



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 03:33 PM UTC

PDB ID : 7YFZ / pdb\_00007yfh  
EMDB ID : EMD-33802  
Title : Cyanophage Pam3 baseplate proteins  
Authors : Yang, F.; Jiang, Y.L.; Zhou, C.Z.  
Deposited on : 2022-07-09  
Resolution : 3.19 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

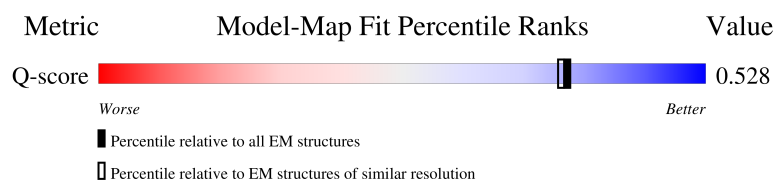
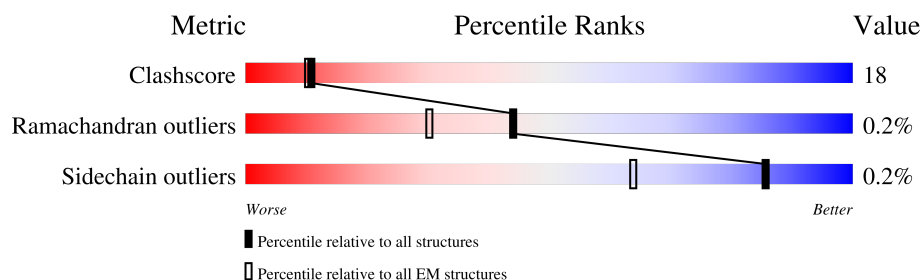
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.19 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.



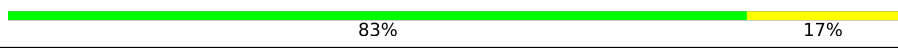
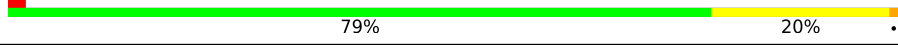
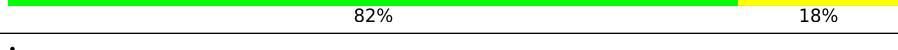
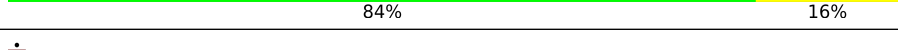
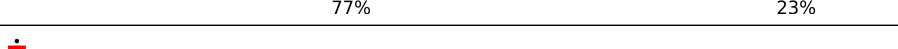
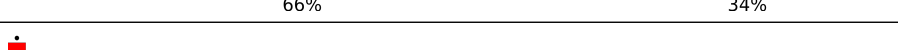
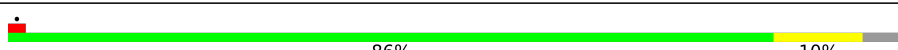
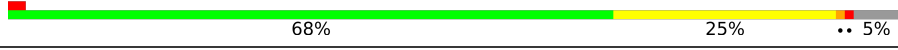
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14455 ( 2.69 - 3.69 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 299    | <br>87% 12%      |
| 1   | B     | 299    | <br>75% 25%      |
| 1   | E     | 299    | <br>76% 24%      |
| 1   | F     | 299    | <br>82% 18%      |

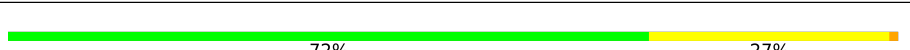
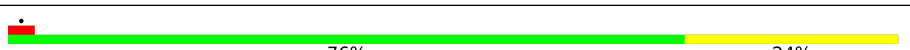
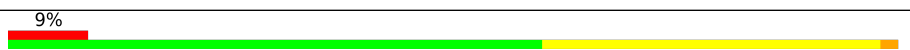
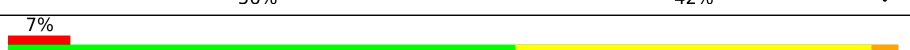
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | H     | 299    |    |
| 1   | I     | 299    |    |
| 1   | K     | 299    |    |
| 1   | L     | 299    |    |
| 1   | O     | 299    |    |
| 1   | P     | 299    |    |
| 1   | Q     | 299    |    |
| 1   | R     | 299    |    |
| 2   | C     | 238    |    |
| 2   | D     | 238    |    |
| 2   | G     | 238    |    |
| 2   | J     | 238    |  |
| 2   | M     | 238    |  |
| 2   | S     | 238    |  |
| 3   | X     | 125    |  |
| 3   | n     | 125    |  |
| 3   | o     | 125    |  |
| 3   | p     | 125    |  |
| 3   | q     | 125    |  |
| 3   | r     | 125    |  |
| 4   | a     | 191    |  |
| 4   | b     | 191    |  |
| 4   | c     | 191    |  |
| 4   | d     | 191    |  |
| 4   | e     | 191    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | f     | 191    |    |
| 5   | h     | 106    |    |
| 5   | i     | 106    |    |
| 5   | j     | 106    |    |
| 5   | k     | 106    |    |
| 5   | l     | 106    |    |
| 5   | m     | 106    |    |
| 6   | t     | 229    |    |
| 6   | u     | 229    |    |
| 6   | v     | 229    |    |
| 7   | w     | 221    |    |
| 7   | x     | 221    |    |
| 7   | y     | 221    |  |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 128850 atoms, of which 61470 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 Pam3 baseplate wedge gp22.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 1   | A     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4519  | 1439 | 2224 | 393 | 453 | 10 |         |       |
| 1   | B     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4565  | 1439 | 2270 | 393 | 453 | 10 |         |       |
| 1   | E     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4519  | 1439 | 2224 | 393 | 453 | 10 |         |       |
| 1   | F     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4565  | 1439 | 2270 | 393 | 453 | 10 |         |       |
| 1   | H     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4519  | 1439 | 2224 | 393 | 453 | 10 |         |       |
| 1   | I     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4565  | 1439 | 2270 | 393 | 453 | 10 |         |       |
| 1   | K     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4519  | 1439 | 2224 | 393 | 453 | 10 |         |       |
| 1   | L     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4551  | 1439 | 2256 | 393 | 453 | 10 |         |       |
| 1   | O     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4512  | 1439 | 2217 | 393 | 453 | 10 |         |       |
| 1   | P     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4565  | 1439 | 2270 | 393 | 453 | 10 |         |       |
| 1   | Q     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4519  | 1439 | 2224 | 393 | 453 | 10 |         |       |
| 1   | R     | 299      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4565  | 1439 | 2270 | 393 | 453 | 10 |         |       |

- Molecule 2 is a protein called Pam3 baseplate wedge gp23.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | C     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 1161 | 1507 | 300 | 353 | 18 |         |       |
| 2   | D     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 1161 | 1507 | 300 | 353 | 18 |         |       |
| 2   | G     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 1161 | 1507 | 300 | 353 | 18 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | J     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 1161 | 1507 | 300 | 353 | 18 |         |       |
| 2   | M     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 1161 | 1507 | 300 | 353 | 18 |         |       |
| 2   | S     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 1161 | 1507 | 300 | 353 | 18 |         |       |

- Molecule 3 is a protein called Pam3 sheath initiator gp21.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 3   | X     | 120      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1869  | 592 | 933 | 160 | 181 | 3 |         |       |
| 3   | n     | 120      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1869  | 592 | 933 | 160 | 181 | 3 |         |       |
| 3   | o     | 120      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1869  | 592 | 933 | 160 | 181 | 3 |         |       |
| 3   | p     | 120      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1869  | 592 | 933 | 160 | 181 | 3 |         |       |
| 3   | q     | 120      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1869  | 592 | 933 | 160 | 181 | 3 |         |       |
| 3   | r     | 120      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1869  | 592 | 933 | 160 | 181 | 3 |         |       |

- Molecule 4 is a protein called Pam3 tube initiator gp17.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 4   | a     | 182      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 2119  | 831 | 777 | 237 | 270 | 4 |         |       |
| 4   | b     | 182      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 2119  | 831 | 777 | 237 | 270 | 4 |         |       |
| 4   | c     | 182      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 2119  | 831 | 777 | 237 | 270 | 4 |         |       |
| 4   | d     | 182      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 2119  | 831 | 777 | 237 | 270 | 4 |         |       |
| 4   | e     | 182      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 2119  | 831 | 777 | 237 | 270 | 4 |         |       |
| 4   | f     | 182      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 2119  | 831 | 777 | 237 | 270 | 4 |         |       |

- Molecule 5 is a protein called Pam3 plug gp18.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 5   | h     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 527 | 833 | 139 | 160 | 1 |         |       |
| 5   | i     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 527 | 833 | 139 | 160 | 1 |         |       |
| 5   | j     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 527 | 833 | 139 | 160 | 1 |         |       |
| 5   | k     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 527 | 833 | 139 | 160 | 1 |         |       |
| 5   | l     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 527 | 833 | 139 | 160 | 1 |         |       |
| 5   | m     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 527 | 833 | 139 | 160 | 1 |         |       |

- Molecule 6 is a protein called Pam3 hub gp19.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6   | t     | 229      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3538  | 1095 | 1776 | 313 | 343 | 11 |         |       |
| 6   | u     | 229      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3538  | 1095 | 1776 | 313 | 343 | 11 |         |       |
| 6   | v     | 229      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3538  | 1095 | 1776 | 313 | 343 | 11 |         |       |

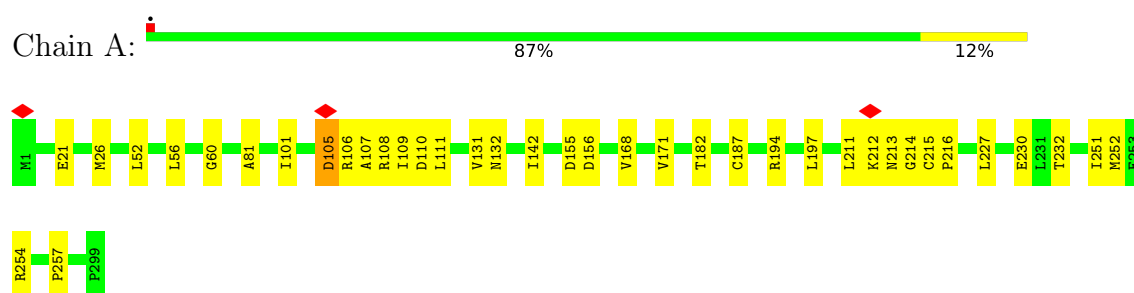
- Molecule 7 is a protein called Pam3 spike gp20.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 7   | w     | 221      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3277  | 1012 | 1633 | 292 | 329 | 11 |         |       |
| 7   | x     | 221      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3277  | 1012 | 1633 | 292 | 329 | 11 |         |       |
| 7   | y     | 221      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3277  | 1012 | 1633 | 292 | 329 | 11 |         |       |

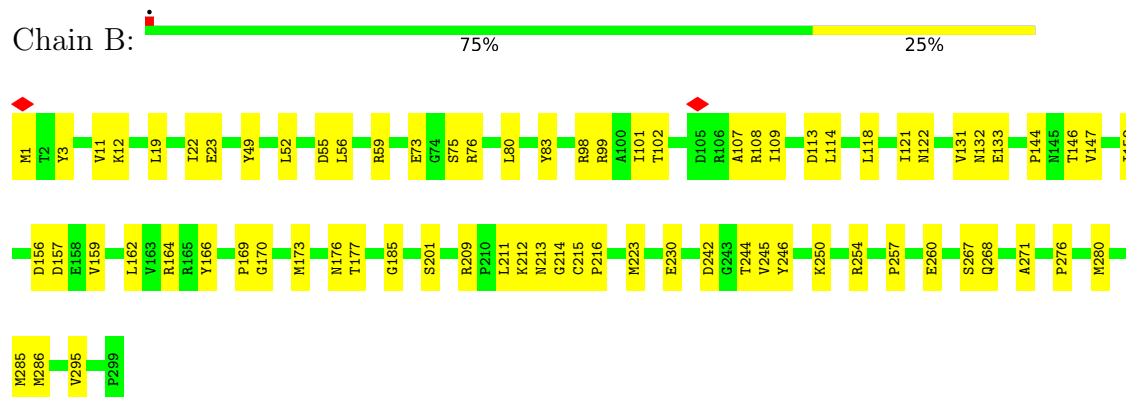
### 3 Residue-property plots

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.

