              |
| 2:5A:996:DA:C2'  | 2:5A:997:DA:H5'  | 2.49                     | 0.40              |
| 2:1A:996:DA:C2'  | 2:1A:997:DA:H5'  | 2.49                     | 0.40              |
| 1:A:651:SER:OG   | 1:A:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:D:472:THR:HG23 | 1:D:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:D:481:VAL:O    | 1:P:445:GLY:HA3  | 2.22                     | 0.40              |
| 1:E:261:ASN:ND2  | 1:F:458:ALA:H    | 2.20                     | 0.40              |
| 1:E:481:VAL:O    | 1:F:445:GLY:HA3  | 2.22                     | 0.40              |
| 1:F:360:VAL:HG11 | 1:G:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:F:433:GLN:O    | 1:F:451:LYS:NZ   | 2.48                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:442:ASN:HB3  | 1:F:448:GLN:NE2  | 2.37                     | 0.40              |
| 1:F:496:GLU:O    | 1:Q:560:ARG:HG2  | 2.20                     | 0.40              |
| 1:G:388:LEU:HD13 | 1:G:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:H:565:VAL:O    | 1:W:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:J:445:GLY:HA3  | 1:L:481:VAL:O    | 2.21                     | 0.40              |
| 1:L:298:ARG:HH12 | 2:BA:996:DA:N6   | 2.20                     | 0.40              |
| 1:O:349:THR:HB   | 1:n:431:VAL:HG23 | 2.04                     | 0.40              |
| 1:P:619:HIS:CA   | 2:FA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:R:651:SER:OG   | 1:R:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:S:388:LEU:HD13 | 1:S:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:S:431:VAL:HG23 | 1:U:349:THR:HB   | 2.04                     | 0.40              |
| 1:V:472:THR:HG23 | 1:V:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:W:472:THR:HG23 | 1:W:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:W:476:ASN:CB   | 1:W:480:GLY:HA3  | 2.47                     | 0.40              |
| 1:Y:358:PRO:HG3  | 1:4:389:GLU:HG3  | 2.04                     | 0.40              |
| 1:Z:227:ASP:O    | 1:Z:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:a:298:ARG:HH12 | 2:RA:996:DA:N6   | 2.20                     | 0.40              |
| 1:a:442:ASN:HB3  | 1:a:448:GLN:NE2  | 2.37                     | 0.40              |
| 1:b:305:LYS:HB3  | 1:b:668:THR:HG22 | 2.04                     | 0.40              |
| 1:b:360:VAL:HG11 | 1:o:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:c:381:GLU:OE1  | 1:s:693:TYR:HD2  | 2.05                     | 0.40              |
| 1:i:651:SER:OG   | 1:i:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:l:651:SER:OG   | 1:l:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:m:633:PRO:HA   | 1:m:634:PRO:HD3  | 1.89                     | 0.40              |
| 1:n:633:PRO:HA   | 1:n:634:PRO:HD3  | 1.89                     | 0.40              |
| 1:q:398:THR:HG22 | 1:y:397:ARG:HH12 | 1.85                     | 0.40              |
| 1:q:472:THR:HG23 | 1:q:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:q:496:GLU:HG3  | 1:s:565:VAL:O    | 2.22                     | 0.40              |
| 1:t:349:THR:HB   | 1:v:431:VAL:HG23 | 2.04                     | 0.40              |
| 1:t:360:VAL:HG11 | 1:6:644:PRO:HG3  | 2.03                     | 0.40              |
| 1:t:442:ASN:HB3  | 1:t:448:GLN:NE2  | 2.37                     | 0.40              |
| 1:t:445:GLY:HA3  | 1:u:481:VAL:O    | 2.22                     | 0.40              |
| 1:u:619:HIS:CA   | 2:nA:997:DA:H2'  | 2.50                     | 0.40              |
| 1:v:354:PRO:HD3  | 1:v:361:PHE:CD2  | 2.57                     | 0.40              |
| 1:v:360:VAL:HG11 | 1:w:644:PRO:HG3  | 2.04                     | 0.40              |
| 1:w:431:VAL:HG23 | 1:x:349:THR:HB   | 2.04                     | 0.40              |
| 1:w:565:VAL:O    | 1:x:496:GLU:HG3  | 2.22                     | 0.40              |
| 1:x:431:VAL:HG23 | 1:y:349:THR:HB   | 2.04                     | 0.40              |
| 1:z:227:ASP:O    | 1:z:675:LEU:HB2  | 2.20                     | 0.40              |
| 1:1:388:LEU:HD13 | 1:1:637:LEU:HD13 | 2.04                     | 0.40              |
| 1:1:619:HIS:CA   | 2:uA:997:DA:O3'  | 2.60                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:651:SER:OG   | 1:1:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:2:472:THR:HG23 | 1:2:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:3:356:PHE:HA   | 1:3:357:PRO:HD3  | 1.92                     | 0.40              |
| 1:3:472:THR:HG23 | 1:3:522:ALA:HB1  | 2.03                     | 0.40              |
| 1:4:227:ASP:O    | 1:4:675:LEU:HB2  | 2.21                     | 0.40              |
| 1:5:496:GLU:O    | 1:7:560:ARG:HG2  | 2.20                     | 0.40              |
| 1:5:651:SER:OG   | 1:5:653:VAL:HG22 | 2.21                     | 0.40              |
| 1:6:292:ASN:O    | 1:6:720:LEU:HD21 | 2.20                     | 0.40              |
| 1:6:619:HIS:CA   | 2:zA:997:DA:H2'  | 2.50                     | 0.40              |
| 2:bA:996:DA:C2'  | 2:bA:997:DA:H5'  | 2.49                     | 0.40              |
| 2:tA:996:DA:C2'  | 2:tA:997:DA:H5'  | 2.49                     | 0.40              |
| 2:0A:996:DA:C2'  | 2:0A:997:DA:H5'  | 2.49                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 1     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 2     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 3     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 4     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 5     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 6     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 7     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 8     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | A     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | B     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | C     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | D     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | E     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | F     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | G     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | H     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | I     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | J     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | K     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | L     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | M     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | N     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | O     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | P     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | Q     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | R     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | S     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | T     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | U     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | V     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | W     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | X     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | Y     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | Z     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | a     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | b     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | c     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | d     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | e     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | f     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | g     | 515/724 (71%) | 499 (97%) | 16 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | h     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | i     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | j     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | k     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | l     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | m     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | n     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | o     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | p     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | q     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | r     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | s     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | t     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | u     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | v     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | w     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | x     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | y     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | z     | 515/724 (71%)     | 499 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| All | All   | 30900/43440 (71%) | 29940 (97%) | 960 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 1   | 