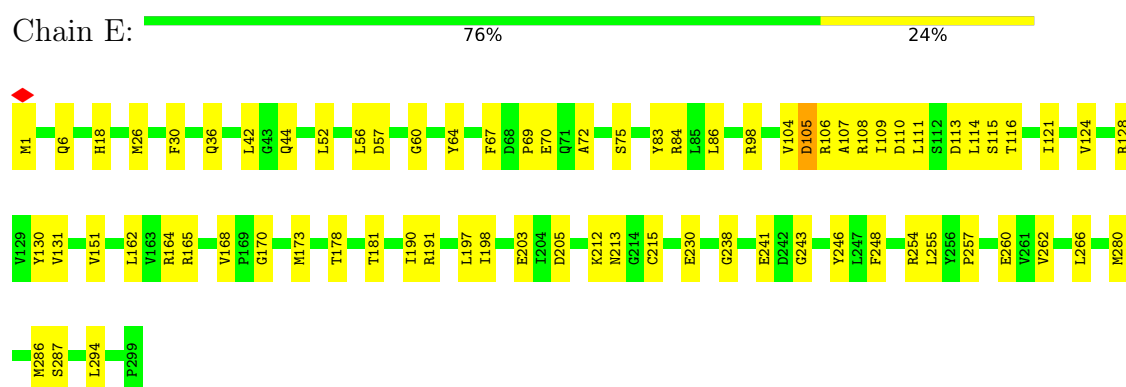
- Molecule 1: Pam3 baseplate wedge gp22



- Molecule 1: Pam3 baseplate wedge gp22

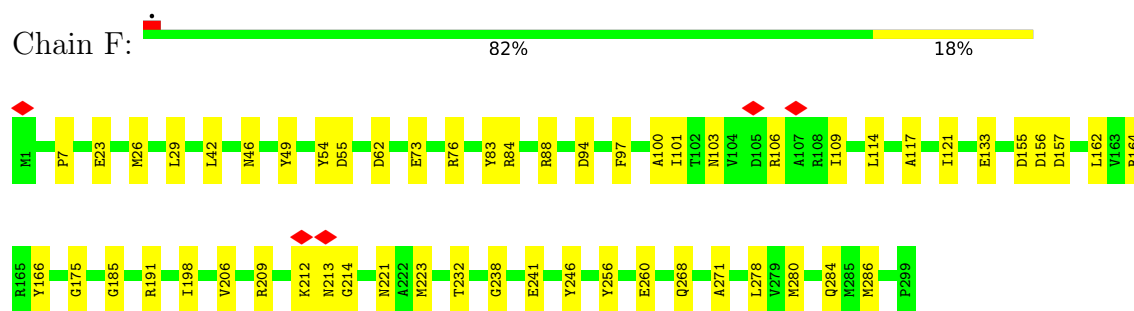


- Molecule 1: Pam3 baseplate wedge gp22

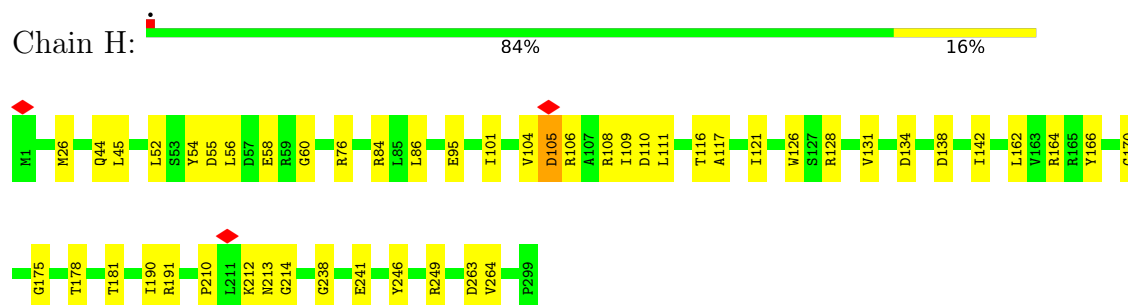




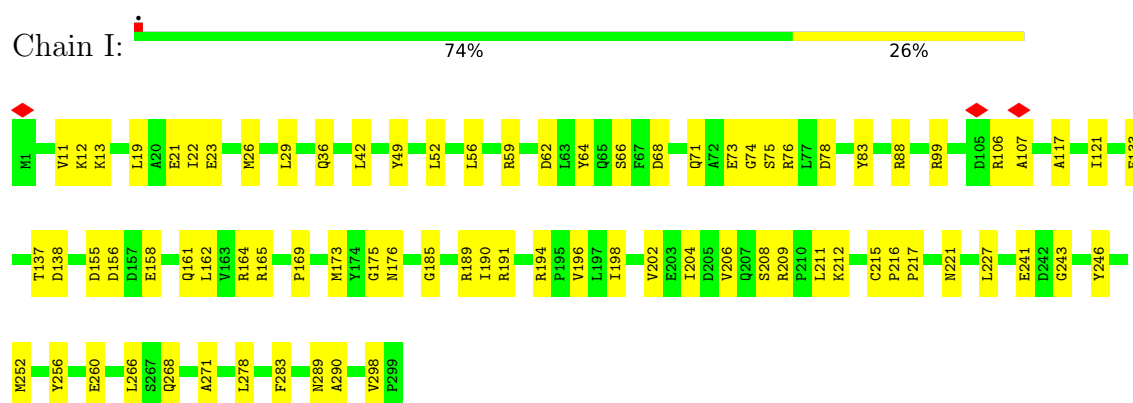
- Molecule 1: Pam3 baseplate wedge gp22



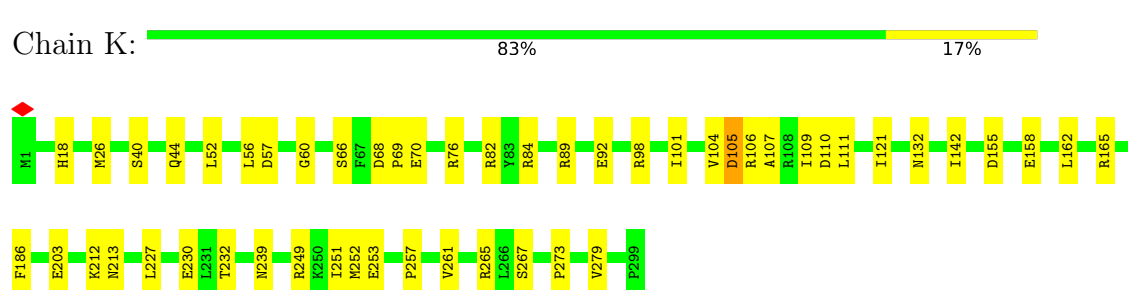
- Molecule 1: Pam3 baseplate wedge gp22



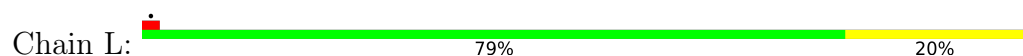
- Molecule 1: Pam3 baseplate wedge gp22

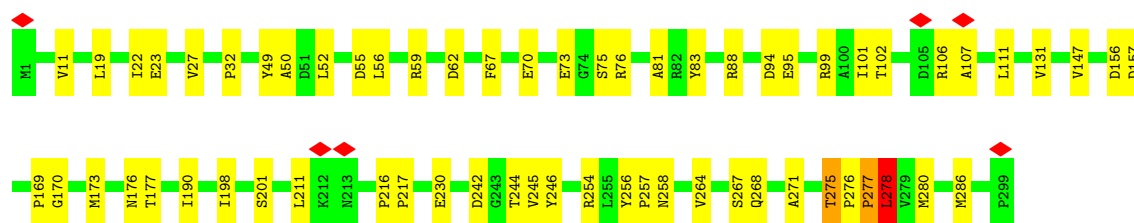


- Molecule 1: Pam3 baseplate wedge gp22



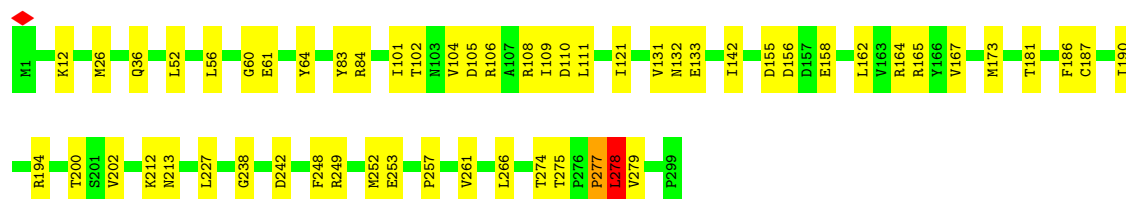
- Molecule 1: Pam3 baseplate wedge gp22





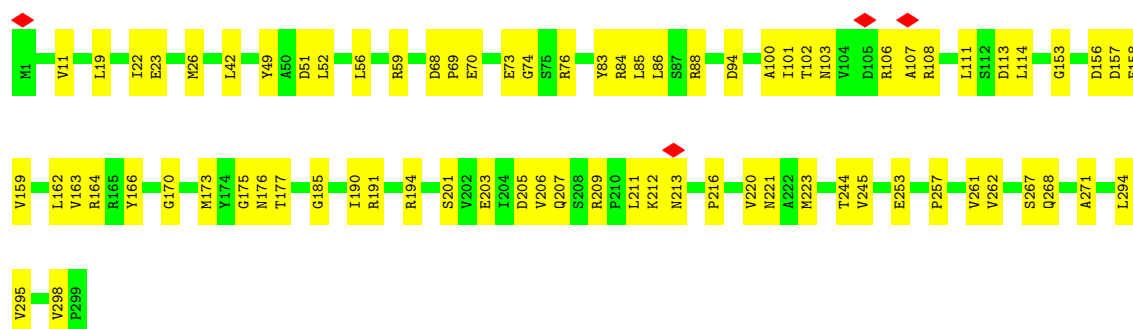
- Molecule 1: Pam3 baseplate wedge gp22

Chain O: 81% 18%



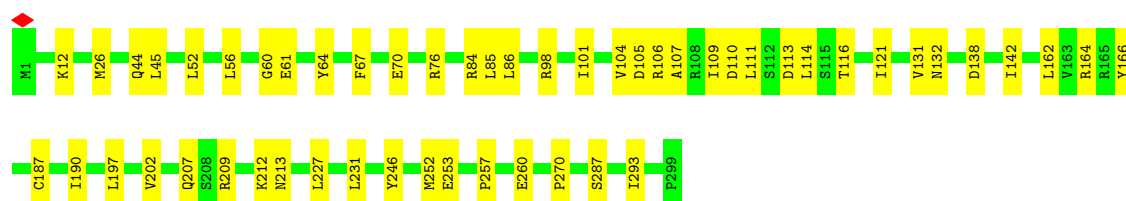
- Molecule 1: Pam3 baseplate wedge gp22

Chain P: 75% 25%



- Molecule 1: Pam3 baseplate wedge gp22

Chain Q: 82% 18%



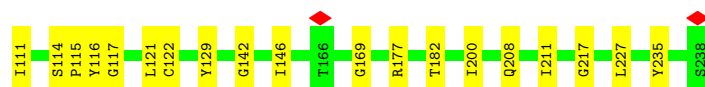
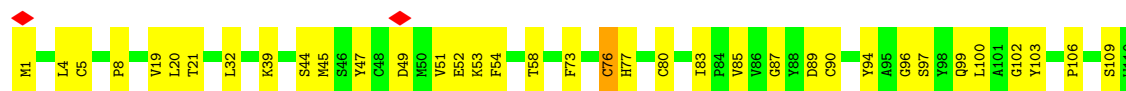
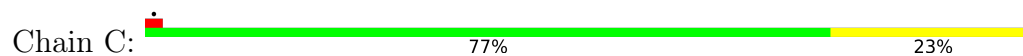
- Molecule 1: Pam3 baseplate wedge gp22

Chain R: 84% 16%

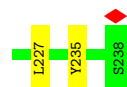
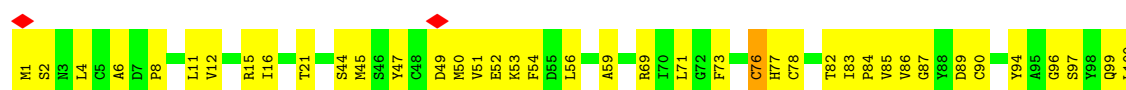




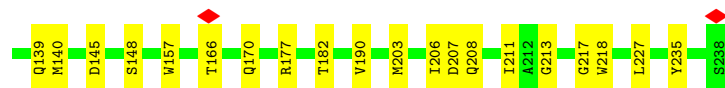
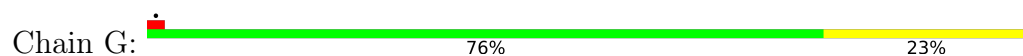
- Molecule 2: Pam3 baseplate wedge gp23