1     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | 2     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 1   | 3     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | 4     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | 5     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | 6     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | 7     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | 8     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | A     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | B     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | C     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | D     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | E     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | F     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | G     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | H     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | I     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | J     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | K     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | L     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | M     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | N     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | O     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | P     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | Q     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | R     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | S     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | T     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | U     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | V     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | W     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | X     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |
| 1   | Y     | 451/613 (74%) | 450 (100%) | 1 (0%)   | 87          | 96 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |    |
|-----|-------|-------------------|--------------|----------|-------------|----|
| 1   | Z     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | a     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | b     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | c     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | d     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | e     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | f     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | g     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | h     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | i     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | j     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | k     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | l     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | m     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | n     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | o     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | p     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | q     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | r     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | s     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | t     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | u     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | v     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | w     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | x     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | y     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| 1   | z     | 451/613 (74%)     | 450 (100%)   | 1 (0%)   | 87          | 96 |
| All | All   | 27060/36780 (74%) | 27000 (100%) | 60 (0%)  | 85          | 96 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 523 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 523 | LEU  |
| 1   | C     | 523 | LEU  |
| 1   | D     | 523 | LEU  |
| 1   | E     | 523 | LEU  |
| 1   | F     | 523 | LEU  |
| 1   | G     | 523 | LEU  |
| 1   | H     | 523 | LEU  |
| 1   | I     | 523 | LEU  |
| 1   | J     | 523 | LEU  |
| 1   | K     | 523 | LEU  |
| 1   | L     | 523 | LEU  |
| 1   | M     | 523 | LEU  |
| 1   | N     | 523 | LEU  |
| 1   | O     | 523 | LEU  |
| 1   | P     | 523 | LEU  |
| 1   | Q     | 523 | LEU  |
| 1   | R     | 523 | LEU  |
| 1   | S     | 523 | LEU  |
| 1   | T     | 523 | LEU  |
| 1   | U     | 523 | LEU  |
| 1   | V     | 523 | LEU  |
| 1   | W     | 523 | LEU  |
| 1   | X     | 523 | LEU  |
| 1   | Y     | 523 | LEU  |
| 1   | Z     | 523 | LEU  |
| 1   | a     | 523 | LEU  |
| 1   | b     | 523 | LEU  |
| 1   | c     | 523 | LEU  |
| 1   | d     | 523 | LEU  |
| 1   | e     | 523 | LEU  |
| 1   | f     | 523 | LEU  |
| 1   | g     | 523 | LEU  |
| 1   | h     | 523 | LEU  |
| 1   | i     | 523 | LEU  |
| 1   | j     | 523 | LEU  |
| 1   | k     | 523 | LEU  |
| 1   | l     | 523 | LEU  |
| 1   | m     | 523 | LEU  |
| 1   | n     | 523 | LEU  |
| 1   | o     | 523 | LEU  |
| 1   | p     | 523 | LEU  |
| 1   | q     | 523 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | r     | 523 | LEU  |
| 1   | s     | 523 | LEU  |
| 1   | t     | 523 | LEU  |
| 1   | u     | 523 | LEU  |
| 1   | v     | 523 | LEU  |
| 1   | w     | 523 | LEU  |
| 1   | x     | 523 | LEU  |
| 1   | y     | 523 | LEU  |
| 1   | z     | 523 | LEU  |
| 1   | 1     | 523 | LEU  |
| 1   | 2     | 523 | LEU  |
| 1   | 3     | 523 | LEU  |
| 1   | 4     | 523 | LEU  |
| 1   | 5     | 523 | LEU  |
| 1   | 6     | 523 | LEU  |
| 1   | 7     | 523 | LEU  |
| 1   | 8     | 523 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (718) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 219 | HIS  |
| 1   | A     | 245 | HIS  |
| 1   | A     | 261 | ASN  |
| 1   | A     | 332 | GLN  |
| 1   | A     | 421 | GLN  |
| 1   | A     | 450 | ASN  |
| 1   | A     | 476 | ASN  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 509 | ASN  |
| 1   | A     | 525 | ASN  |
| 1   | A     | 535 | ASN  |
| 1   | A     | 631 | HIS  |
| 1   | A     | 679 | ASN  |
| 1   | B     | 219 | HIS  |
| 1   | B     | 245 | HIS  |
| 1   | B     | 261 | ASN  |
| 1   | B     | 332 | GLN  |
| 1   | B     | 421 | GLN  |
| 1   | B     | 450 | ASN  |
| 1   | B     | 476 | ASN  |
| 1   | B     | 507 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 509 | ASN  |
| 1   | B     | 525 | ASN  |
| 1   | B     | 535 | ASN  |
| 1   | B     | 631 | HIS  |
| 1   | C     | 219 | HIS  |
| 1   | C     | 245 | HIS  |
| 1   | C     | 261 | ASN  |
| 1   | C     | 332 | GLN  |
| 1   | C     | 421 | GLN  |
| 1   | C     | 450 | ASN  |
| 1   | C     | 476 | ASN  |
| 1   | C     | 507 | GLN  |
| 1   | C     | 509 | ASN  |
| 1   | C     | 525 | ASN  |
| 1   | C     | 535 | ASN  |
| 1   | C     | 631 | HIS  |
| 1   | D     | 219 | HIS  |
| 1   | D     | 245 | HIS  |
| 1   | D     | 261 | ASN  |
| 1   | D     | 332 | GLN  |
| 1   | D     | 421 | GLN  |
| 1   | D     | 476 | ASN  |
| 1   | D     | 507 | GLN  |
| 1   | D     | 509 | ASN  |
| 1   | D     | 525 | ASN  |
| 1   | D     | 535 | ASN  |
| 1   | D     | 573 | ASN  |
| 1   | D     | 631 | HIS  |
| 1   | E     | 219 | HIS  |
| 1   | E     | 245 | HIS  |
| 1   | E     | 261 | ASN  |
| 1   | E     | 332 | GLN  |
| 1   | E     | 421 | GLN  |
| 1   | E     | 450 | ASN  |
| 1   | E     | 476 | ASN  |
| 1   | E     | 507 | GLN  |
| 1   | E     | 509 | ASN  |
| 1   | E     | 525 | ASN  |
| 1   | E     | 535 | ASN  |
| 1   | E     | 631 | HIS  |
| 1   | F     | 219 | HIS  |
| 1   | F     | 245 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 261 | ASN  |
| 1   | F     | 332 | GLN  |
| 1   | F     | 421 | GLN  |
| 1   | F     | 476 | ASN  |
| 1   | F     | 507 | GLN  |
| 1   | F     | 509 | ASN  |
| 1   | F     | 525 | ASN  |
| 1   | F     | 535 | ASN  |
| 1   | F     | 631 | HIS  |
| 1   | G     | 219 | HIS  |
| 1   | G     | 245 | HIS  |
| 1   | G     | 261 | ASN  |
| 1   | G     | 332 | GLN  |
| 1   | G     | 421 | GLN  |
| 1   | G     | 476 | ASN  |
| 1   | G     | 507 | GLN  |
| 1   | G     | 509 | ASN  |
| 1   | G     | 525 | ASN  |
| 1   | G     | 535 | ASN  |
| 1   | G     | 631 | HIS  |
| 1   | H     | 219 | HIS  |
| 1   | H     | 245 | HIS  |
| 1   | H     | 261 | ASN  |
| 1   | H     | 332 | GLN  |
| 1   | H     | 421 | GLN  |
| 1   | H     | 450 | ASN  |
| 1   | H     | 476 | ASN  |
| 1   | H     | 507 | GLN  |
| 1   | H     | 509 | ASN  |
| 1   | H     | 525 | ASN  |
| 1   | H     | 631 | HIS  |
| 1   | I     | 219 | HIS  |
| 1   | I     | 245 | HIS  |
| 1   | I     | 261 | ASN  |
| 1   | I     | 332 | GLN  |
| 1   | I     | 421 | GLN  |
| 1   | I     | 476 | ASN  |
| 1   | I     | 507 | GLN  |
| 1   | I     | 509 | ASN  |
| 1   | I     | 525 | ASN  |
| 1   | I     | 535 | ASN  |
| 1   | I     | 631 | HIS  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 679 | ASN  |
| 1   | J     | 219 | HIS  |
| 1   | J     | 245 | HIS  |