- Molecule 2: Pam3 baseplate wedge gp23



- Molecule 2: Pam3 baseplate wedge gp23

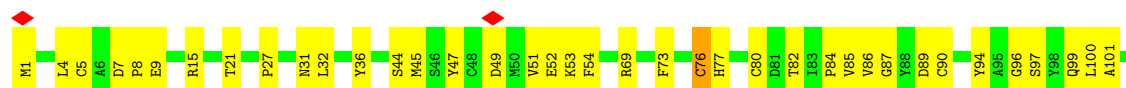


- Molecule 2: Pam3 baseplate wedge gp23

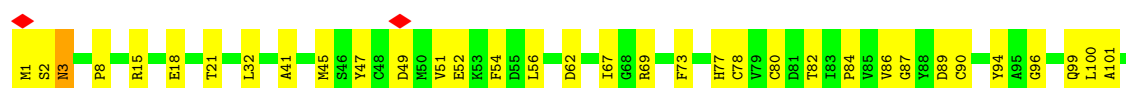
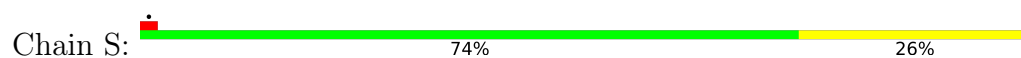




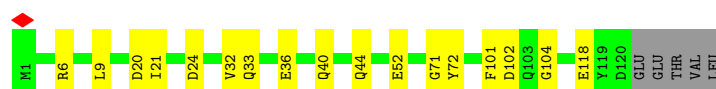
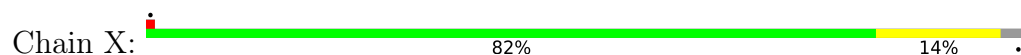
- Molecule 2: Pam3 baseplate wedge gp23



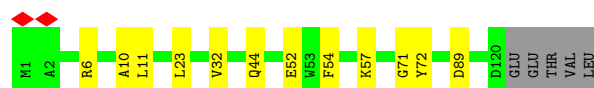
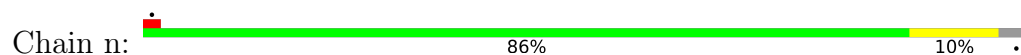
- Molecule 2: Pam3 baseplate wedge gp23



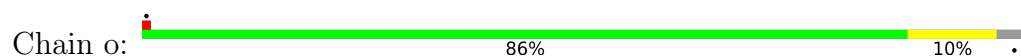
- Molecule 3: Pam3 sheath initiator gp21



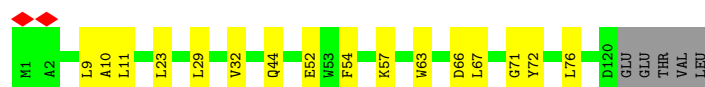
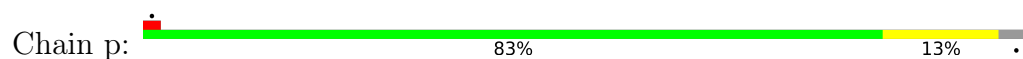
- Molecule 3: Pam3 sheath initiator gp21



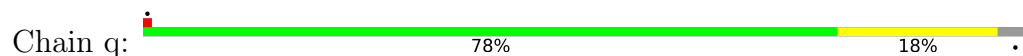
- Molecule 3: Pam3 sheath initiator gp21



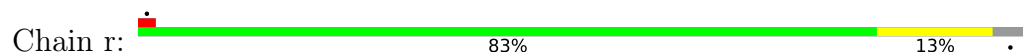
- Molecule 3: Pam3 sheath initiator gp21



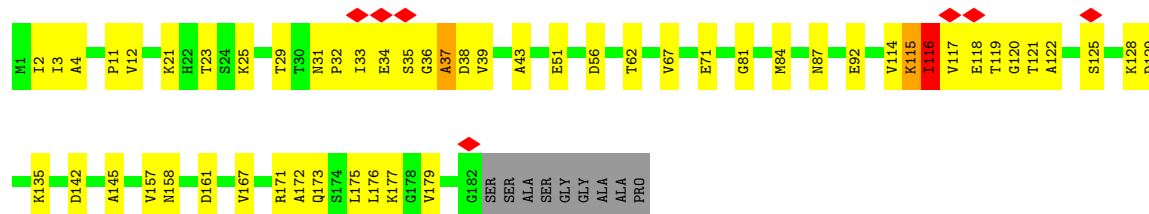
- Molecule 3: Pam3 sheath initiator gp21



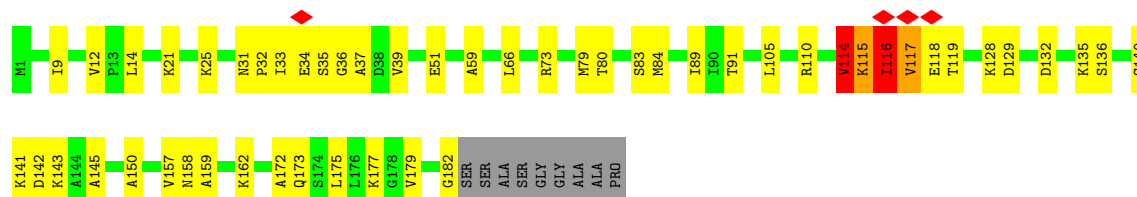
- Molecule 3: Pam3 sheath initiator gp21



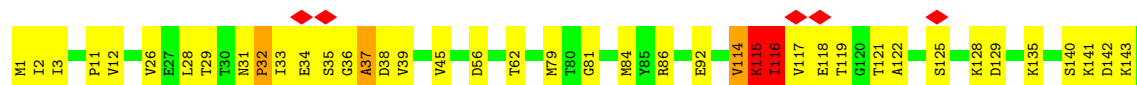
- Molecule 4: Pam3 tube initiator gp17



- Molecule 4: Pam3 tube initiator gp17



- Molecule 4: Pam3 tube initiator gp17





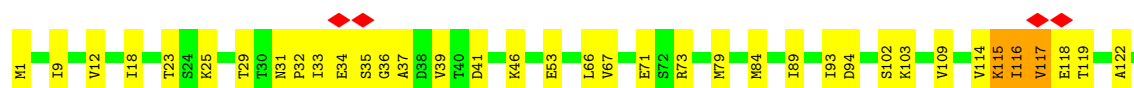
• Molecule 4: Pam3 tube initiator gp17



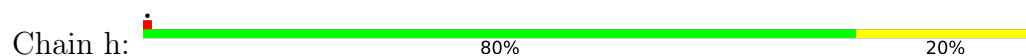
• Molecule 4: Pam3 tube initiator gp17



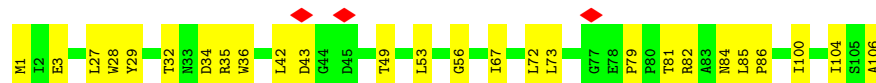
• Molecule 4: Pam3 tube initiator gp17



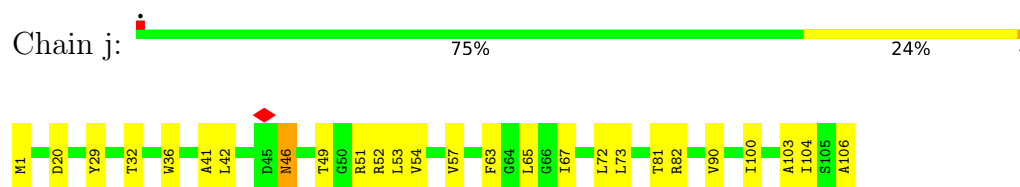
• Molecule 5: Pam3 plug gp18



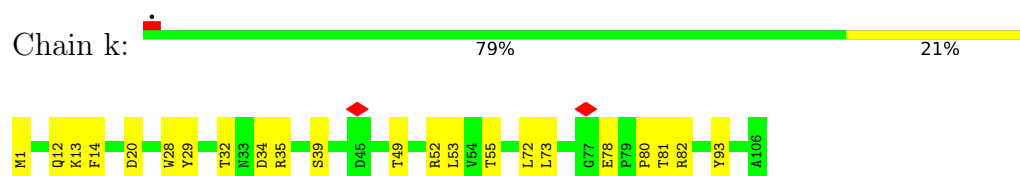
• Molecule 5: Pam3 plug gp18



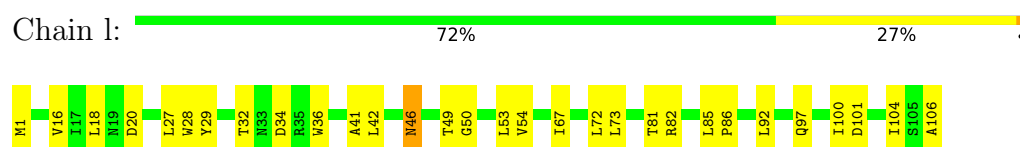
- Molecule 5: Pam3 plug gp18



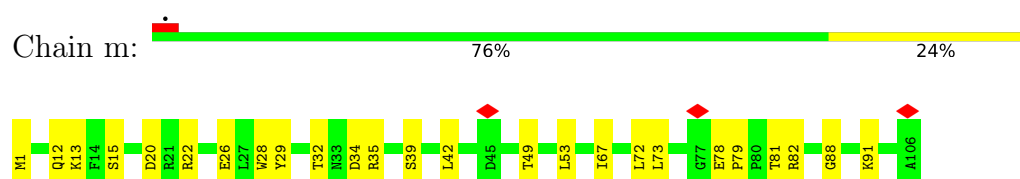
- Molecule 5: Pam3 plug gp18



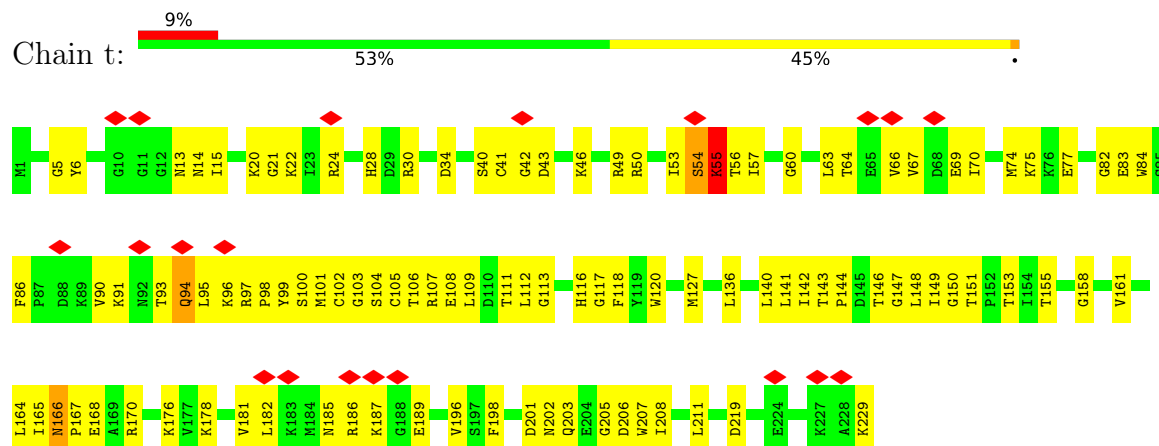
- Molecule 5: Pam3 plug gp18



- Molecule 5: Pam3 plug gp18

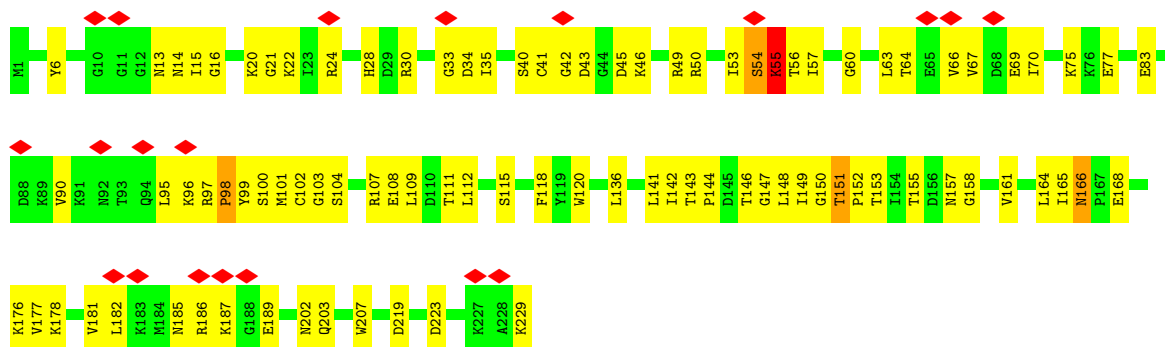


- Molecule 6: Pam3 hub gp19

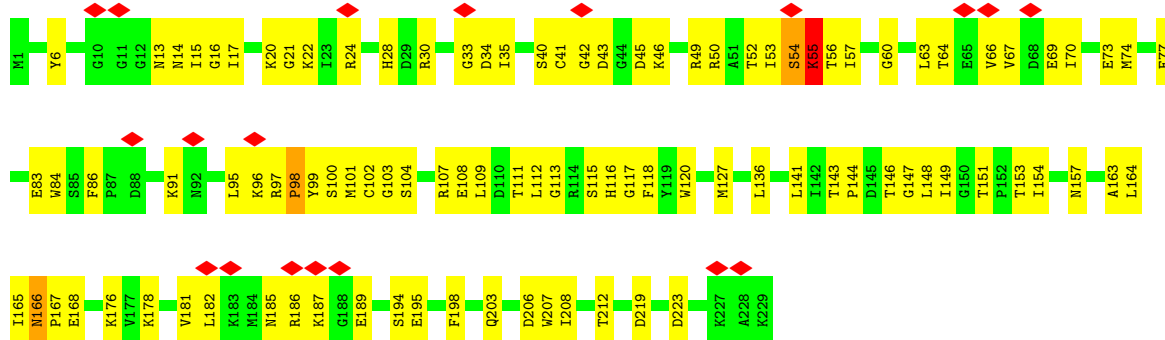


- Molecule 6: Pam3 hub gp19

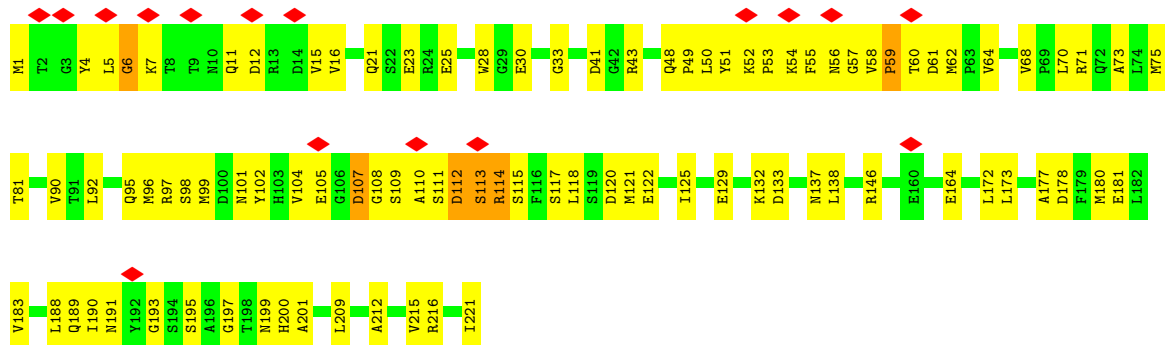




• Molecule 6: Pam3 hub gp19



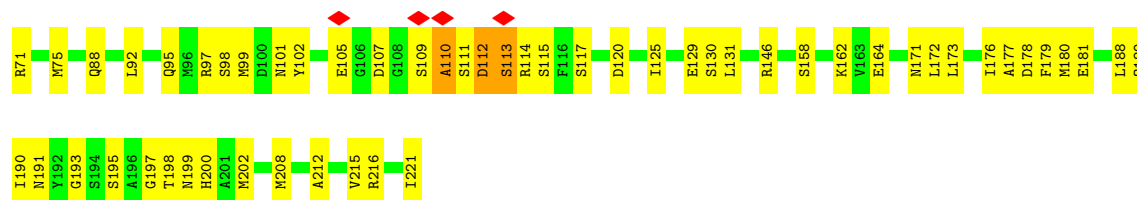
• Molecule 7: Pam3 spike gp20



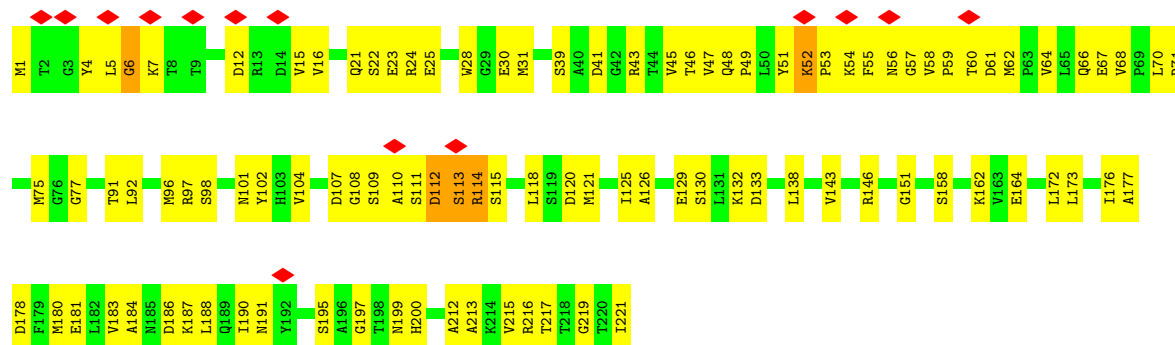
• Molecule 7: Pam3 spike gp20







• Molecule 7: Pam3 spike gp20



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 45155                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY             | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                              | Depositor |
| Minimum defocus (nm)                 | 1000                            | Depositor |
| Maximum defocus (nm)                 | 2000                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)       | Depositor |
| Maximum map value                    | 0.060                           | Depositor |
| Minimum map value                    | -0.023                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.003                           | Depositor |
| Recommended contour level            | 0.008                           | Depositor |
| Map size ( $\text{\AA}$ )            | 513.60004, 513.60004, 513.60004 | wwPDB     |
| Map dimensions                       | 480, 480, 480                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.07, 1.07, 1.07                | 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   | A     | 0.26         | 0/2339        | 0.43        | 0/3188        |
| 1   | B     | 0.23         | 0/2339        | 0.41        | 0/3188        |
| 1   | E     | 0.23         | 0/2339        | 0.41        | 0/3188        |
| 1   | F     | 0.23         | 0/2339        | 0.40        | 0/3188        |
| 1   | H     | 0.22         | 0/2339        | 0.42        | 0/3188        |
| 1   | I     | 0.24         | 0/2339        | 0.41        | 0/3188        |
| 1   | K     | 0.22         | 0/2339        | 0.40        | 0/3188        |
| 1   | L     | 0.26         | 0/2339        | 0.45        | 0/3188        |
| 1   | O     | 0.28         | 0/2339        | 0.46        | 1/3188 (0.0%) |
| 1   | P     | 0.25         | 0/2339        | 0.41        | 0/3188        |
| 1   | Q     | 0.25         | 0/2339        | 0.46        | 2/3188 (0.1%) |
| 1   | R     | 0.23         | 0/2339        | 0.40        | 0/3188        |
| 2   | C     | 0.27         | 0/1876        | 0.49        | 1/2554 (0.0%) |
| 2   | D     | 0.27         | 0/1876        | 0.52        | 1/2554 (0.0%) |
| 2   | G     | 0.26         | 0/1876        | 0.48        | 1/2554 (0.0%) |
| 2   | J     | 0.25         | 0/1876        | 0.44        | 0/2554        |
| 2   | M     | 0.28         | 0/1876        | 0.51        | 1/2554 (0.0%) |
| 2   | S     | 0.26         | 0/1876        | 0.46        | 0/2554        |
| 3   | X     | 0.24         | 0/951         | 0.42        | 0/1287        |
| 3   | n     | 0.24         | 0/951         | 0.41        | 0/1287        |
| 3   | o     | 0.23         | 0/951         | 0.43        | 0/1287        |
| 3   | p     | 0.24         | 0/951         | 0.41        | 0/1287        |
| 3   | q     | 0.24         | 0/951         | 0.42        | 0/1287        |
| 3   | r     | 0.24         | 0/951         | 0.39        | 0/1287        |
| 4   | a     | 0.32         | 0/1358        | 0.64        | 5/1835 (0.3%) |
| 4   | b     | 0.40         | 2/1358 (0.1%) | 0.63        | 3/1835 (0.2%) |
| 4   | c     | 0.41         | 1/1358 (0.1%) | 0.70        | 6/1835 (0.3%) |
| 4   | d     | 0.39         | 1/1358 (0.1%) | 0.65        | 3/1835 (0.2%) |
| 4   | e     | 0.31         | 0/1358        | 0.62        | 3/1835 (0.2%) |
| 4   | f     | 0.29         | 0/1358        | 0.56        | 0/1835        |
| 5   | h     | 0.26         | 0/841         | 0.41        | 0/1143        |
| 5   | i     | 0.28         | 0/841         | 0.43        | 0/1143        |
| 5   | j     | 0.27         | 0/841         | 0.41        | 0/1143        |
| 5   | k     | 0.25         | 0/841         | 0.43        | 0/1143        |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 5   | l     | 0.27         | 0/841          | 0.41        | 0/1143          |
| 5   | m     | 0.26         | 0/841          | 0.44        | 0/1143          |
| 6   | t     | 0.34         | 0/1792         | 0.74        | 3/2408 (0.1%)   |
| 6   | u     | 0.34         | 0/1792         | 0.77        | 4/2408 (0.2%)   |
| 6   | v     | 0.36         | 0/1792         | 0.78        | 4/2408 (0.2%)   |
| 7   | w     | 0.35         | 0/1669         | 0.76        | 3/2258 (0.1%)   |
| 7   | x     | 0.36         | 0/1669         | 0.72        | 3/2258 (0.1%)   |
| 7   | y     | 0.33         | 0/1669         | 0.75        | 6/2258 (0.3%)   |
| All | All   | 0.28         | 4/68607 (0.0%) | 0.52        | 50/93168 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | X     | 0                   | 1                   |
| 4   | b     | 0                   | 1                   |
| 4   | c     | 0                   | 1                   |
| 4   | d     | 0                   | 1                   |
| 6   | t     | 0                   | 3                   |
| 6   | u     | 0                   | 3                   |
| 6   | v     | 0                   | 2                   |
| 7   | w     | 0                   | 3                   |
| All | All   | 0                   | 15                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | c     | 116 | ILE  | N-CA  | 6.37 | 1.54        | 1.46     |
| 4   | b     | 116 | ILE  | N-CA  | 6.17 | 1.54        | 1.46     |
| 4   | d     | 116 | ILE  | N-CA  | 5.75 | 1.53        | 1.46     |
| 4   | b     | 115 | LYS  | N-CA  | 5.43 | 1.52        | 1.45     |