| 1   | J     | 261 | ASN  |
| 1   | J     | 332 | GLN  |
| 1   | J     | 421 | GLN  |
| 1   | J     | 476 | ASN  |
| 1   | J     | 507 | GLN  |
| 1   | J     | 509 | ASN  |
| 1   | J     | 525 | ASN  |
| 1   | J     | 535 | ASN  |
| 1   | J     | 573 | ASN  |
| 1   | J     | 631 | HIS  |
| 1   | K     | 219 | HIS  |
| 1   | K     | 245 | HIS  |
| 1   | K     | 261 | ASN  |
| 1   | K     | 332 | GLN  |
| 1   | K     | 421 | GLN  |
| 1   | K     | 476 | ASN  |
| 1   | K     | 507 | GLN  |
| 1   | K     | 509 | ASN  |
| 1   | K     | 525 | ASN  |
| 1   | K     | 535 | ASN  |
| 1   | K     | 573 | ASN  |
| 1   | K     | 631 | HIS  |
| 1   | L     | 219 | HIS  |
| 1   | L     | 245 | HIS  |
| 1   | L     | 261 | ASN  |
| 1   | L     | 332 | GLN  |
| 1   | L     | 421 | GLN  |
| 1   | L     | 476 | ASN  |
| 1   | L     | 507 | GLN  |
| 1   | L     | 509 | ASN  |
| 1   | L     | 525 | ASN  |
| 1   | L     | 535 | ASN  |
| 1   | L     | 631 | HIS  |
| 1   | L     | 679 | ASN  |
| 1   | M     | 219 | HIS  |
| 1   | M     | 245 | HIS  |
| 1   | M     | 261 | ASN  |
| 1   | M     | 332 | GLN  |
| 1   | M     | 421 | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 476 | ASN  |
| 1   | M     | 507 | GLN  |
| 1   | M     | 509 | ASN  |
| 1   | M     | 525 | ASN  |
| 1   | M     | 535 | ASN  |
| 1   | M     | 573 | ASN  |
| 1   | M     | 631 | HIS  |
| 1   | N     | 219 | HIS  |
| 1   | N     | 245 | HIS  |
| 1   | N     | 261 | ASN  |
| 1   | N     | 332 | GLN  |
| 1   | N     | 421 | GLN  |
| 1   | N     | 476 | ASN  |
| 1   | N     | 507 | GLN  |
| 1   | N     | 509 | ASN  |
| 1   | N     | 525 | ASN  |
| 1   | N     | 535 | ASN  |
| 1   | N     | 631 | HIS  |
| 1   | O     | 219 | HIS  |
| 1   | O     | 245 | HIS  |
| 1   | O     | 261 | ASN  |
| 1   | O     | 332 | GLN  |
| 1   | O     | 421 | GLN  |
| 1   | O     | 450 | ASN  |
| 1   | O     | 476 | ASN  |
| 1   | O     | 507 | GLN  |
| 1   | O     | 509 | ASN  |
| 1   | O     | 525 | ASN  |
| 1   | O     | 535 | ASN  |
| 1   | O     | 573 | ASN  |
| 1   | O     | 631 | HIS  |
| 1   | P     | 219 | HIS  |
| 1   | P     | 245 | HIS  |
| 1   | P     | 261 | ASN  |
| 1   | P     | 332 | GLN  |
| 1   | P     | 421 | GLN  |
| 1   | P     | 476 | ASN  |
| 1   | P     | 507 | GLN  |
| 1   | P     | 509 | ASN  |
| 1   | P     | 525 | ASN  |
| 1   | P     | 535 | ASN  |
| 1   | P     | 546 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 631 | HIS  |
| 1   | Q     | 219 | HIS  |
| 1   | Q     | 245 | HIS  |
| 1   | Q     | 261 | ASN  |
| 1   | Q     | 332 | GLN  |
| 1   | Q     | 421 | GLN  |
| 1   | Q     | 450 | ASN  |
| 1   | Q     | 476 | ASN  |
| 1   | Q     | 507 | GLN  |
| 1   | Q     | 509 | ASN  |
| 1   | Q     | 525 | ASN  |
| 1   | Q     | 631 | HIS  |
| 1   | R     | 219 | HIS  |
| 1   | R     | 245 | HIS  |
| 1   | R     | 261 | ASN  |
| 1   | R     | 332 | GLN  |
| 1   | R     | 421 | GLN  |
| 1   | R     | 450 | ASN  |
| 1   | R     | 476 | ASN  |
| 1   | R     | 507 | GLN  |
| 1   | R     | 509 | ASN  |
| 1   | R     | 525 | ASN  |
| 1   | R     | 535 | ASN  |
| 1   | R     | 573 | ASN  |
| 1   | R     | 631 | HIS  |
| 1   | R     | 679 | ASN  |
| 1   | S     | 219 | HIS  |
| 1   | S     | 245 | HIS  |
| 1   | S     | 261 | ASN  |
| 1   | S     | 332 | GLN  |
| 1   | S     | 421 | GLN  |
| 1   | S     | 450 | ASN  |
| 1   | S     | 476 | ASN  |
| 1   | S     | 507 | GLN  |
| 1   | S     | 509 | ASN  |
| 1   | S     | 525 | ASN  |
| 1   | S     | 535 | ASN  |
| 1   | S     | 631 | HIS  |
| 1   | T     | 219 | HIS  |
| 1   | T     | 245 | HIS  |
| 1   | T     | 261 | ASN  |
| 1   | T     | 332 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 421 | GLN  |
| 1   | T     | 476 | ASN  |
| 1   | T     | 507 | GLN  |
| 1   | T     | 509 | ASN  |
| 1   | T     | 525 | ASN  |
| 1   | T     | 535 | ASN  |
| 1   | T     | 631 | HIS  |
| 1   | U     | 219 | HIS  |
| 1   | U     | 245 | HIS  |
| 1   | U     | 261 | ASN  |
| 1   | U     | 332 | GLN  |
| 1   | U     | 421 | GLN  |
| 1   | U     | 450 | ASN  |
| 1   | U     | 476 | ASN  |
| 1   | U     | 507 | GLN  |
| 1   | U     | 509 | ASN  |
| 1   | U     | 525 | ASN  |
| 1   | U     | 631 | HIS  |
| 1   | V     | 219 | HIS  |
| 1   | V     | 245 | HIS  |
| 1   | V     | 261 | ASN  |
| 1   | V     | 332 | GLN  |
| 1   | V     | 421 | GLN  |
| 1   | V     | 450 | ASN  |
| 1   | V     | 476 | ASN  |
| 1   | V     | 507 | GLN  |
| 1   | V     | 509 | ASN  |
| 1   | V     | 525 | ASN  |
| 1   | V     | 535 | ASN  |
| 1   | V     | 631 | HIS  |
| 1   | W     | 219 | HIS  |
| 1   | W     | 245 | HIS  |
| 1   | W     | 261 | ASN  |
| 1   | W     | 332 | GLN  |
| 1   | W     | 421 | GLN  |
| 1   | W     | 450 | ASN  |
| 1   | W     | 476 | ASN  |
| 1   | W     | 507 | GLN  |
| 1   | W     | 509 | ASN  |
| 1   | W     | 525 | ASN  |
| 1   | W     | 535 | ASN  |
| 1   | W     | 631 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 219 | HIS  |
| 1   | X     | 245 | HIS  |
| 1   | X     | 261 | ASN  |
| 1   | X     | 332 | GLN  |
| 1   | X     | 421 | GLN  |
| 1   | X     | 476 | ASN  |
| 1   | X     | 507 | GLN  |
| 1   | X     | 509 | ASN  |
| 1   | X     | 525 | ASN  |
| 1   | X     | 535 | ASN  |
| 1   | X     | 631 | HIS  |
| 1   | Y     | 219 | HIS  |
| 1   | Y     | 245 | HIS  |
| 1   | Y     | 261 | ASN  |
| 1   | Y     | 332 | GLN  |
| 1   | Y     | 421 | GLN  |
| 1   | Y     | 476 | ASN  |
| 1   | Y     | 507 | GLN  |
| 1   | Y     | 509 | ASN  |
| 1   | Y     | 525 | ASN  |
| 1   | Y     | 535 | ASN  |
| 1   | Y     | 631 | HIS  |
| 1   | Z     | 219 | HIS  |
| 1   | Z     | 245 | HIS  |
| 1   | Z     | 261 | ASN  |
| 1   | Z     | 332 | GLN  |
| 1   | Z     | 421 | GLN  |
| 1   | Z     | 450 | ASN  |
| 1   | Z     | 476 | ASN  |
| 1   | Z     | 507 | GLN  |
| 1   | Z     | 509 | ASN  |
| 1   | Z     | 525 | ASN  |
| 1   | Z     | 535 | ASN  |
| 1   | Z     | 631 | HIS  |
| 1   | Z     | 679 | ASN  |
| 1   | a     | 219 | HIS  |
| 1   | a     | 245 | HIS  |
| 1   | a     | 261 | ASN  |
| 1   | a     | 332 | GLN  |
| 1   | a     | 421 | GLN  |
| 1   | a     | 450 | ASN  |
| 1   | a     | 476 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 507 | GLN  |
| 1   | a     | 509 | ASN  |
| 1   | a     | 525 | ASN  |
| 1   | a     | 535 | ASN  |
| 1   | a     | 631 | HIS  |
| 1   | a     | 679 | ASN  |
| 1   | b     | 219 | HIS  |
| 1   | b     | 245 | HIS  |
| 1   | b     | 261 | ASN  |
| 1   | b     | 332 | GLN  |
| 1   | b     | 421 | GLN  |
| 1   | b     | 450 | ASN  |
| 1   | b     | 476 | ASN  |
| 1   | b     | 507 | GLN  |
| 1   | b     | 509 | ASN  |
| 1   | b     | 525 | ASN  |
| 1   | b     | 535 | ASN  |
| 1   | b     | 631 | HIS  |
| 1   | b     | 679 | ASN  |
| 1   | c     | 219 | HIS  |
| 1   | c     | 245 | HIS  |
| 1   | c     | 261 | ASN  |
| 1   | c     | 332 | GLN  |
| 1   | c     | 421 | GLN  |
| 1   | c     | 476 | ASN  |
| 1   | c     | 507 | GLN  |
| 1   | c     | 509 | ASN  |
| 1   | c     | 525 | ASN  |
| 1   | c     | 535 | ASN  |
| 1   | c     | 631 | HIS  |
| 1   | d     | 219 | HIS  |
| 1   | d     | 245 | HIS  |
| 1   | d     | 261 | ASN  |
| 1   | d     | 332 | GLN  |
| 1   | d     | 421 | GLN  |
| 1   | d     | 450 | ASN  |
| 1   | d     | 476 | ASN  |
| 1   | d     | 507 | GLN  |
| 1   | d     | 509 | ASN  |
| 1   | d     | 525 | ASN  |
| 1   | d     | 530 | ASN  |
| 1   | d     | 535 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | d     | 631 | HIS  |
| 1   | e     | 219 | HIS  |
| 1   | e     | 245 | HIS  |
| 1   | e     | 261 | ASN  |
| 1   | e     | 332 | GLN  |
| 1   | e     | 421 | GLN  |
| 1   | e     | 450 | ASN  |
| 1   | e     | 476 | ASN  |
| 1   | e     | 507 | GLN  |
| 1   | e     | 509 | ASN  |
| 1   | e     | 525 | ASN  |
| 1   | e     | 535 | ASN  |
| 1   | e     | 631 | HIS  |
| 1   | f     | 219 | HIS  |
| 1   | f     | 245 | HIS  |
| 1   | f     | 261 | ASN  |
| 1   | f     | 332 | GLN  |
| 1   | f     | 421 | GLN  |
| 1   | f     | 450 | ASN  |
| 1   | f     | 476 | ASN  |
| 1   | f     | 507 | GLN  |
| 1   | f     | 509 | ASN  |
| 1   | f     | 525 | ASN  |
| 1   | f     | 535 | ASN  |
| 1   | f     | 631 | HIS  |
| 1   | g     | 219 | HIS  |
| 1   | g     | 245 | HIS  |
| 1   | g     | 261 | ASN  |
| 1   | g     | 332 | GLN  |
| 1   | g     | 421 | GLN  |
| 1   | g     | 450 | ASN  |
| 1   | g     | 476 | ASN  |
| 1   | g     | 507 | GLN  |
| 1   | g     | 509 | ASN  |
| 1   | g     | 525 | ASN  |
| 1   | g     | 535 | ASN  |
| 1   | g     | 573 | ASN  |
| 1   | g     | 631 | HIS  |
| 1   | h     | 219 | HIS  |
| 1   | h     | 245 | HIS  |
| 1   | h     | 261 | ASN  |
| 1   | h     | 332 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | h     | 421 | GLN  |
| 1   | h     | 476 | ASN  |
| 1   | h     | 507 | GLN  |
| 1   | h     | 509 | ASN  |
| 1   | h     | 525 | ASN  |
| 1   | h     | 535 | ASN  |
| 1   | h     | 631 | HIS  |
| 1   | i     | 219 | HIS  |
| 1   | i     | 245 | HIS  |
| 1   | i     | 261 | ASN  |
| 1   | i     | 332 | GLN  |
| 1   | i     | 421 | GLN  |
| 1   | i     | 450 | ASN  |
| 1   | i     | 476 | ASN  |
| 1   | i     | 507 | GLN  |
| 1   | i     | 509 | ASN  |