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | b     | 114 | VAL  | O-C-N  | -15.28 | 106.08      | 123.03   |
| 4   | d     | 114 | VAL  | O-C-N  | -14.36 | 107.09      | 123.03   |
| 4   | c     | 114 | VAL  | O-C-N  | -12.85 | 108.55      | 122.81   |
| 7   | w     | 6   | GLY  | N-CA-C | 9.83   | 123.84      | 110.58   |
| 6   | t     | 54  | SER  | CA-C-N | -8.73  | 108.58      | 121.76   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | t     | 54  | SER  | C-N-CA   | -8.73 | 108.58      | 121.76   |
| 7   | y     | 114 | ARG  | CA-CB-CG | 8.44  | 130.98      | 114.10   |
| 7   | y     | 6   | GLY  | N-CA-C   | 8.22  | 123.83      | 111.42   |
| 6   | v     | 54  | SER  | CA-C-N   | -8.03 | 110.80      | 122.44   |
| 6   | v     | 54  | SER  | C-N-CA   | -8.03 | 110.80      | 122.44   |
| 6   | u     | 54  | SER  | CA-C-N   | -8.02 | 110.81      | 122.44   |
| 6   | u     | 54  | SER  | C-N-CA   | -8.02 | 110.81      | 122.44   |
| 7   | x     | 6   | GLY  | N-CA-C   | 7.96  | 123.97      | 111.08   |
| 2   | M     | 76  | CYS  | CA-CB-SG | 7.38  | 131.38      | 114.40   |
| 1   | O     | 277 | PRO  | N-CA-C   | -7.31 | 105.33      | 114.68   |
| 2   | C     | 76  | CYS  | CA-CB-SG | 7.15  | 130.85      | 114.40   |
| 2   | D     | 76  | CYS  | CA-CB-SG | 6.93  | 130.34      | 114.40   |
| 1   | Q     | 270 | PRO  | CA-N-CD  | -6.92 | 101.82      | 111.50   |
| 7   | x     | 113 | SER  | N-CA-C   | 6.69  | 120.34      | 107.44   |
| 7   | w     | 112 | ASP  | CB-CA-C  | 6.31  | 122.98      | 110.42   |
| 7   | x     | 112 | ASP  | CB-CA-C  | 6.29  | 122.94      | 110.42   |
| 4   | a     | 37  | ALA  | CA-C-N   | 6.19  | 131.65      | 122.74   |
| 4   | a     | 37  | ALA  | C-N-CA   | 6.19  | 131.65      | 122.74   |
| 7   | y     | 113 | SER  | N-CA-C   | 6.12  | 120.50      | 107.70   |
| 4   | b     | 115 | LYS  | CA-C-O   | -5.95 | 114.79      | 121.81   |
| 6   | v     | 98  | PRO  | N-CA-C   | 5.94  | 120.59      | 111.57   |
| 4   | d     | 116 | ILE  | CA-C-O   | -5.91 | 113.39      | 120.78   |
| 6   | t     | 55  | LYS  | N-CA-C   | 5.88  | 117.84      | 107.61   |
| 7   | w     | 113 | SER  | N-CA-C   | 5.78  | 119.78      | 107.70   |
| 4   | c     | 115 | LYS  | CA-C-O   | -5.73 | 114.52      | 121.05   |
| 7   | y     | 112 | ASP  | CB-CA-C  | 5.71  | 121.79      | 110.42   |
| 6   | u     | 98  | PRO  | N-CA-C   | 5.63  | 120.13      | 111.57   |
| 7   | y     | 52  | LYS  | CA-CB-CG | 5.61  | 125.31      | 114.10   |
| 6   | v     | 55  | LYS  | N-CA-C   | 5.60  | 117.49      | 107.80   |
| 6   | u     | 55  | LYS  | N-CA-C   | 5.43  | 117.19      | 107.80   |
| 1   | Q     | 270 | PRO  | N-CD-CG  | -5.31 | 97.42       | 103.80   |
| 4   | e     | 120 | GLY  | N-CA-C   | 5.31  | 125.77      | 113.18   |
| 4   | c     | 11  | PRO  | CA-C-N   | -5.27 | 118.79      | 122.59   |
| 4   | c     | 11  | PRO  | C-N-CA   | -5.27 | 118.79      | 122.59   |
| 4   | e     | 11  | PRO  | CA-C-N   | -5.27 | 118.79      | 122.59   |
| 4   | e     | 11  | PRO  | C-N-CA   | -5.27 | 118.79      | 122.59   |
| 7   | y     | 114 | ARG  | CB-CA-C  | -5.21 | 102.47      | 112.43   |
| 4   | d     | 115 | LYS  | CA-C-O   | -5.20 | 115.12      | 121.36   |
| 4   | c     | 37  | ALA  | CA-C-N   | 5.17  | 130.18      | 122.74   |
| 4   | c     | 37  | ALA  | C-N-CA   | 5.17  | 130.18      | 122.74   |
| 4   | a     | 11  | PRO  | CA-C-N   | -5.14 | 118.89      | 122.59   |
| 4   | a     | 11  | PRO  | C-N-CA   | -5.14 | 118.89      | 122.59   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 106 | PRO  | CA-N-CD | -5.12 | 104.83      | 112.00   |
| 4   | b     | 116 | ILE  | CA-C-O  | -5.05 | 114.46      | 120.78   |
| 4   | a     | 120 | GLY  | N-CA-C  | 5.02  | 125.08      | 113.18   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | X     | 33  | GLN  | Peptide   |
| 4   | b     | 114 | VAL  | Mainchain |
| 4   | c     | 114 | VAL  | Mainchain |
| 4   | d     | 114 | VAL  | Mainchain |
| 6   | t     | 166 | ASN  | Peptide   |
| 6   | t     | 55  | LYS  | Peptide   |
| 6   | t     | 94  | GLN  | Peptide   |
| 6   | u     | 151 | THR  | Peptide   |
| 6   | u     | 166 | ASN  | Peptide   |
| 6   | u     | 55  | LYS  | Peptide   |
| 6   | v     | 166 | ASN  | Peptide   |
| 6   | v     | 55  | LYS  | Peptide   |
| 7   | w     | 107 | ASP  | Peptide   |
| 7   | w     | 114 | ARG  | Peptide   |
| 7   | w     | 59  | PRO  | Peptide   |

## 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   | A     | 2295  | 2224     | 2269     | 48      | 0            |
| 1   | B     | 2295  | 2270     | 2269     | 65      | 0            |
| 1   | E     | 2295  | 2224     | 2269     | 71      | 0            |
| 1   | F     | 2295  | 2270     | 2270     | 56      | 0            |
| 1   | H     | 2295  | 2224     | 2268     | 62      | 0            |
| 1   | I     | 2295  | 2270     | 2269     | 80      | 0            |
| 1   | K     | 2295  | 2224     | 2269     | 50      | 0            |
| 1   | L     | 2295  | 2256     | 2270     | 68      | 0            |
| 1   | O     | 2295  | 2217     | 2269     | 59      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | P     | 2295  | 2270     | 2269     | 66      | 0            |
| 1   | Q     | 2295  | 2224     | 2270     | 56      | 0            |
| 1   | R     | 2295  | 2270     | 2269     | 47      | 0            |
| 2   | C     | 1832  | 1507     | 1766     | 67      | 0            |
| 2   | D     | 1832  | 1507     | 1767     | 85      | 0            |
| 2   | G     | 1832  | 1507     | 1766     | 63      | 0            |
| 2   | J     | 1832  | 1507     | 1766     | 70      | 0            |
| 2   | M     | 1832  | 1507     | 1766     | 75      | 0            |
| 2   | S     | 1832  | 1507     | 1767     | 68      | 0            |
| 3   | X     | 936   | 933      | 933      | 11      | 0            |
| 3   | n     | 936   | 933      | 933      | 9       | 0            |
| 3   | o     | 936   | 933      | 933      | 11      | 0            |
| 3   | p     | 936   | 933      | 933      | 17      | 0            |
| 3   | q     | 936   | 933      | 933      | 16      | 0            |
| 3   | r     | 936   | 933      | 933      | 12      | 0            |
| 4   | a     | 1342  | 777      | 1368     | 128     | 0            |
| 4   | b     | 1342  | 777      | 1368     | 121     | 0            |
| 4   | c     | 1342  | 777      | 1368     | 116     | 0            |
| 4   | d     | 1342  | 777      | 1368     | 118     | 0            |
| 4   | e     | 1342  | 777      | 1368     | 138     | 0            |
| 4   | f     | 1342  | 777      | 1368     | 131     | 0            |
| 5   | h     | 827   | 833      | 833      | 16      | 0            |
| 5   | i     | 827   | 833      | 833      | 27      | 0            |
| 5   | j     | 827   | 833      | 833      | 27      | 0            |
| 5   | k     | 827   | 833      | 833      | 22      | 0            |
| 5   | l     | 827   | 833      | 833      | 27      | 0            |
| 5   | m     | 827   | 833      | 833      | 28      | 0            |
| 6   | t     | 1762  | 1776     | 1776     | 290     | 0            |
| 6   | u     | 1762  | 1776     | 1776     | 262     | 0            |
| 6   | v     | 1762  | 1776     | 1776     | 293     | 0            |
| 7   | w     | 1644  | 1633     | 1633     | 260     | 0            |
| 7   | x     | 1644  | 1633     | 1633     | 260     | 0            |
| 7   | y     | 1644  | 1633     | 1633     | 255     | 0            |
| All | All   | 67380 | 61470    | 66859    | 2481    | 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 18.

All (2481) 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:109:ILE:HD13 | 2:J:73:PHE:CE1   | 1.49                     | 1.45              |
| 1:E:109:ILE:HD13 | 2:G:73:PHE:CE1   | 1.53                     | 1.42              |
| 1:Q:109:ILE:HD13 | 2:S:73:PHE:CE1   | 1.54                     | 1.40              |
| 1:E:109:ILE:HD13 | 2:G:73:PHE:CD1   | 1.67                     | 1.30              |
| 1:E:109:ILE:CD1  | 2:G:73:PHE:CE1   | 2.17                     | 1.25              |
| 1:H:109:ILE:CD1  | 2:J:73:PHE:CE1   | 2.22                     | 1.22              |
| 1:H:109:ILE:CD1  | 2:J:73:PHE:HE1   | 1.53                     | 1.20              |
| 4:a:35:SER:HA    | 4:f:118:GLU:HB2  | 1.21                     | 1.17              |
| 4:b:118:GLU:HB2  | 4:c:35:SER:HA    | 1.21                     | 1.14              |
| 4:d:118:GLU:HB2  | 4:e:35:SER:HA    | 1.24                     | 1.12              |
| 1:K:109:ILE:HD11 | 2:M:77:HIS:HE1   | 1.06                     | 1.11              |
| 4:c:115:LYS:CG   | 4:d:34:GLU:HB3   | 1.81                     | 1.11              |
| 1:H:109:ILE:HD13 | 2:J:73:PHE:CD1   | 1.85                     | 1.10              |
| 1:Q:109:ILE:CD1  | 2:S:73:PHE:CE1   | 2.35                     | 1.10              |
| 4:a:36:GLY:HA3   | 4:f:116:ILE:HG23 | 1.24                     | 1.09              |
| 4:e:116:ILE:HB   | 4:f:36:GLY:HA3   | 1.32                     | 1.08              |
| 1:L:275:THR:O    | 1:L:277:PRO:HD3  | 1.53                     | 1.07              |
| 4:c:31:ASN:HB3   | 4:c:32:PRO:HD2   | 1.31                     | 1.06              |
| 4:e:116:ILE:CB   | 4:f:36:GLY:HA3   | 1.84                     | 1.06              |
| 6:t:57:ILE:HG21  | 7:y:59:PRO:HG2   | 1.33                     | 1.06              |
| 4:a:173:GLN:HE22 | 4:a:177:LYS:HE2  | 1.20                     | 1.06              |
| 4:a:36:GLY:HA3   | 4:f:116:ILE:CG2  | 1.86                     | 1.05              |
| 1:L:275:THR:C    | 1:L:277:PRO:HD3  | 1.81                     | 1.05              |
| 1:H:56:LEU:O     | 2:J:47:TYR:OH    | 1.75                     | 1.04              |
| 6:t:151:THR:HG23 | 6:v:30:ARG:HE    | 1.16                     | 1.04              |
| 1:Q:56:LEU:O     | 2:S:47:TYR:OH    | 1.75                     | 1.04              |
| 4:a:31:ASN:HB3   | 4:a:32:PRO:HD2   | 1.34                     | 1.04              |
| 4:e:31:ASN:HB3   | 4:e:32:PRO:HD2   | 1.34                     | 1.03              |
| 4:c:115:LYS:HG2  | 4:d:34:GLU:HB3   | 1.39                     | 1.02              |
| 1:E:56:LEU:O     | 2:G:47:TYR:OH    | 1.77                     | 1.02              |
| 1:K:109:ILE:HD11 | 2:M:77:HIS:CE1   | 1.93                     | 1.01              |
| 6:u:99:TYR:HB2   | 7:w:52:LYS:HD2   | 1.42                     | 1.01              |
| 4:a:116:ILE:CB   | 4:b:36:GLY:HA3   | 1.89                     | 1.01              |
| 5:k:13:LYS:O     | 6:v:186:ARG:NH1  | 1.92                     | 1.01              |
| 4:a:36:GLY:H     | 4:f:118:GLU:H    | 1.05                     | 1.00              |
| 5:m:13:LYS:O     | 6:u:186:ARG:NH1  | 1.93                     | 1.00              |
| 6:t:102:CYS:O    | 7:w:114:ARG:N    | 1.94                     | 1.00              |
| 5:h:13:LYS:O     | 6:t:186:ARG:NH1  | 1.96                     | 0.99              |
| 4:b:118:GLU:H    | 4:c:36:GLY:H     | 1.05                     | 0.99              |
| 6:t:99:TYR:OH    | 7:y:55:PHE:N     | 1.95                     | 0.99              |
| 4:d:158:ASN:HA   | 6:v:186:ARG:NH1  | 1.78                     | 0.99              |
| 4:d:118:GLU:H    | 4:e:36:GLY:H     | 1.07                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:c:121:THR:HG22 | 6:u:166:ASN:CG   | 1.87                     | 0.98              |
| 1:R:55:ASP:OD2   | 2:S:15:ARG:NH2   | 1.96                     | 0.98              |
| 1:K:56:LEU:O     | 2:M:47:TYR:OH    | 1.81                     | 0.98              |
| 6:u:96:LYS:N     | 7:w:61:ASP:OD2   | 1.96                     | 0.97              |
| 1:Q:109:ILE:HD13 | 2:S:73:PHE:HE1   | 1.15                     | 0.97              |
| 6:v:102:CYS:O    | 7:y:114:ARG:N    | 1.97                     | 0.97              |
| 2:D:47:TYR:OH    | 1:O:56:LEU:O     | 1.81                     | 0.97              |
| 7:y:191:ASN:ND2  | 7:y:199:ASN:O    | 1.97                     | 0.96              |
| 1:A:109:ILE:HD13 | 2:C:73:PHE:CD1   | 2.01                     | 0.96              |
| 6:t:103:GLY:N    | 7:w:112:ASP:OD1  | 1.98                     | 0.96              |
| 4:d:116:ILE:O    | 4:d:117:VAL:HG12 | 1.63                     | 0.95              |
| 2:S:21:THR:OG1   | 3:X:52:GLU:OE2   | 1.82                     | 0.95              |
| 4:a:36:GLY:CA    | 4:f:116:ILE:HG23 | 1.97                     | 0.95              |
| 4:e:92:GLU:OE1   | 4:e:110:ARG:NH1  | 1.99                     | 0.95              |
| 6:v:103:GLY:N    | 7:y:112:ASP:OD1  | 1.99                     | 0.95              |
| 1:Q:109:ILE:HD13 | 2:S:73:PHE:CD1   | 2.01                     | 0.95              |
| 4:f:116:ILE:HG22 | 4:f:117:VAL:H    | 1.32                     | 0.94              |
| 4:a:116:ILE:HB   | 4:b:36:GLY:HA3   | 1.46                     | 0.93              |
| 6:u:103:GLY:N    | 7:x:112:ASP:OD1  | 2.00                     | 0.93              |
| 4:f:116:ILE:O    | 4:f:117:VAL:HG12 | 1.66                     | 0.93              |
| 2:G:51:VAL:HG23  | 2:G:52:GLU:OE2   | 1.68                     | 0.93              |
| 1:E:109:ILE:CD1  | 2:G:73:PHE:HE1   | 1.69                     | 0.93              |
| 1:A:56:LEU:O     | 2:C:47:TYR:OH    | 1.85                     | 0.93              |
| 1:Q:109:ILE:CD1  | 2:S:73:PHE:HE1   | 1.77                     | 0.93              |
| 4:b:157:VAL:HG13 | 6:u:186:ARG:NH2  | 1.83                     | 0.93              |
| 7:x:191:ASN:ND2  | 7:x:199:ASN:O    | 2.03                     | 0.92              |
| 1:I:241:GLU:OE2  | 1:K:212:LYS:NZ   | 2.01                     | 0.92              |
| 4:f:157:VAL:HG13 | 6:t:186:ARG:NH2  | 1.84                     | 0.92              |
| 4:b:116:ILE:H    | 4:c:34:GLU:HB2   | 1.34                     | 0.92              |
| 1:L:76:ARG:NH2   | 2:M:1:MET:SD     | 2.43                     | 0.92              |
| 2:D:21:THR:OG1   | 3:p:52:GLU:OE2   | 1.87                     | 0.92              |
| 4:d:9:ILE:HD12   | 4:d:14:LEU:HD11  | 1.49                     | 0.91              |
| 6:v:97:ARG:NH2   | 7:x:62:MET:SD    | 2.43                     | 0.91              |
| 4:b:116:ILE:O    | 4:b:117:VAL:HG12 | 1.71                     | 0.91              |
| 4:d:116:ILE:CG2  | 4:e:36:GLY:HA3   | 1.99                     | 0.91              |
| 1:B:250:LYS:NZ   | 1:E:257:PRO:O    | 2.04                     | 0.91              |
| 4:f:29:THR:OG1   | 6:v:206:ASP:OD1  | 1.88                     | 0.91              |
| 4:a:118:GLU:HB2  | 4:b:35:SER:HA    | 1.50                     | 0.90              |
| 4:f:140:SER:OG   | 4:f:142:ASP:OD1  | 1.90                     | 0.90              |
| 1:Q:113:ASP:OD2  | 1:R:106:ARG:NH1  | 2.05                     | 0.90              |
| 2:M:76:CYS:HB3   | 2:M:122:CYS:HA   | 1.54                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:118:GLU:HB3  | 6:v:147:GLY:HA2  | 1.53                     | 0.89              |
| 6:t:56:THR:OG1   | 7:w:101:ASN:OD1  | 1.90                     | 0.89              |
| 6:t:63:LEU:HD11  | 7:y:60:THR:OG1   | 1.72                     | 0.89              |
| 4:b:118:GLU:N    | 4:c:36:GLY:H     | 1.69                     | 0.89              |
| 2:C:76:CYS:HB3   | 2:C:122:CYS:HA   | 1.54                     | 0.89              |
| 6:u:46:LYS:NZ    | 6:u:77:GLU:OE1   | 2.05                     | 0.89              |
| 1:I:227:LEU:HD13 | 1:I:252:MET:HE3  | 1.53                     | 0.88              |
| 3:q:105:ARG:NH2  | 3:q:109:GLU:OE2  | 2.07                     | 0.88              |
| 1:O:275:THR:O    | 1:O:277:PRO:HD3  | 1.74                     | 0.88              |
| 6:u:102:CYS:O    | 7:x:114:ARG:N    | 2.05                     | 0.88              |
| 6:v:97:ARG:NH2   | 7:x:62:MET:O     | 2.05                     | 0.88              |
| 4:b:140:SER:OG   | 4:b:142:ASP:OD1  | 1.91                     | 0.88              |
| 6:t:107:ARG:NH2  | 7:w:115:SER:OG   | 2.07                     | 0.88              |
| 4:a:36:GLY:H     | 4:f:118:GLU:N    | 1.71                     | 0.87              |
| 4:d:115:LYS:C    | 4:d:116:ILE:HG13 | 1.99                     | 0.87              |
| 1:L:245:VAL:CG1  | 1:L:276:PRO:HG2  | 2.04                     | 0.87              |
| 4:a:121:THR:HA   | 6:t:140:LEU:HD11 | 1.56                     | 0.87              |
| 4:b:172:ALA:HA   | 5:m:1:MET:HE2    | 1.57                     | 0.87              |
| 4:d:118:GLU:N    | 4:e:36:GLY:H     | 1.72                     | 0.87              |
| 6:t:143:THR:HG1  | 6:t:146:THR:HG1  | 1.15                     | 0.87              |
| 2:J:21:THR:OG1   | 3:q:52:GLU:OE2   | 1.92                     | 0.86              |
| 4:a:21:LYS:NZ    | 4:f:94:ASP:OD1   | 2.08                     | 0.86              |
| 6:t:96:LYS:N     | 7:y:61:ASP:OD2   | 2.07                     | 0.86              |
| 2:D:76:CYS:HB3   | 2:D:122:CYS:HA   | 1.58                     | 0.86              |
| 4:a:118:GLU:HB3  | 6:t:147:GLY:HA2  | 1.57                     | 0.86              |
| 4:a:32:PRO:HA    | 6:v:203:GLN:CD   | 2.00                     | 0.86              |
| 6:v:102:CYS:N    | 7:y:112:ASP:O    | 2.08                     | 0.86              |
| 1:L:275:THR:O    | 1:L:277:PRO:CD   | 2.24                     | 0.86              |
| 1:F:83:TYR:OH    | 2:G:54:PHE:O     | 1.94                     | 0.86              |
| 4:c:118:GLU:HB3  | 6:u:147:GLY:HA2  | 1.57                     | 0.85              |
| 6:u:20:LYS:O     | 7:w:7:LYS:NZ     | 2.09                     | 0.85              |
| 4:b:31:ASN:HB3   | 4:b:32:PRO:HD2   | 1.59                     | 0.85              |
| 4:b:175:LEU:HD12 | 5:m:1:MET:HE1    | 1.59                     | 0.85              |
| 2:J:90:CYS:HB2   | 2:J:94:TYR:HB3   | 1.59                     | 0.85              |
| 4:c:118:GLU:HB2  | 4:d:35:SER:HA    | 1.59                     | 0.85              |
| 4:d:141:LYS:HG2  | 4:d:150:ALA:HB1  | 1.57                     | 0.85              |
| 2:M:21:THR:OG1   | 3:r:52:GLU:OE2   | 1.95                     | 0.85              |
| 4:a:119:THR:HG22 | 6:t:166:ASN:ND2  | 1.91                     | 0.85              |
| 4:d:116:ILE:HG23 | 4:e:36:GLY:HA3   | 1.58                     | 0.85              |
| 2:C:21:THR:OG1   | 3:n:52:GLU:OE2   | 1.94                     | 0.84              |
| 1:I:13:LYS:NZ    | 1:I:21:GLU:OE2   | 2.10                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:a:115:LYS:HG2  | 4:b:34:GLU:HB3   | 1.57                     | 0.84              |
| 4:c:31:ASN:HB3   | 4:c:32:PRO:CD    | 2.06                     | 0.84              |
| 4:e:32:PRO:O     | 6:u:203:GLN:NE2  | 2.10                     | 0.84              |
| 1:O:266:LEU:HD13 | 1:O:278:LEU:HD22 | 1.59                     | 0.84              |
| 1:R:83:TYR:OH    | 2:S:54:PHE:O     | 1.95                     | 0.84              |