| 1   | i     | 525 | ASN  |
| 1   | i     | 530 | ASN  |
| 1   | i     | 535 | ASN  |
| 1   | i     | 546 | ASN  |
| 1   | i     | 631 | HIS  |
| 1   | j     | 219 | HIS  |
| 1   | j     | 245 | HIS  |
| 1   | j     | 261 | ASN  |
| 1   | j     | 332 | GLN  |
| 1   | j     | 421 | GLN  |
| 1   | j     | 476 | ASN  |
| 1   | j     | 507 | GLN  |
| 1   | j     | 509 | ASN  |
| 1   | j     | 525 | ASN  |
| 1   | j     | 535 | ASN  |
| 1   | j     | 631 | HIS  |
| 1   | k     | 219 | HIS  |
| 1   | k     | 245 | HIS  |
| 1   | k     | 261 | ASN  |
| 1   | k     | 332 | GLN  |
| 1   | k     | 421 | GLN  |
| 1   | k     | 476 | ASN  |
| 1   | k     | 507 | GLN  |
| 1   | k     | 509 | ASN  |
| 1   | k     | 525 | ASN  |
| 1   | k     | 535 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | k     | 631 | HIS  |
| 1   | l     | 219 | HIS  |
| 1   | l     | 245 | HIS  |
| 1   | l     | 261 | ASN  |
| 1   | l     | 332 | GLN  |
| 1   | l     | 421 | GLN  |
| 1   | l     | 450 | ASN  |
| 1   | l     | 476 | ASN  |
| 1   | l     | 507 | GLN  |
| 1   | l     | 509 | ASN  |
| 1   | l     | 525 | ASN  |
| 1   | l     | 530 | ASN  |
| 1   | l     | 535 | ASN  |
| 1   | l     | 546 | ASN  |
| 1   | l     | 631 | HIS  |
| 1   | m     | 219 | HIS  |
| 1   | m     | 245 | HIS  |
| 1   | m     | 261 | ASN  |
| 1   | m     | 332 | GLN  |
| 1   | m     | 421 | GLN  |
| 1   | m     | 450 | ASN  |
| 1   | m     | 476 | ASN  |
| 1   | m     | 507 | GLN  |
| 1   | m     | 509 | ASN  |
| 1   | m     | 525 | ASN  |
| 1   | m     | 535 | ASN  |
| 1   | m     | 631 | HIS  |
| 1   | n     | 219 | HIS  |
| 1   | n     | 245 | HIS  |
| 1   | n     | 261 | ASN  |
| 1   | n     | 332 | GLN  |
| 1   | n     | 421 | GLN  |
| 1   | n     | 476 | ASN  |
| 1   | n     | 507 | GLN  |
| 1   | n     | 509 | ASN  |
| 1   | n     | 525 | ASN  |
| 1   | n     | 530 | ASN  |
| 1   | n     | 535 | ASN  |
| 1   | n     | 631 | HIS  |
| 1   | o     | 219 | HIS  |
| 1   | o     | 245 | HIS  |
| 1   | o     | 261 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | o     | 332 | GLN  |
| 1   | o     | 421 | GLN  |
| 1   | o     | 450 | ASN  |
| 1   | o     | 476 | ASN  |
| 1   | o     | 507 | GLN  |
| 1   | o     | 509 | ASN  |
| 1   | o     | 525 | ASN  |
| 1   | o     | 535 | ASN  |
| 1   | o     | 631 | HIS  |
| 1   | p     | 219 | HIS  |
| 1   | p     | 245 | HIS  |
| 1   | p     | 261 | ASN  |
| 1   | p     | 332 | GLN  |
| 1   | p     | 421 | GLN  |
| 1   | p     | 450 | ASN  |
| 1   | p     | 476 | ASN  |
| 1   | p     | 507 | GLN  |
| 1   | p     | 509 | ASN  |
| 1   | p     | 525 | ASN  |
| 1   | p     | 535 | ASN  |
| 1   | p     | 631 | HIS  |
| 1   | q     | 219 | HIS  |
| 1   | q     | 245 | HIS  |
| 1   | q     | 261 | ASN  |
| 1   | q     | 332 | GLN  |
| 1   | q     | 421 | GLN  |
| 1   | q     | 450 | ASN  |
| 1   | q     | 476 | ASN  |
| 1   | q     | 507 | GLN  |
| 1   | q     | 509 | ASN  |
| 1   | q     | 525 | ASN  |
| 1   | q     | 535 | ASN  |
| 1   | q     | 546 | ASN  |
| 1   | q     | 573 | ASN  |
| 1   | q     | 631 | HIS  |
| 1   | r     | 219 | HIS  |
| 1   | r     | 245 | HIS  |
| 1   | r     | 261 | ASN  |
| 1   | r     | 332 | GLN  |
| 1   | r     | 421 | GLN  |
| 1   | r     | 476 | ASN  |
| 1   | r     | 507 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | r     | 509 | ASN  |
| 1   | r     | 525 | ASN  |
| 1   | r     | 535 | ASN  |
| 1   | r     | 573 | ASN  |
| 1   | r     | 631 | HIS  |
| 1   | s     | 219 | HIS  |
| 1   | s     | 245 | HIS  |
| 1   | s     | 261 | ASN  |
| 1   | s     | 332 | GLN  |
| 1   | s     | 421 | GLN  |
| 1   | s     | 450 | ASN  |
| 1   | s     | 476 | ASN  |
| 1   | s     | 507 | GLN  |
| 1   | s     | 509 | ASN  |
| 1   | s     | 525 | ASN  |
| 1   | s     | 535 | ASN  |
| 1   | s     | 631 | HIS  |
| 1   | t     | 219 | HIS  |
| 1   | t     | 245 | HIS  |
| 1   | t     | 261 | ASN  |
| 1   | t     | 332 | GLN  |
| 1   | t     | 421 | GLN  |
| 1   | t     | 476 | ASN  |
| 1   | t     | 507 | GLN  |
| 1   | t     | 509 | ASN  |
| 1   | t     | 525 | ASN  |
| 1   | t     | 535 | ASN  |
| 1   | t     | 631 | HIS  |
| 1   | u     | 219 | HIS  |
| 1   | u     | 245 | HIS  |
| 1   | u     | 261 | ASN  |
| 1   | u     | 332 | GLN  |
| 1   | u     | 421 | GLN  |
| 1   | u     | 476 | ASN  |
| 1   | u     | 507 | GLN  |
| 1   | u     | 509 | ASN  |
| 1   | u     | 525 | ASN  |
| 1   | u     | 535 | ASN  |
| 1   | u     | 631 | HIS  |
| 1   | v     | 219 | HIS  |
| 1   | v     | 245 | HIS  |
| 1   | v     | 261 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | v     | 332 | GLN  |
| 1   | v     | 421 | GLN  |
| 1   | v     | 450 | ASN  |
| 1   | v     | 476 | ASN  |
| 1   | v     | 507 | GLN  |
| 1   | v     | 509 | ASN  |
| 1   | v     | 525 | ASN  |
| 1   | v     | 631 | HIS  |
| 1   | w     | 219 | HIS  |
| 1   | w     | 245 | HIS  |
| 1   | w     | 261 | ASN  |
| 1   | w     | 332 | GLN  |
| 1   | w     | 421 | GLN  |
| 1   | w     | 450 | ASN  |
| 1   | w     | 476 | ASN  |
| 1   | w     | 507 | GLN  |
| 1   | w     | 509 | ASN  |
| 1   | w     | 525 | ASN  |
| 1   | w     | 535 | ASN  |
| 1   | w     | 631 | HIS  |
| 1   | x     | 219 | HIS  |
| 1   | x     | 245 | HIS  |
| 1   | x     | 261 | ASN  |
| 1   | x     | 332 | GLN  |
| 1   | x     | 421 | GLN  |
| 1   | x     | 450 | ASN  |
| 1   | x     | 476 | ASN  |
| 1   | x     | 507 | GLN  |
| 1   | x     | 509 | ASN  |
| 1   | x     | 525 | ASN  |
| 1   | x     | 535 | ASN  |
| 1   | x     | 631 | HIS  |
| 1   | y     | 219 | HIS  |
| 1   | y     | 245 | HIS  |
| 1   | y     | 261 | ASN  |
| 1   | y     | 332 | GLN  |
| 1   | y     | 421 | GLN  |
| 1   | y     | 450 | ASN  |
| 1   | y     | 476 | ASN  |
| 1   | y     | 507 | GLN  |
| 1   | y     | 509 | ASN  |
| 1   | y     | 525 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | y     | 535 | ASN  |
| 1   | y     | 573 | ASN  |
| 1   | y     | 631 | HIS  |
| 1   | y     | 679 | ASN  |
| 1   | z     | 219 | HIS  |
| 1   | z     | 245 | HIS  |
| 1   | z     | 261 | ASN  |
| 1   | z     | 332 | GLN  |
| 1   | z     | 421 | GLN  |
| 1   | z     | 476 | ASN  |
| 1   | z     | 507 | GLN  |
| 1   | z     | 509 | ASN  |
| 1   | z     | 525 | ASN  |
| 1   | z     | 535 | ASN  |
| 1   | z     | 631 | HIS  |
| 1   | 1     | 219 | HIS  |
| 1   | 1     | 245 | HIS  |
| 1   | 1     | 261 | ASN  |
| 1   | 1     | 332 | GLN  |
| 1   | 1     | 421 | GLN  |
| 1   | 1     | 476 | ASN  |
| 1   | 1     | 507 | GLN  |
| 1   | 1     | 509 | ASN  |
| 1   | 1     | 525 | ASN  |
| 1   | 1     | 535 | ASN  |
| 1   | 1     | 546 | ASN  |
| 1   | 1     | 631 | HIS  |
| 1   | 2     | 219 | HIS  |
| 1   | 2     | 245 | HIS  |
| 1   | 2     | 261 | ASN  |
| 1   | 2     | 332 | GLN  |
| 1   | 2     | 421 | GLN  |
| 1   | 2     | 476 | ASN  |
| 1   | 2     | 507 | GLN  |
| 1   | 2     | 509 | ASN  |
| 1   | 2     | 525 | ASN  |
| 1   | 2     | 535 | ASN  |
| 1   | 2     | 573 | ASN  |
| 1   | 2     | 631 | HIS  |
| 1   | 3     | 219 | HIS  |
| 1   | 3     | 245 | HIS  |
| 1   | 3     | 261 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3     | 332 | GLN  |
| 1   | 3     | 421 | GLN  |
| 1   | 3     | 450 | ASN  |
| 1   | 3     | 476 | ASN  |
| 1   | 3     | 507 | GLN  |
| 1   | 3     | 509 | ASN  |
| 1   | 3     | 525 | ASN  |
| 1   | 3     | 530 | ASN  |
| 1   | 3     | 535 | ASN  |
| 1   | 3     | 631 | HIS  |
| 1   | 4     | 219 | HIS  |
| 1   | 4     | 245 | HIS  |
| 1   | 4     | 261 | ASN  |
| 1   | 4     | 332 | GLN  |
| 1   | 4     | 421 | GLN  |
| 1   | 4     | 476 | ASN  |
| 1   | 4     | 507 | GLN  |
| 1   | 4     | 509 | ASN  |
| 1   | 4     | 525 | ASN  |
| 1   | 4     | 535 | ASN  |
| 1   | 4     | 631 | HIS  |
| 1   | 5     | 219 | HIS  |
| 1   | 5     | 245 | HIS  |
| 1   | 5     | 261 | ASN  |
| 1   | 5     | 332 | GLN  |
| 1   | 5     | 421 | GLN  |
| 1   | 5     | 476 | ASN  |
| 1   | 5     | 507 | GLN  |
| 1   | 5     | 509 | ASN  |
| 1   | 5     | 525 | ASN  |
| 1   | 5     | 535 | ASN  |
| 1   | 5     | 631 | HIS  |
| 1   | 5     | 679 | ASN  |
| 1   | 6     | 219 | HIS  |
| 1   | 6     | 245 | HIS  |
| 1   | 6     | 261 | ASN  |
| 1   | 6     | 332 | GLN  |
| 1   | 6     | 421 | GLN  |
| 1   | 6     | 476 | ASN  |
| 1   | 6     | 507 | GLN  |
| 1   | 6     | 509 | ASN  |
| 1   | 6     | 525 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 535 | ASN  |
| 1   | 6     | 631 | HIS  |
| 1   | 7     | 219 | HIS  |
| 1   | 7     | 245 | HIS  |
| 1   | 7     | 261 | ASN  |
| 1   | 7     | 332 | GLN  |
| 1   | 7     | 421 | GLN  |
| 1   | 7     | 476 | ASN  |
| 1   | 7     | 507 | GLN  |
| 1   | 7     | 509 | ASN  |
| 1   | 7     | 525 | ASN  |
| 1   | 7     | 535 | ASN  |
| 1   | 7     | 631 | HIS  |
| 1   | 8     | 219 | HIS  |
| 1   | 8     | 245 | HIS  |
| 1   | 8     | 261 | ASN  |
| 1   | 8     | 332 | GLN  |
| 1   | 8     | 421 | GLN  |
| 1   | 8     | 450 | ASN  |
| 1   | 8     | 476 | ASN  |
| 1   | 8     | 507 | GLN  |
| 1   | 8     | 509 | ASN  |
| 1   | 8     | 525 | ASN  |
| 1   | 8     | 535 | ASN  |
| 1   | 8     | 631 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

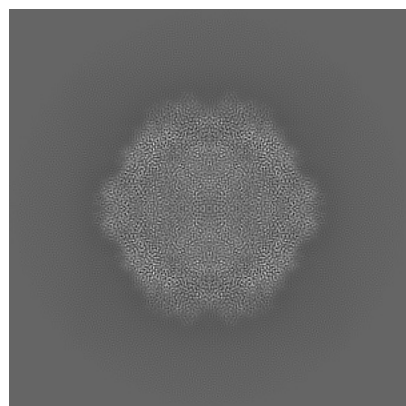
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46748. These allow visual inspection of the internal detail of the map and identification of artifacts.

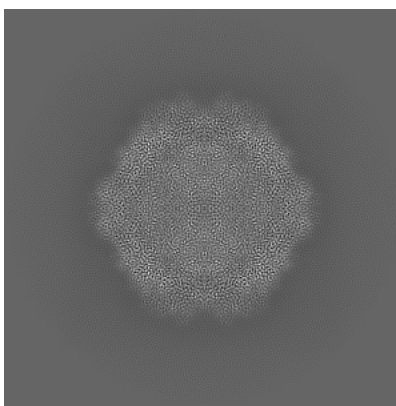
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

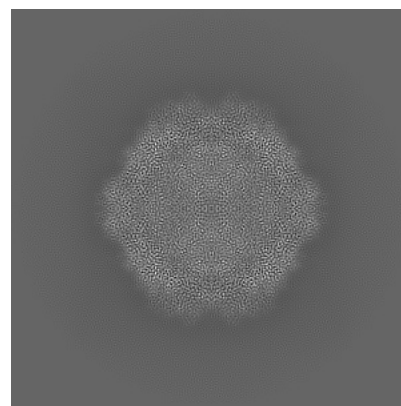
#### 6.1.1 Primary map



X

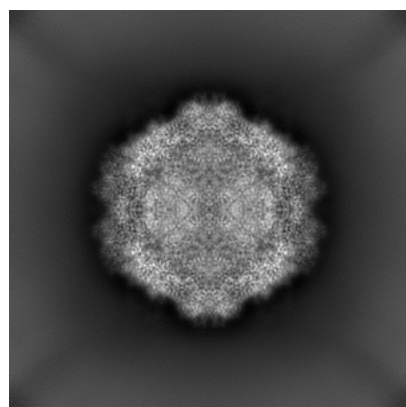


Y

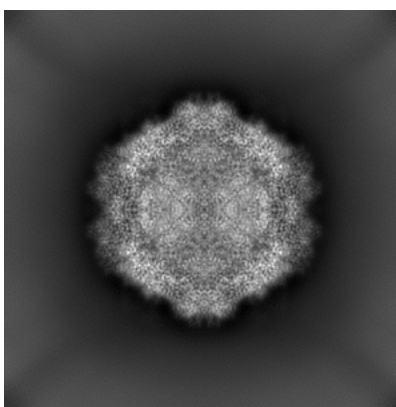


Z

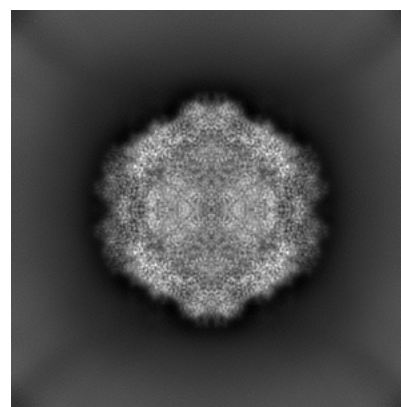
#### 6.1.2 Raw map



X



Y

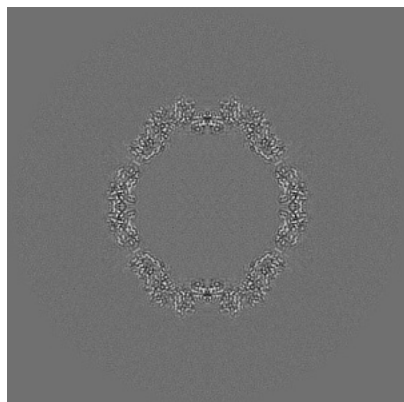


Z

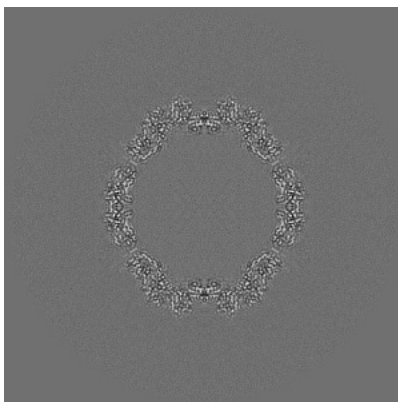
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

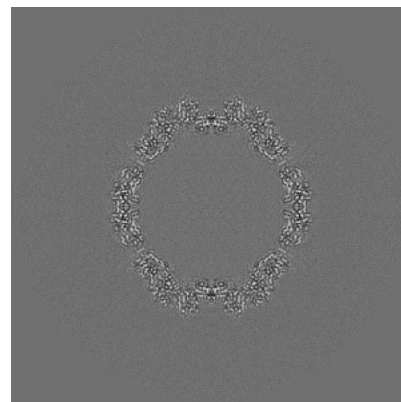
### 6.2.1 Primary map



X Index: 250

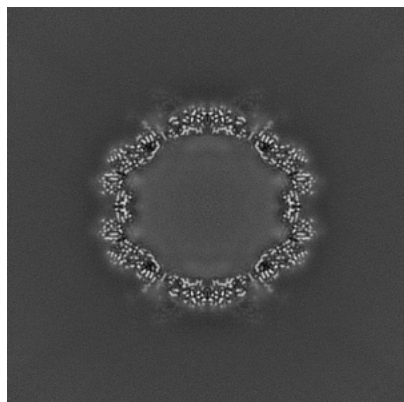


Y Index: 250

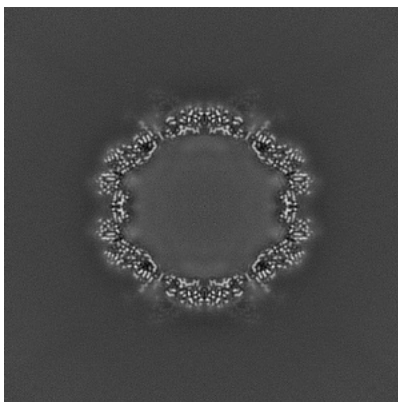


Z Index: 250

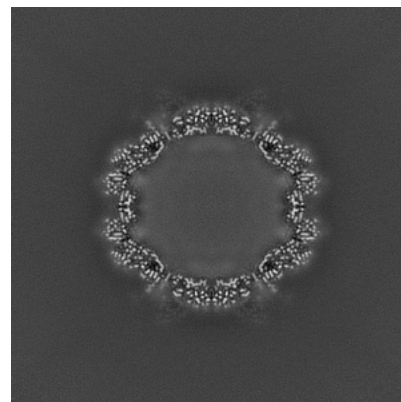
### 6.2.2 Raw map



X Index: 250



Y Index: 250

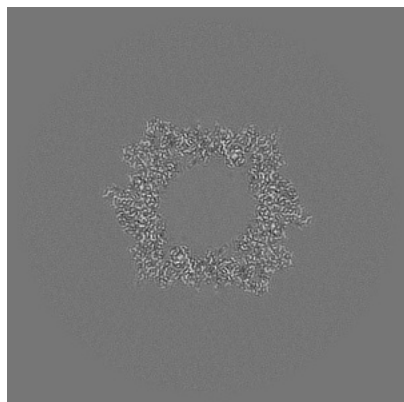


Z Index: 250

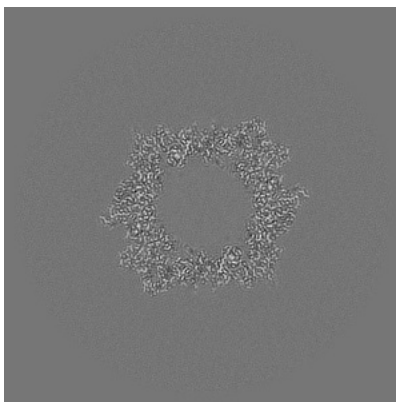
The images above show central slices of the map in three orthogonal directions.

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

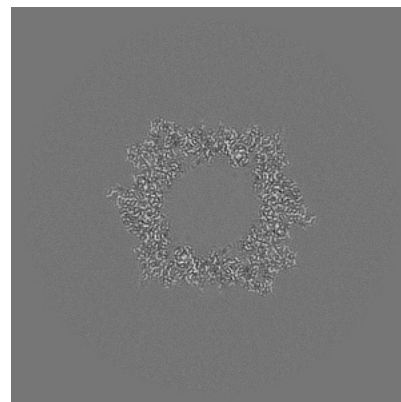
### 6.3.1 Primary map



X Index: 320

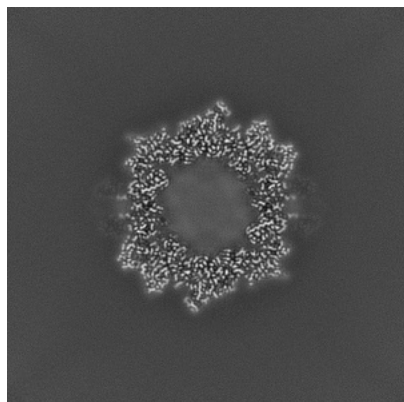


Y Index: 180

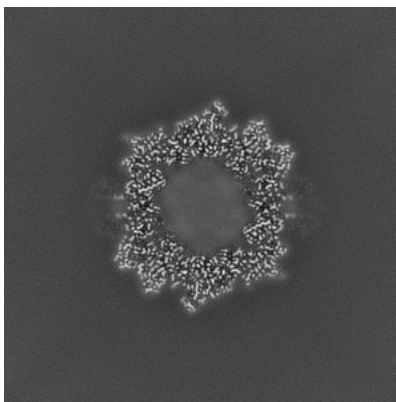


Z Index: 320

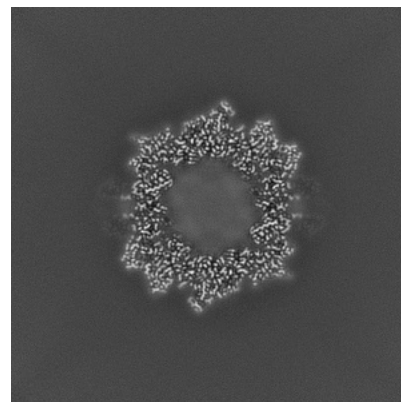
### 6.3.2 Raw map



X Index: 320



Y Index: 320

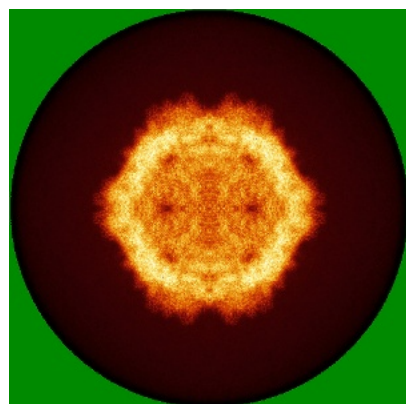


Z Index: 320

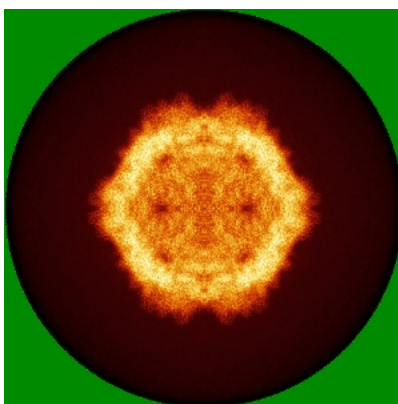
The images above show the largest variance slices of the map in three orthogonal directions.