| 4:d:140:SER:OG   | 4:d:142:ASP:OD1  | 1.94                     | 0.84              |
| 4:d:94:ASP:OD1   | 4:e:21:LYS:NZ    | 2.10                     | 0.84              |
| 2:D:51:VAL:O     | 1:P:76:ARG:NH1   | 2.08                     | 0.84              |
| 4:c:173:GLN:OE1  | 4:c:177:LYS:HE2  | 1.77                     | 0.84              |
| 6:t:63:LEU:HA    | 7:y:58:VAL:HG11  | 1.59                     | 0.84              |
| 7:x:178:ASP:OD1  | 7:y:216:ARG:NH2  | 2.11                     | 0.84              |
| 4:d:157:VAL:HG13 | 6:v:186:ARG:NH2  | 1.92                     | 0.84              |
| 6:v:20:LYS:O     | 7:x:7:LYS:NZ     | 2.11                     | 0.84              |
| 6:t:55:LYS:O     | 7:w:109:SER:OG   | 1.96                     | 0.84              |
| 2:D:1:MET:N      | 1:P:73:GLU:O     | 2.11                     | 0.83              |
| 2:D:73:PHE:CD1   | 1:O:109:ILE:HD13 | 2.11                     | 0.83              |
| 6:t:151:THR:HG23 | 6:v:30:ARG:NE    | 1.91                     | 0.83              |
| 6:v:104:SER:N    | 7:y:113:SER:O    | 2.10                     | 0.83              |
| 4:e:119:THR:HG22 | 6:v:166:ASN:ND2  | 1.93                     | 0.83              |
| 1:F:198:ILE:HD11 | 1:F:284:GLN:OE1  | 1.78                     | 0.83              |
| 1:A:257:PRO:O    | 1:R:246:TYR:OH   | 1.97                     | 0.83              |
| 1:K:109:ILE:HD13 | 2:M:73:PHE:CD1   | 2.14                     | 0.83              |
| 1:L:83:TYR:OH    | 2:M:54:PHE:O     | 1.94                     | 0.83              |
| 6:t:67:VAL:HG23  | 7:y:58:VAL:HG23  | 1.58                     | 0.83              |
| 4:f:31:ASN:HB3   | 4:f:32:PRO:HD2   | 1.61                     | 0.83              |
| 6:u:97:ARG:NE    | 7:w:51:TYR:O     | 2.11                     | 0.83              |
| 4:f:158:ASN:HA   | 6:t:186:ARG:NH1  | 1.93                     | 0.82              |
| 6:u:165:ILE:HD12 | 6:u:207:TRP:HE3  | 1.43                     | 0.82              |
| 6:v:67:VAL:HG23  | 7:x:58:VAL:HG23  | 1.60                     | 0.82              |
| 6:v:99:TYR:HB2   | 7:x:52:LYS:HD2   | 1.61                     | 0.82              |
| 4:e:118:GLU:HB2  | 4:f:35:SER:HA    | 1.60                     | 0.82              |
| 2:G:82:THR:O     | 2:G:99:GLN:NE2   | 2.13                     | 0.82              |
| 1:I:209:ARG:NH1  | 1:I:260:GLU:OE1  | 2.12                     | 0.82              |
| 1:L:278:LEU:HD22 | 1:L:280:MET:HE2  | 1.59                     | 0.82              |
| 4:a:116:ILE:CA   | 4:b:36:GLY:HA3   | 2.09                     | 0.82              |
| 4:e:142:ASP:O    | 3:n:57:LYS:NZ    | 2.12                     | 0.82              |
| 4:d:162:LYS:HD3  | 6:v:186:ARG:HB3  | 1.60                     | 0.82              |
| 4:a:32:PRO:O     | 6:v:203:GLN:NE2  | 2.12                     | 0.82              |
| 4:a:173:GLN:NE2  | 4:a:177:LYS:HE2  | 1.94                     | 0.82              |
| 1:A:109:ILE:CD1  | 2:C:73:PHE:CE1   | 2.63                     | 0.81              |
| 1:P:223:MET:HE3  | 1:P:295:VAL:HG11 | 1.61                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:c:119:THR:OG1  | 4:d:37:ALA:O     | 1.97                     | 0.81              |
| 6:v:101:MET:C    | 7:y:112:ASP:O    | 2.23                     | 0.81              |
| 1:E:83:TYR:O     | 1:F:84:ARG:NH1   | 2.13                     | 0.81              |
| 4:c:32:PRO:O     | 6:t:203:GLN:NE2  | 2.13                     | 0.81              |
| 6:v:97:ARG:NH1   | 7:x:48:GLN:OE1   | 2.12                     | 0.81              |
| 6:v:98:PRO:HA    | 7:x:52:LYS:HE3   | 1.62                     | 0.81              |
| 7:w:95:GLN:NE2   | 7:w:122:GLU:OE2  | 2.13                     | 0.81              |
| 4:b:158:ASN:HA   | 6:u:186:ARG:NH1  | 1.94                     | 0.81              |
| 6:u:97:ARG:O     | 7:w:52:LYS:HE3   | 1.80                     | 0.81              |
| 7:w:178:ASP:OD1  | 7:x:216:ARG:NH2  | 2.13                     | 0.81              |
| 6:v:97:ARG:O     | 7:x:52:LYS:HE3   | 1.80                     | 0.81              |
| 6:t:102:CYS:N    | 7:w:112:ASP:O    | 2.14                     | 0.81              |
| 7:x:129:GLU:OE1  | 7:y:71:ARG:NH2   | 2.13                     | 0.81              |
| 6:t:14:ASN:ND2   | 6:t:166:ASN:OD1  | 2.14                     | 0.81              |
| 6:t:101:MET:C    | 7:w:112:ASP:O    | 2.23                     | 0.81              |
| 4:b:118:GLU:H    | 4:c:36:GLY:N     | 1.78                     | 0.80              |
| 4:f:116:ILE:HG22 | 4:f:117:VAL:N    | 1.96                     | 0.80              |
| 6:u:22:LYS:O     | 6:u:42:GLY:N     | 2.14                     | 0.80              |
| 6:v:55:LYS:O     | 7:y:109:SER:OG   | 2.00                     | 0.80              |
| 1:L:76:ARG:NH1   | 2:M:4:LEU:HD21   | 1.97                     | 0.80              |
| 4:e:115:LYS:HG2  | 4:f:34:GLU:HB3   | 1.60                     | 0.80              |
| 2:D:59:ALA:O     | 2:D:130:ARG:NH2  | 2.14                     | 0.80              |
| 6:v:22:LYS:O     | 6:v:42:GLY:N     | 2.14                     | 0.80              |
| 1:H:249:ARG:NH1  | 1:P:253:GLU:OE1  | 2.14                     | 0.80              |
| 4:a:36:GLY:N     | 4:f:118:GLU:H    | 1.79                     | 0.80              |
| 6:u:102:CYS:HB2  | 7:x:110:ALA:HB1  | 1.64                     | 0.80              |
| 4:e:116:ILE:CA   | 4:f:36:GLY:HA3   | 2.12                     | 0.79              |
| 4:e:122:ALA:HB1  | 4:e:157:VAL:HA   | 1.63                     | 0.79              |
| 6:u:103:GLY:HA3  | 7:x:114:ARG:HB3  | 1.64                     | 0.79              |
| 4:e:172:ALA:HA   | 5:i:1:MET:HE2    | 1.64                     | 0.79              |
| 6:t:20:LYS:O     | 7:y:7:LYS:NZ     | 2.13                     | 0.79              |
| 1:L:264:VAL:O    | 1:L:276:PRO:HG3  | 1.82                     | 0.79              |
| 6:u:101:MET:C    | 7:x:112:ASP:O    | 2.25                     | 0.79              |
| 2:M:45:MET:HE2   | 2:M:45:MET:HA    | 1.63                     | 0.79              |
| 4:c:116:ILE:O    | 4:c:117:VAL:HG12 | 1.82                     | 0.79              |
| 6:v:96:LYS:N     | 7:x:61:ASP:OD2   | 2.15                     | 0.79              |
| 2:G:21:THR:OG1   | 3:o:52:GLU:OE2   | 2.01                     | 0.79              |
| 2:S:94:TYR:HE1   | 2:S:96:GLY:HA3   | 1.48                     | 0.78              |
| 6:t:46:LYS:NZ    | 6:t:77:GLU:OE2   | 2.16                     | 0.78              |
| 7:w:216:ARG:NH2  | 7:y:178:ASP:OD1  | 2.17                     | 0.78              |
| 4:d:116:ILE:HG22 | 4:d:117:VAL:H    | 1.46                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:76:ARG:NH1   | 2:C:4:LEU:HD21   | 1.98                     | 0.78              |
| 1:F:55:ASP:OD2   | 2:G:15:ARG:NH2   | 2.15                     | 0.78              |
| 4:e:31:ASN:HB3   | 4:e:32:PRO:CD    | 2.11                     | 0.78              |
| 1:E:109:ILE:HD11 | 2:G:77:HIS:CE1   | 2.19                     | 0.78              |
| 1:Q:109:ILE:HD11 | 2:S:77:HIS:CE1   | 2.18                     | 0.78              |
| 4:e:118:GLU:H    | 4:f:36:GLY:C     | 1.92                     | 0.78              |
| 2:J:82:THR:O     | 2:J:99:GLN:NE2   | 2.17                     | 0.78              |
| 6:v:107:ARG:NH2  | 7:y:115:SER:OG   | 2.17                     | 0.78              |
| 1:F:76:ARG:NH1   | 2:G:4:LEU:HD21   | 1.99                     | 0.78              |
| 4:a:121:THR:HG22 | 6:t:166:ASN:CG   | 2.09                     | 0.78              |
| 6:u:101:MET:O    | 7:x:111:SER:C    | 2.27                     | 0.78              |
| 2:G:157:TRP:O    | 2:G:177:ARG:NH2  | 2.16                     | 0.78              |
| 4:d:118:GLU:H    | 4:e:36:GLY:N     | 1.81                     | 0.78              |
| 6:t:22:LYS:O     | 6:t:42:GLY:N     | 2.17                     | 0.77              |
| 1:A:109:ILE:CD1  | 2:C:73:PHE:CD1   | 2.66                     | 0.77              |
| 6:v:56:THR:HA    | 7:y:109:SER:OG   | 1.84                     | 0.77              |
| 7:w:215:VAL:HG11 | 7:y:180:MET:HE1  | 1.67                     | 0.77              |
| 4:e:158:ASN:HB3  | 6:v:168:GLU:OE2  | 1.85                     | 0.77              |
| 6:t:86:PHE:O     | 6:t:91:LYS:NZ    | 2.17                     | 0.77              |
| 6:t:104:SER:N    | 7:w:113:SER:O    | 2.17                     | 0.77              |
| 1:L:245:VAL:HG13 | 1:L:276:PRO:HG2  | 1.65                     | 0.77              |
| 2:S:87:GLY:C     | 2:S:100:LEU:HD12 | 2.10                     | 0.77              |
| 4:a:116:ILE:HG22 | 4:b:36:GLY:HA2   | 1.65                     | 0.77              |
| 6:u:102:CYS:N    | 7:x:112:ASP:O    | 2.18                     | 0.77              |
| 7:w:137:ASN:O    | 7:w:146:ARG:NH2  | 2.18                     | 0.77              |
| 4:f:116:ILE:CG2  | 4:f:117:VAL:H    | 1.99                     | 0.77              |
| 6:t:99:TYR:HD1   | 7:y:52:LYS:HB3   | 1.49                     | 0.77              |
| 7:x:56:ASN:O     | 7:x:58:VAL:HG23  | 1.85                     | 0.76              |
| 4:c:141:LYS:HG3  | 4:c:150:ALA:HB1  | 1.67                     | 0.76              |
| 4:a:31:ASN:HB3   | 4:a:32:PRO:CD    | 2.15                     | 0.76              |
| 4:c:142:ASP:O    | 3:r:57:LYS:NZ    | 2.18                     | 0.76              |
| 6:t:99:TYR:CD1   | 7:y:59:PRO:HA    | 2.21                     | 0.76              |
| 4:c:172:ALA:HA   | 5:j:1:MET:HE2    | 1.67                     | 0.76              |
| 1:Q:84:ARG:NH2   | 1:Q:101:ILE:O    | 2.18                     | 0.76              |
| 4:c:118:GLU:H    | 4:d:36:GLY:C     | 1.94                     | 0.76              |
| 5:k:34:ASP:O     | 5:k:35:ARG:NE    | 2.18                     | 0.76              |
| 2:D:109:SER:OG   | 2:D:116:TYR:HB2  | 1.85                     | 0.76              |
| 1:E:238:GLY:N    | 1:E:241:GLU:OE2  | 2.18                     | 0.75              |
| 2:G:87:GLY:C     | 2:G:100:LEU:HD12 | 2.12                     | 0.75              |
| 1:E:230:GLU:OE1  | 1:E:254:ARG:NH2  | 2.18                     | 0.75              |
| 4:f:162:LYS:HE3  | 6:t:186:ARG:HG2  | 1.65                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:97:ARG:O     | 7:y:52:LYS:NZ    | 2.19                     | 0.75              |
| 1:I:99:ARG:NH1   | 4:b:182:GLY:O    | 2.20                     | 0.75              |
| 3:q:78:GLU:OE2   | 3:q:82:LYS:NZ    | 2.14                     | 0.75              |
| 6:v:49:ARG:HG3   | 6:v:50:ARG:HG3   | 1.68                     | 0.75              |
| 4:b:142:ASP:O    | 3:q:57:LYS:NZ    | 2.20                     | 0.74              |
| 2:J:87:GLY:C     | 2:J:100:LEU:HD12 | 2.11                     | 0.74              |
| 6:v:14:ASN:ND2   | 6:v:166:ASN:OD1  | 2.18                     | 0.74              |
| 4:f:141:LYS:HG2  | 4:f:150:ALA:HB1  | 1.67                     | 0.74              |
| 1:I:246:TYR:OH   | 1:K:257:PRO:O    | 2.04                     | 0.74              |
| 4:a:119:THR:OG1  | 4:b:37:ALA:O     | 2.05                     | 0.74              |
| 6:u:99:TYR:O     | 7:x:109:SER:HB2  | 1.88                     | 0.74              |
| 4:b:116:ILE:N    | 4:c:34:GLU:HB2   | 2.02                     | 0.74              |