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

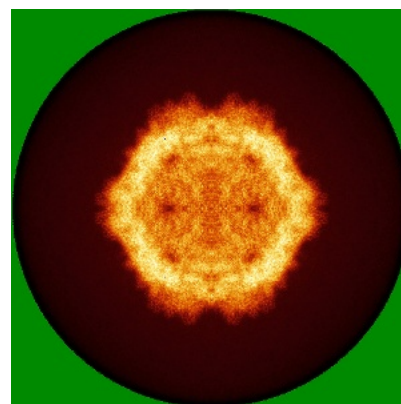
### 6.4.1 Primary map



X

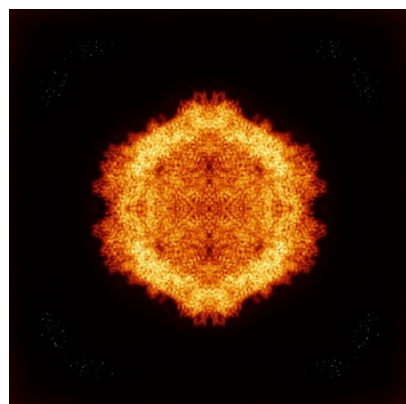


Y

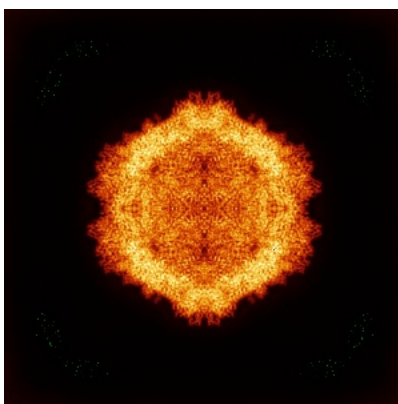


Z

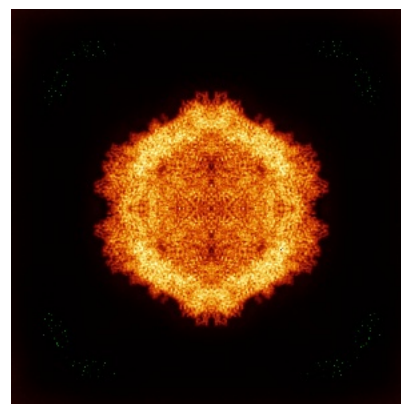
### 6.4.2 Raw map



X



Y

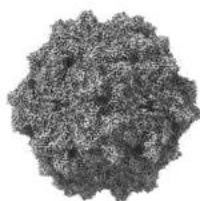


Z

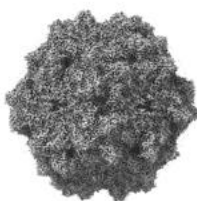
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

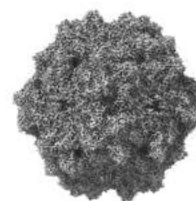
### 6.5.1 Primary map



X



Y



Z

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

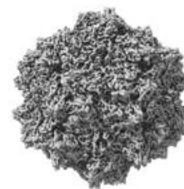
### 6.5.2 Raw map



X



Y



Z

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

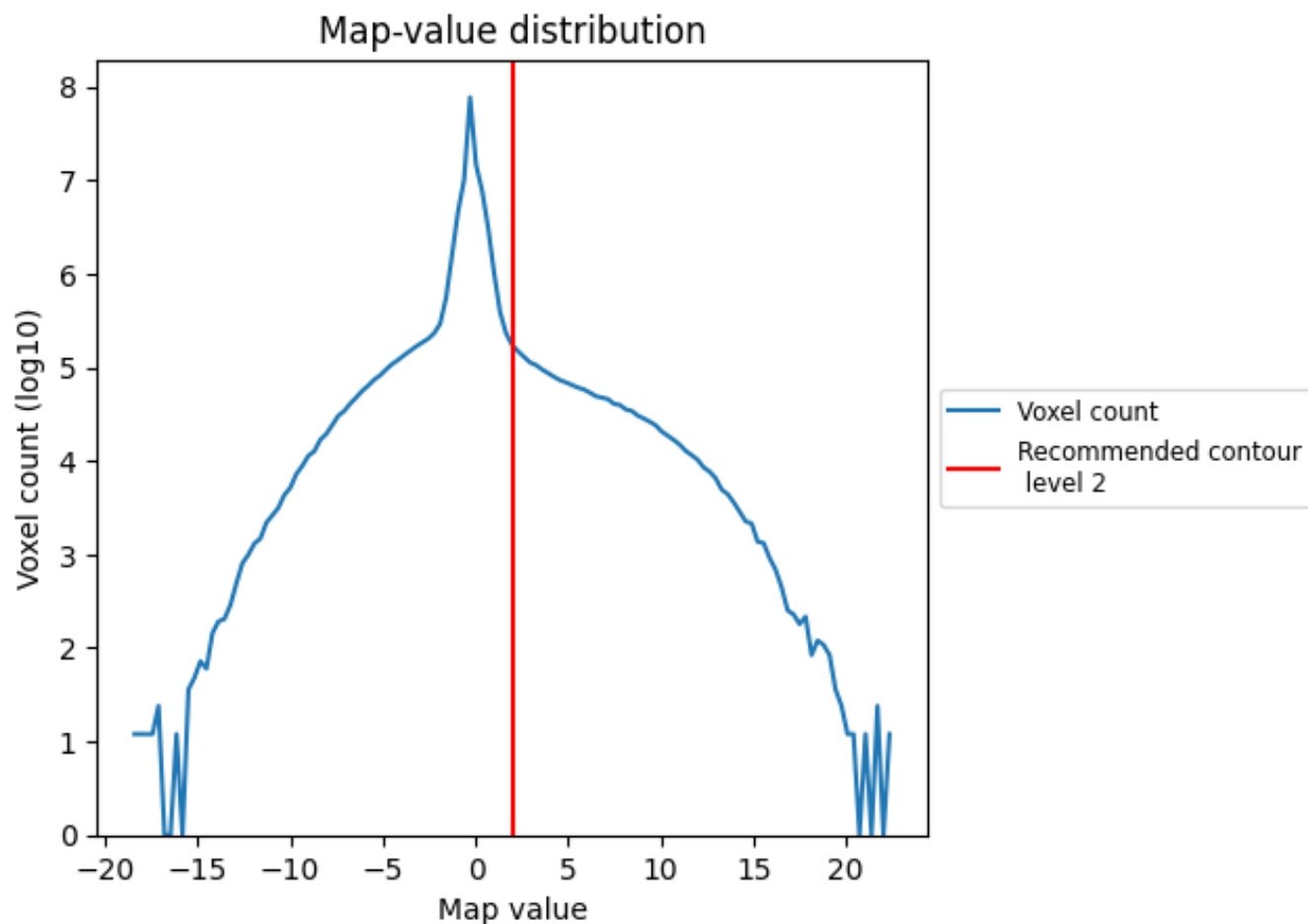
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

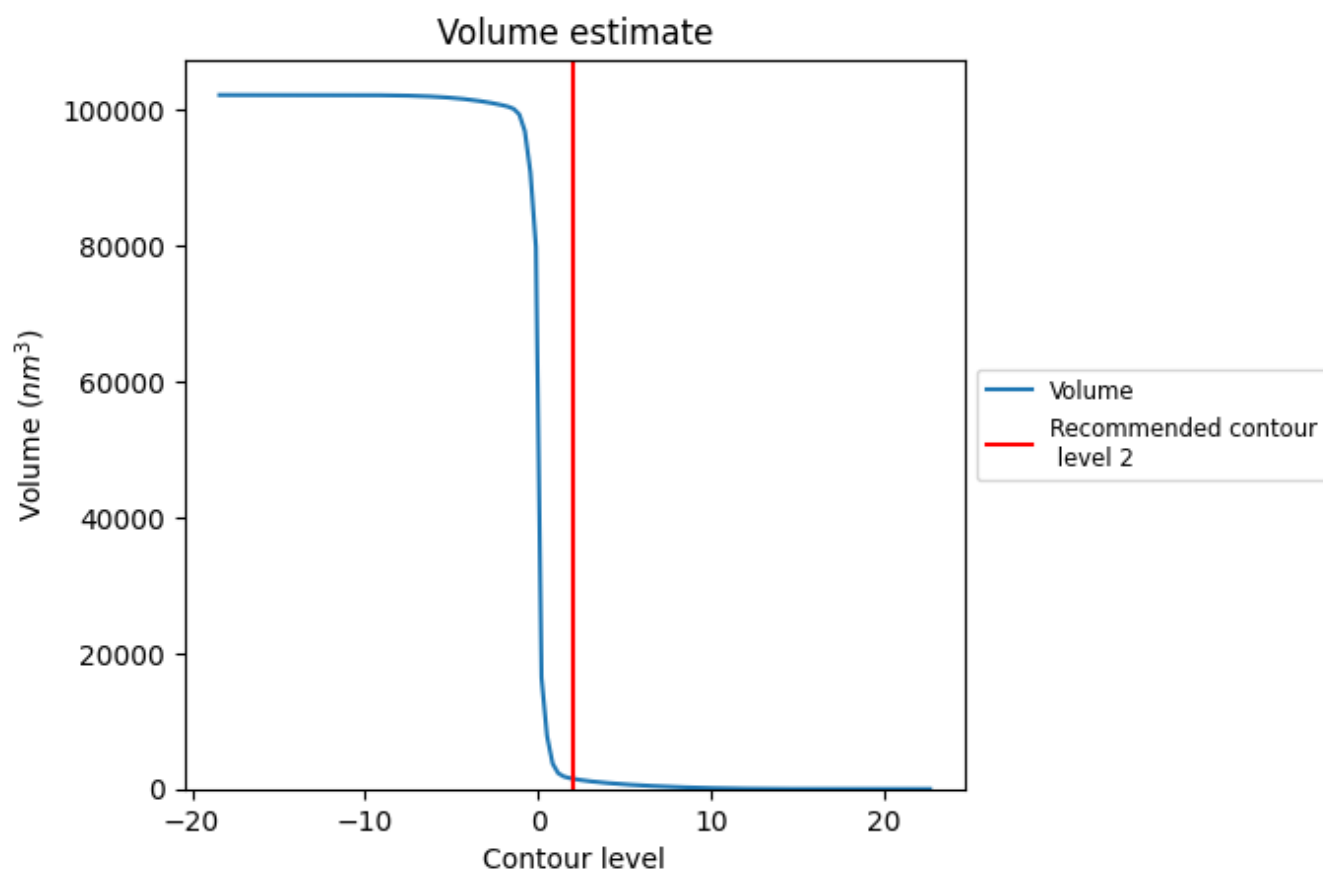
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

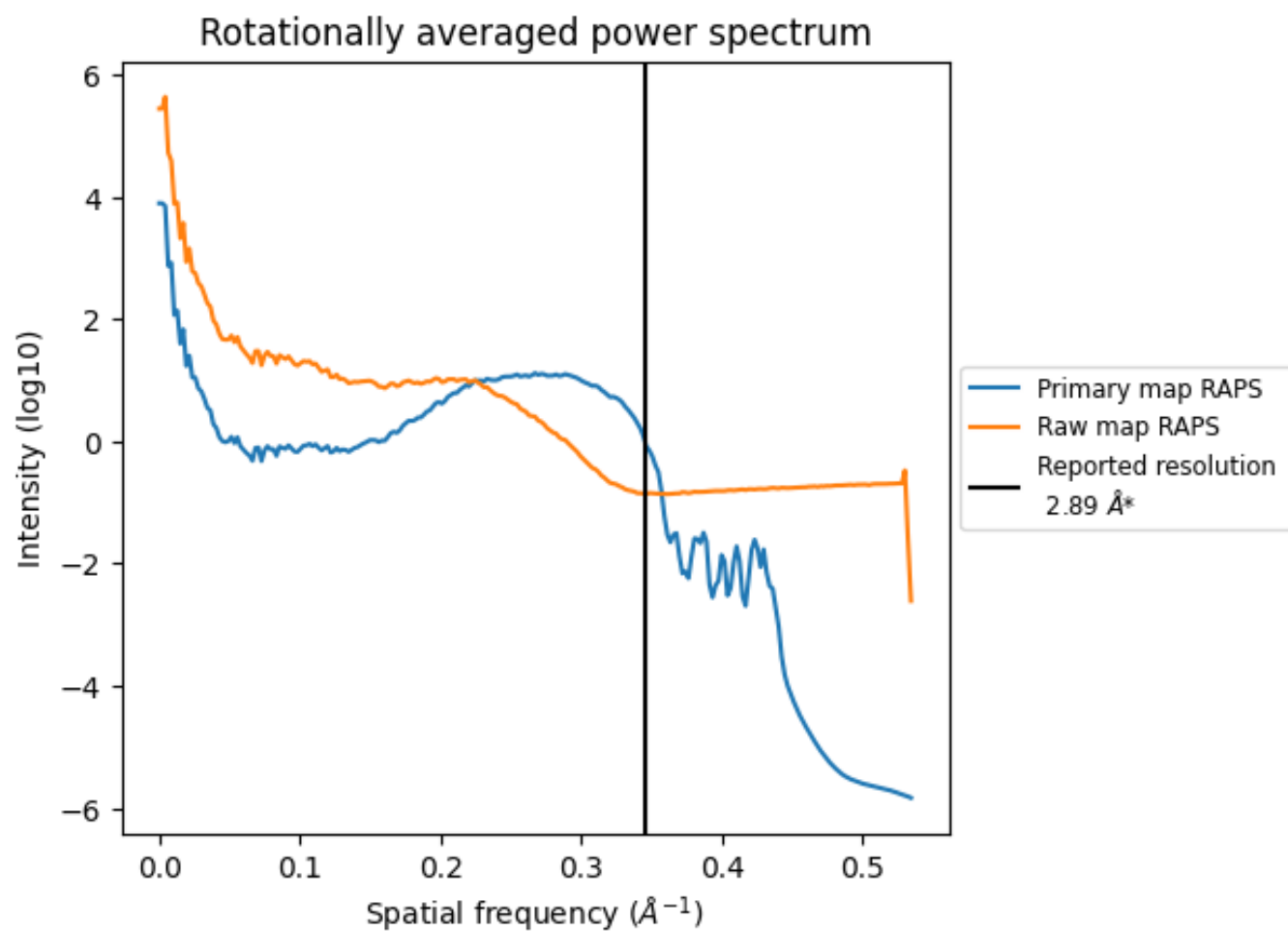


The volume at the recommended contour level is 1513  $\text{nm}^3$ ; this corresponds to an approximate mass of 1367 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

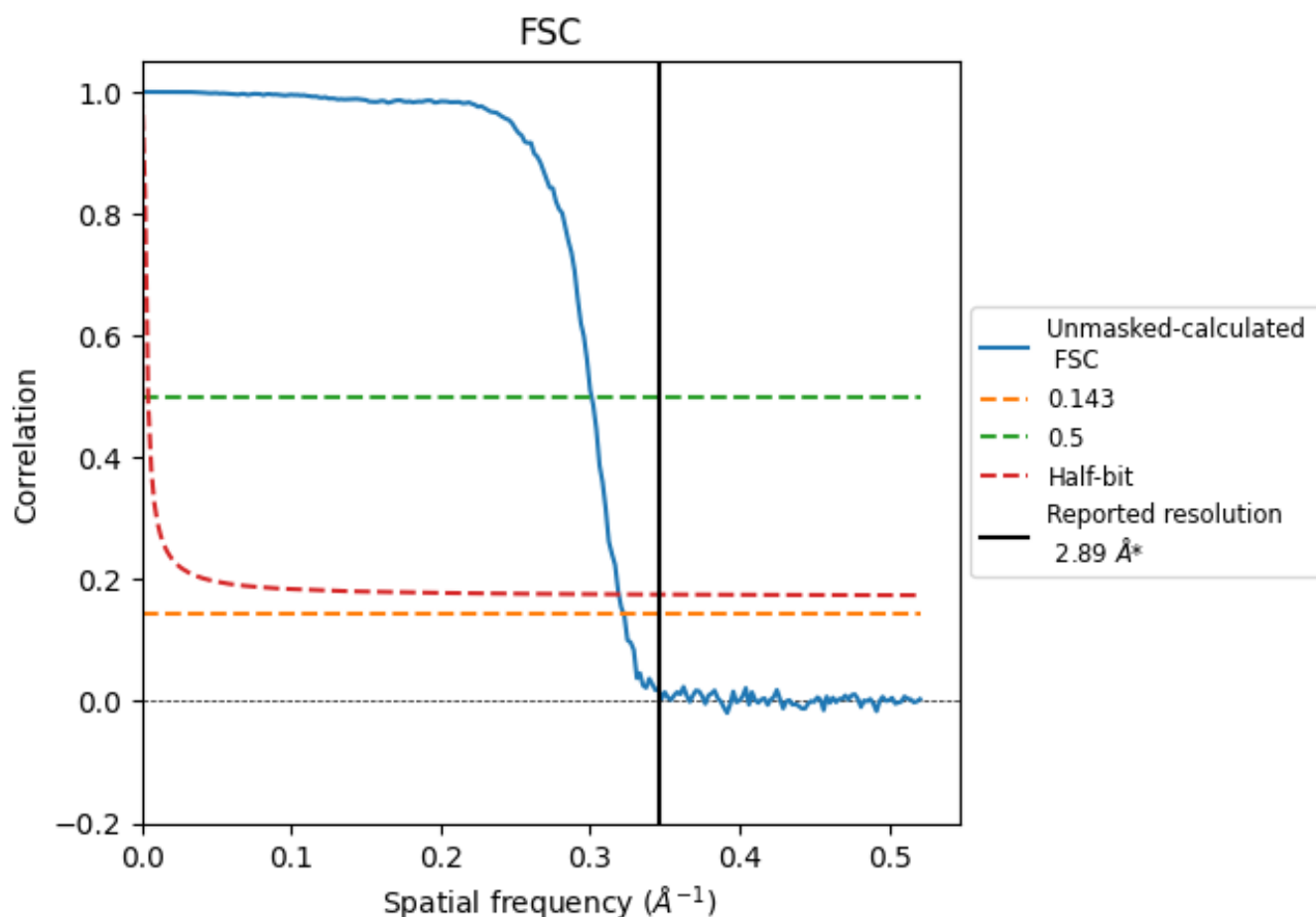


\*Reported resolution corresponds to spatial frequency of 0.346  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.346  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

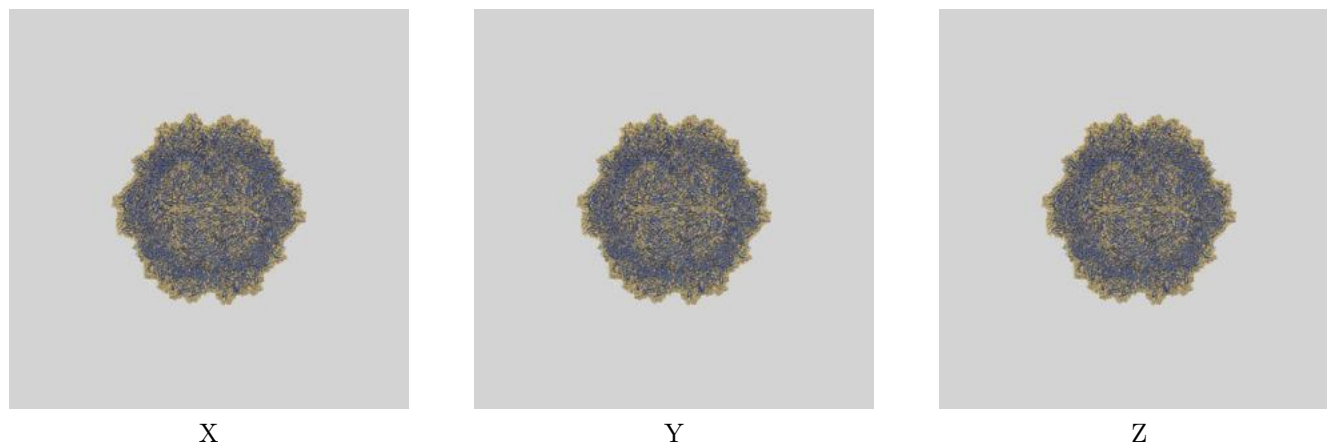
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.89                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.10                               | 3.32 | 3.13     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

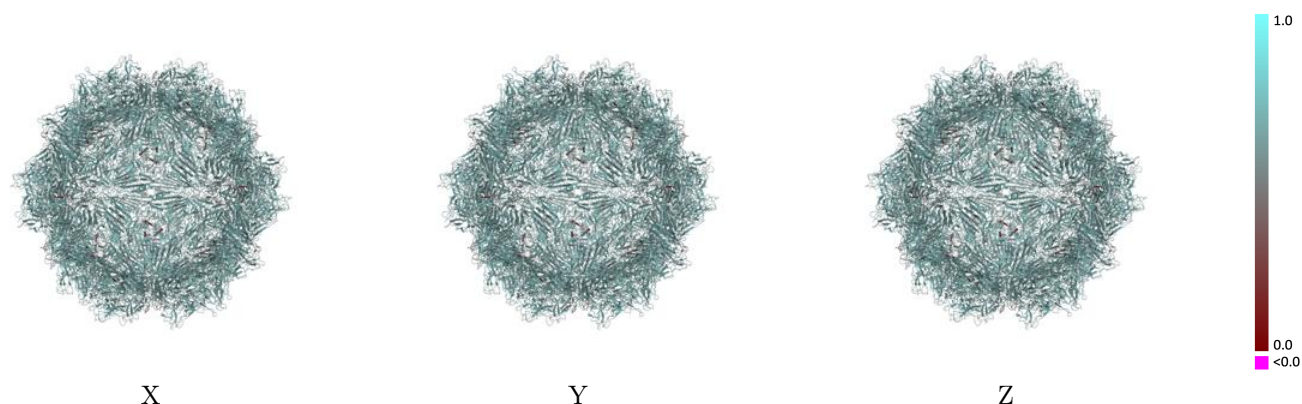
This section contains information regarding the fit between EMDB map EMD-46748 and PDB model 9DCB. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



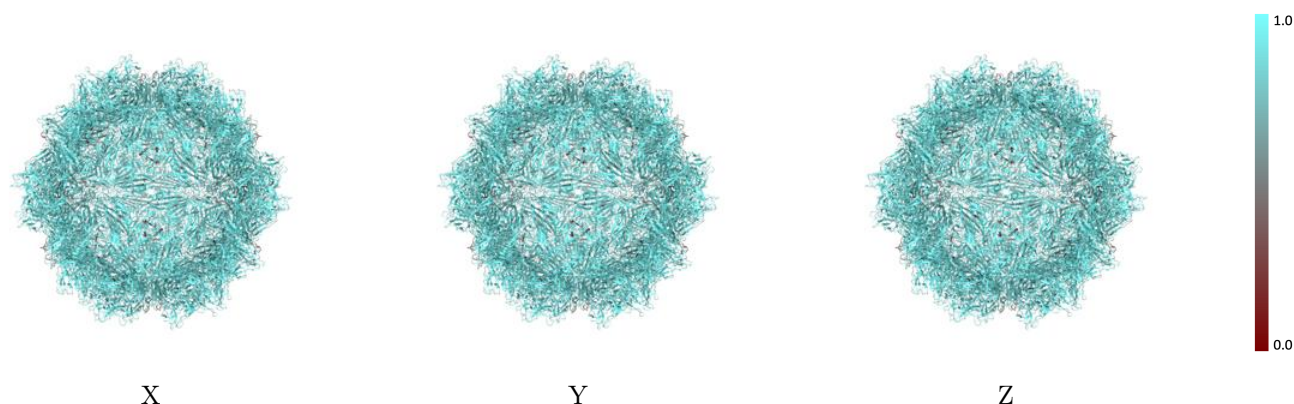
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



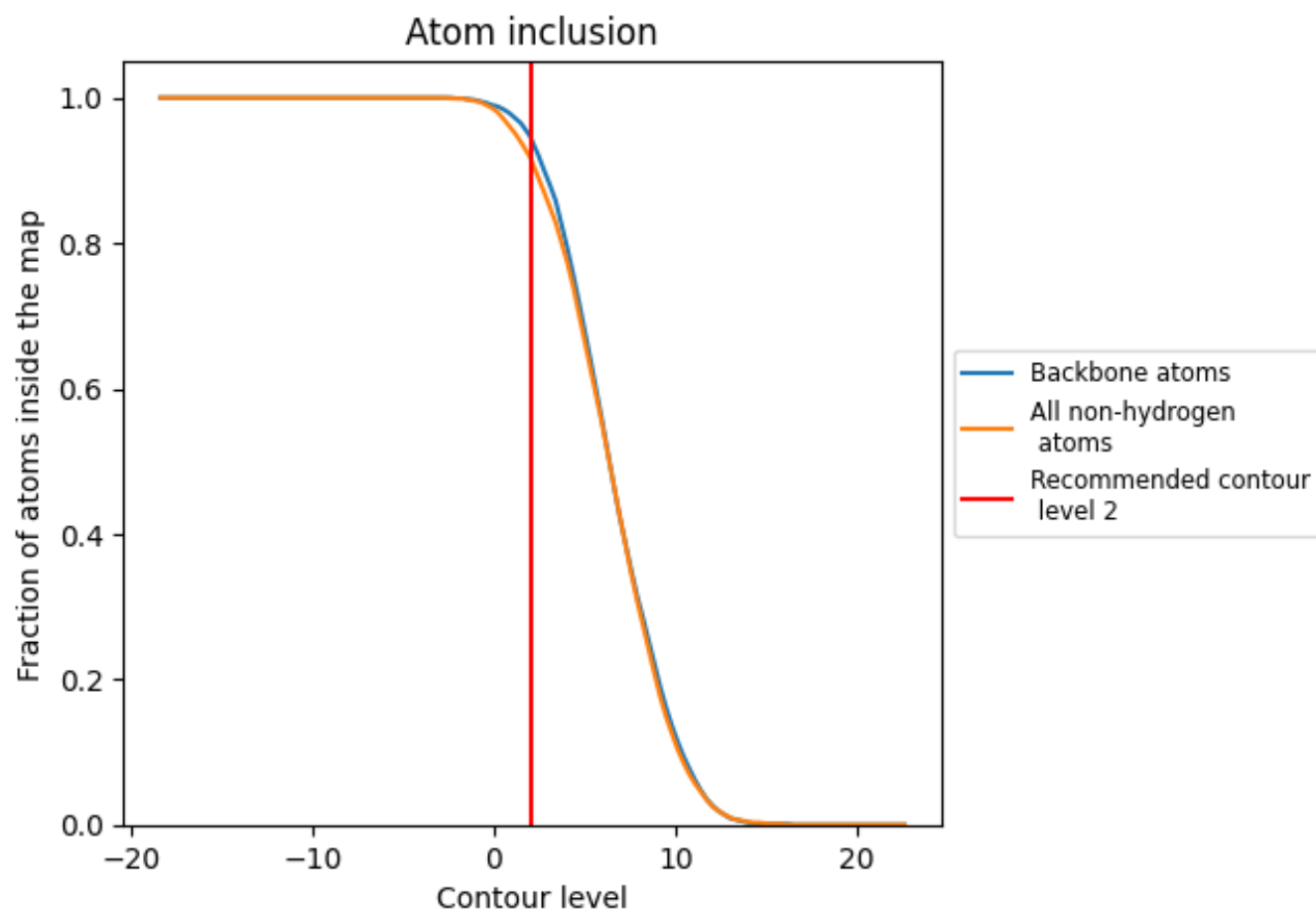
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































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

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9180   |  0.6230   |
| 0     |  0.3330   |  0.1870   |
| 0A    |  0.3330   |  0.1970   |
| 1     |  0.9240   |  0.6270   |
| 1A    |  0.3330   |  0.1980   |
| 2     |  0.9250   |  0.6280   |
| 2A    |  0.3330   |  0.1860   |
| 3     |  0.9230   |  0.6270   |
| 3A    |  0.3330   |  0.1900   |
| 4     |  0.9230   |  0.6270   |
| 4A    |  0.3330   |  0.1840   |
| 5     |  0.9230   |  0.6280   |
| 5A    |  0.3330   |  0.1800   |
| 6     |  0.9230   |  0.6270   |
| 7     |  0.9230  |  0.6280  |
| 8     |  0.9230 |  0.6270 |
| 9     |  0.3090 |  0.1940 |
| A     |  0.9230 |  0.6270 |
| AA    |  0.3090 |  0.1810 |
| B     |  0.9230 |  0.6270 |
| BA    |  0.3090 |  0.1790 |
| C     |  0.9230 |  0.6280 |
| CA    |  0.3330 |  0.1730 |
| D     |  0.9250 |  0.6270 |
| DA    |  0.3330 |  0.1880 |
| E     |  0.9240 |  0.6270 |
| EA    |  0.3330 |  0.1720 |
| F     |  0.9230 |  0.6270 |
| FA    |  0.3090 |  0.1930 |
| G     |  0.9230 |  0.6270 |
| GA    |  0.3090 |  0.1820 |
| H     |  0.9230 |  0.6280 |
| HA    |  0.3330 |  0.1790 |
| I     |  0.9230 |  0.6270 |
| IA    |  0.3330 |  0.1770 |



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

































































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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| J     |  0.9240   |  0.6270   |
| JA    |  0.3330   |  0.1900   |
| K     |  0.9240   |  0.6280   |
| KA    |  0.3090   |  0.1750   |
| L     |  0.9250   |  0.6270   |
| LA    |  0.3330   |  0.1830   |
| M     |  0.9230   |  0.6270   |
| MA    |  0.3090   |  0.1880   |
| N     |  0.9230   |  0.6270   |
| NA    |  0.3090   |  0.1900   |
| O     |  0.9230   |  0.6280   |
| OA    |  0.3090   |  0.1910   |
| P     |  0.9240   |  0.6270   |
| PA    |  0.3090   |  0.1930   |
| Q     |  0.9250   |  0.6270   |
| QA    |  0.3330   |  0.1820   |
| R     |  0.9230   |  0.6270   |
| RA    |  0.3090  |  0.1800  |
| S     |  0.9230 |  0.6270 |
| SA    |  0.3330 |  0.1940 |
| T     |  0.9250 |  0.6270 |
| TA    |  0.3090 |  0.1750 |
| U     |  0.9230 |  0.6280 |
| UA    |  0.3330 |  0.1850 |
| V     |  0.9240 |  0.6280 |
| VA    |  0.3330 |  0.1920 |
| W     |  0.9240 |  0.6270 |
| WA    |  0.3330 |  0.1970 |
| X     |  0.9240 |  0.6280 |
| XA    |  0.3330 |  0.1900 |
| Y     |  0.9240 |  0.6270 |
| YA    |  0.3330 |  0.1730 |
| Z     |  0.9230 |  0.6270 |
| ZA    |  0.3330 |  0.1850 |
| a     |  0.9250 |  0.6270 |
| aA    |  0.3090 |  0.1970 |
| b     |  0.9230 |  0.6270 |
| bA    |  0.3090 |  0.1830 |
| c     |  0.9240 |  0.6280 |
| cA    |  0.3330 |  0.1930 |
| d     |  0.9230 |  0.6270 |
| dA    |  0.3090 |  0.1830 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| e     |  0.9230   |  0.6270   |
| eA    |  0.3330   |  0.1910   |
| f     |  0.9230   |  0.6280   |
| fA    |  0.3090   |  0.1830   |
| g     |  0.9230   |  0.6270   |
| gA    |  0.3330   |  0.1880   |
| h     |  0.9230   |  0.6270   |
| hA    |  0.3330   |  0.1950   |
| i     |  0.9240   |  0.6280   |
| iA    |  0.3090   |  0.1890   |
| j     |  0.9250   |  0.6270   |
| jA    |  0.3090   |  0.1820   |
| k     |  0.9230   |  0.6270   |
| kA    |  0.3330   |  0.2000   |
| l     |  0.9240   |  0.6280   |
| lA    |  0.3090   |  0.1900   |
| m     |  0.9230   |  0.6280   |
| mA    |  0.3330   |  0.1950   |
| n     |  0.9230  |  0.6270  |
| nA    |  0.3090 |  0.1880 |
| o     |  0.9230 |  0.6280 |
| oA    |  0.3090 |  0.1810 |
| p     |  0.9240 |  0.6270 |
| pA    |  0.3330 |  0.1870 |
| q     |  0.9240 |  0.6280 |
| qA    |  0.3090 |  0.1820 |
| r     |  0.9230 |  0.6270 |
| rA    |  0.3330 |  0.1910 |
| s     |  0.9230 |  0.6280 |
| sA    |  0.3330 |  0.1790 |
| t     |  0.9230 |  0.6270 |
| tA    |  0.3330 |  0.1950 |
| u     |  0.9240 |  0.6270 |
| uA    |  0.3090 |  0.2040 |
| v     |  0.9250 |  0.6260 |
| vA    |  0.3090 |  0.1830 |
| w     |  0.9230 |  0.6270 |
| wA    |  0.3330 |  0.1840 |
| x     |  0.9240 |  0.6270 |
| xA    |  0.3330 |  0.1820 |
| y     |  0.9230 |  0.6270 |
| yA    |  0.3330 |  0.1790 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| z     |  0.9230 |  0.6270 |
| zA    |  0.3330 |  0.1810 |