| 4:a:172:ALA:O    | 4:a:176:LEU:HD23 | 1.88                     | 0.74              |
| 6:v:157:ASN:ND2  | 6:v:223:ASP:OD2  | 2.20                     | 0.74              |
| 1:F:246:TYR:OH   | 1:O:257:PRO:O    | 2.05                     | 0.74              |
| 2:S:3:ASN:O      | 2:S:3:ASN:ND2    | 2.16                     | 0.74              |
| 4:a:173:GLN:HE22 | 4:a:177:LYS:CE   | 1.98                     | 0.74              |
| 6:u:101:MET:O    | 7:x:110:ALA:C    | 2.31                     | 0.73              |
| 2:C:177:ARG:N    | 2:C:208:GLN:O    | 2.21                     | 0.73              |
| 5:i:81:THR:N     | 5:i:84:ASN:OD1   | 2.21                     | 0.73              |
| 2:J:94:TYR:CE2   | 2:J:96:GLY:HA3   | 2.23                     | 0.73              |
| 1:O:200:THR:HG23 | 1:O:278:LEU:HD21 | 1.70                     | 0.73              |
| 6:t:143:THR:HG22 | 6:t:178:LYS:HB2  | 1.70                     | 0.73              |
| 6:u:54:SER:HA    | 7:x:111:SER:C    | 2.13                     | 0.73              |
| 4:a:118:GLU:H    | 4:b:36:GLY:C     | 1.95                     | 0.73              |
| 6:t:57:ILE:HG21  | 7:y:59:PRO:CG    | 2.15                     | 0.73              |
| 7:x:12:ASP:O     | 7:x:16:VAL:HG23  | 1.88                     | 0.73              |
| 1:A:107:ALA:HB2  | 1:R:215:CYS:SG   | 2.29                     | 0.73              |
| 6:u:55:LYS:O     | 7:x:109:SER:OG   | 2.06                     | 0.73              |
| 6:v:100:SER:HA   | 7:y:109:SER:HB2  | 1.71                     | 0.73              |
| 1:O:227:LEU:HD13 | 1:O:252:MET:SD   | 2.29                     | 0.73              |
| 2:S:86:VAL:HA    | 2:S:101:ALA:HB3  | 1.71                     | 0.73              |
| 4:d:115:LYS:O    | 4:d:116:ILE:HG13 | 1.89                     | 0.73              |
| 2:D:76:CYS:CB    | 2:D:122:CYS:HA   | 2.20                     | 0.72              |
| 6:t:102:CYS:SG   | 7:w:98:SER:OG    | 2.44                     | 0.72              |
| 6:v:154:ILE:HD12 | 6:v:187:LYS:HG3  | 1.69                     | 0.72              |
| 1:E:280:MET:HE3  | 1:E:286:MET:HG3  | 1.71                     | 0.72              |
| 1:A:109:ILE:HD12 | 2:C:73:PHE:CE1   | 2.23                     | 0.72              |
| 1:H:175:GLY:O    | 1:H:191:ARG:NH2  | 2.22                     | 0.72              |
| 1:A:109:ILE:HD11 | 2:C:77:HIS:CE1   | 2.25                     | 0.72              |
| 1:R:11:VAL:HG22  | 5:k:49:THR:HG21  | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:173:MET:HE1  | 1:P:190:ILE:HG23 | 1.71                     | 0.72              |
| 1:R:73:GLU:OE1   | 5:k:52:ARG:NH1   | 2.22                     | 0.72              |
| 4:a:115:LYS:CG   | 4:b:34:GLU:HB3   | 2.19                     | 0.72              |
| 4:a:172:ALA:HA   | 5:l:1:MET:HE2    | 1.71                     | 0.72              |
| 1:E:109:ILE:HD12 | 2:G:73:PHE:HE1   | 1.53                     | 0.72              |
| 6:v:97:ARG:O     | 7:x:52:LYS:CE    | 2.38                     | 0.72              |
| 4:b:159:ALA:HB3  | 6:u:186:ARG:HD2  | 1.72                     | 0.72              |
| 4:f:157:VAL:O    | 6:t:186:ARG:NH2  | 2.22                     | 0.72              |
| 6:t:97:ARG:HG3   | 7:y:52:LYS:HG3   | 1.71                     | 0.72              |
| 6:t:99:TYR:CD1   | 7:y:52:LYS:HB3   | 2.24                     | 0.72              |
| 2:J:86:VAL:HA    | 2:J:101:ALA:HB3  | 1.70                     | 0.72              |
| 6:v:54:SER:HA    | 7:y:111:SER:C    | 2.14                     | 0.72              |
| 7:y:96:MET:HE3   | 7:y:97:ARG:HG3   | 1.69                     | 0.72              |
| 4:e:116:ILE:O    | 4:e:117:VAL:HG12 | 1.89                     | 0.72              |
| 7:w:191:ASN:ND2  | 7:w:199:ASN:O    | 2.23                     | 0.72              |
| 1:P:59:ARG:HG3   | 5:l:32:THR:HG21  | 1.72                     | 0.72              |
| 4:e:177:LYS:HE2  | 5:i:106:ALA:OXT  | 1.89                     | 0.72              |
| 4:f:138:ASN:O    | 4:f:143:LYS:NZ   | 2.23                     | 0.72              |
| 2:M:177:ARG:N    | 2:M:208:GLN:O    | 2.23                     | 0.71              |
| 6:t:109:LEU:HD23 | 6:t:112:LEU:HD11 | 1.72                     | 0.71              |
| 2:C:76:CYS:CB    | 2:C:122:CYS:HA   | 2.19                     | 0.71              |
| 6:u:98:PRO:HA    | 7:w:52:LYS:HE3   | 1.72                     | 0.71              |
| 1:B:59:ARG:HG3   | 5:i:32:THR:HG21  | 1.71                     | 0.71              |
| 2:D:106:PRO:HG3  | 2:D:182:THR:HG22 | 1.72                     | 0.71              |
| 4:c:56:ASP:OD2   | 4:c:62:THR:OG1   | 2.07                     | 0.71              |
| 1:A:26:MET:HE1   | 2:C:32:LEU:HD12  | 1.71                     | 0.71              |
| 4:a:56:ASP:OD2   | 4:a:62:THR:OG1   | 2.08                     | 0.71              |
| 7:w:189:GLN:NE2  | 7:w:190:ILE:O    | 2.23                     | 0.71              |
| 2:M:76:CYS:CB    | 2:M:122:CYS:HA   | 2.20                     | 0.71              |
| 4:e:119:THR:OG1  | 4:f:37:ALA:O     | 2.08                     | 0.71              |
| 6:t:101:MET:O    | 7:w:111:SER:C    | 2.33                     | 0.71              |
| 6:u:103:GLY:H    | 7:x:112:ASP:CG   | 1.98                     | 0.71              |
| 6:v:97:ARG:N     | 7:x:61:ASP:OD2   | 2.24                     | 0.71              |
| 7:x:52:LYS:HG2   | 7:x:61:ASP:OD1   | 1.91                     | 0.71              |
| 6:t:67:VAL:HG23  | 7:y:58:VAL:CG2   | 2.21                     | 0.71              |
| 7:w:12:ASP:O     | 7:w:16:VAL:HG23  | 1.91                     | 0.71              |
| 1:H:26:MET:HE1   | 2:J:32:LEU:HD12  | 1.73                     | 0.71              |
| 3:q:40:GLN:O     | 3:q:44:GLN:NE2   | 2.24                     | 0.70              |
| 6:t:108:GLU:OE1  | 6:t:111:THR:HG21 | 1.90                     | 0.70              |
| 1:A:111:LEU:HD11 | 1:A:131:VAL:HG21 | 1.71                     | 0.70              |
| 2:S:94:TYR:CE1   | 2:S:96:GLY:HA3   | 2.26                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:103:GLY:HA2  | 7:y:114:ARG:HD2  | 1.73                     | 0.70              |
| 1:O:275:THR:C    | 1:O:277:PRO:HD3  | 2.15                     | 0.70              |
| 4:c:121:THR:HG21 | 6:u:166:ASN:C    | 2.16                     | 0.70              |
| 1:A:108:ARG:HG3  | 2:C:235:TYR:CE1  | 2.26                     | 0.70              |
| 4:d:116:ILE:H    | 4:e:34:GLU:HB2   | 1.55                     | 0.70              |
| 5:h:20:ASP:N     | 6:t:219:ASP:OD2  | 2.23                     | 0.70              |
| 6:t:103:GLY:H    | 7:w:112:ASP:CG   | 1.99                     | 0.70              |
| 1:B:83:TYR:OH    | 2:C:54:PHE:O     | 2.08                     | 0.70              |
| 1:P:207:GLN:OE1  | 1:P:209:ARG:NH2  | 2.25                     | 0.70              |
| 4:d:116:ILE:HG22 | 4:e:37:ALA:H     | 1.55                     | 0.70              |
| 4:d:157:VAL:O    | 6:v:186:ARG:NH2  | 2.24                     | 0.70              |
| 4:e:118:GLU:HB3  | 6:v:147:GLY:CA   | 2.22                     | 0.70              |
| 6:t:104:SER:O    | 7:w:113:SER:OG   | 2.08                     | 0.70              |
| 1:F:76:ARG:NH2   | 2:G:1:MET:SD     | 2.65                     | 0.70              |
| 1:L:107:ALA:HB2  | 2:M:142:GLY:O    | 1.92                     | 0.70              |
| 4:c:118:GLU:N    | 4:d:36:GLY:H     | 1.90                     | 0.70              |
| 1:A:211:LEU:O    | 1:A:214:GLY:N    | 2.25                     | 0.70              |
| 1:P:201:SER:OG   | 1:P:267:SER:OG   | 2.08                     | 0.70              |
| 4:a:2:ILE:HG22   | 4:a:4:ALA:H      | 1.56                     | 0.70              |
| 6:u:14:ASN:ND2   | 6:u:166:ASN:OD1  | 2.25                     | 0.70              |
| 4:a:29:THR:OG1   | 6:v:34:ASP:OD1   | 2.08                     | 0.70              |
| 1:L:280:MET:HE3  | 1:L:286:MET:HG2  | 1.74                     | 0.70              |
| 3:X:40:GLN:O     | 3:X:44:GLN:NE2   | 2.25                     | 0.70              |
| 7:w:133:ASP:O    | 7:x:43:ARG:NH1   | 2.25                     | 0.70              |
| 1:A:109:ILE:HD13 | 2:C:73:PHE:HD1   | 1.56                     | 0.69              |
| 2:D:2:SER:O      | 2:D:4:LEU:HD12   | 1.92                     | 0.69              |
| 1:I:121:ILE:HD11 | 1:I:162:LEU:HD13 | 1.74                     | 0.69              |
| 4:e:29:THR:OG1   | 6:u:34:ASP:OD1   | 2.08                     | 0.69              |
| 2:G:106:PRO:HG2  | 2:G:182:THR:HG23 | 1.73                     | 0.69              |
| 6:v:101:MET:O    | 7:y:111:SER:C    | 2.35                     | 0.69              |
| 2:C:94:TYR:CE2   | 2:C:96:GLY:HA3   | 2.28                     | 0.69              |
| 2:C:114:SER:OG   | 2:C:115:PRO:HD3  | 1.93                     | 0.69              |
| 4:b:162:LYS:HE3  | 6:u:186:ARG:CB   | 2.22                     | 0.69              |
| 6:v:103:GLY:CA   | 7:y:114:ARG:HD2  | 2.23                     | 0.69              |
| 7:w:190:ILE:HD11 | 7:x:200:HIS:CE1  | 2.28                     | 0.69              |
| 7:y:46:THR:HG23  | 7:y:66:GLN:OE1   | 1.91                     | 0.69              |
| 1:K:227:LEU:HD13 | 1:K:252:MET:SD   | 2.33                     | 0.69              |
| 4:d:33:ILE:HD11  | 6:t:30:ARG:HH12  | 1.56                     | 0.69              |
| 6:u:99:TYR:CB    | 7:w:52:LYS:HD2   | 2.19                     | 0.69              |
| 4:c:115:LYS:HG3  | 4:d:34:GLU:HB3   | 1.74                     | 0.69              |
| 4:e:121:THR:HG21 | 6:v:167:PRO:HD2  | 1.73                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:103:GLY:HA3  | 7:y:114:ARG:N    | 2.08                     | 0.69              |
| 4:c:119:THR:HG23 | 4:d:39:VAL:HG21  | 1.73                     | 0.69              |
| 2:D:177:ARG:N    | 2:D:208:GLN:O    | 2.25                     | 0.69              |
| 6:t:99:TYR:CE1   | 7:y:59:PRO:HA    | 2.28                     | 0.69              |
| 1:I:212:LYS:NZ   | 1:K:239:ASN:O    | 2.25                     | 0.69              |
| 1:K:109:ILE:CD1  | 2:M:77:HIS:CE1   | 2.75                     | 0.69              |
| 4:a:116:ILE:O    | 4:a:117:VAL:HG12 | 1.93                     | 0.69              |
| 4:f:159:ALA:HB3  | 6:t:186:ARG:HD2  | 1.74                     | 0.69              |
| 6:t:30:ARG:HG3   | 6:u:151:THR:HG23 | 1.74                     | 0.69              |
| 4:a:121:THR:HG22 | 6:t:166:ASN:OD1  | 1.93                     | 0.69              |
| 5:k:20:ASP:N     | 6:v:219:ASP:OD2  | 2.25                     | 0.69              |
| 6:t:74:MET:CE    | 6:t:109:LEU:HD11 | 2.23                     | 0.69              |
| 6:t:151:THR:HG22 | 6:t:181:VAL:HG21 | 1.75                     | 0.69              |
| 6:v:101:MET:O    | 7:y:110:ALA:C    | 2.36                     | 0.69              |
| 1:B:107:ALA:HB2  | 2:C:142:GLY:O    | 1.93                     | 0.68              |
| 6:v:86:PHE:O     | 6:v:91:LYS:NZ    | 2.25                     | 0.68              |
| 2:D:77:HIS:CE1   | 1:O:109:ILE:HD11 | 2.28                     | 0.68              |
| 2:M:94:TYR:CE2   | 2:M:96:GLY:HA3   | 2.28                     | 0.68              |
| 6:v:24:ARG:N     | 6:v:40:SER:O     | 2.24                     | 0.68              |
| 1:F:97:PHE:O     | 1:F:101:ILE:HD12 | 1.93                     | 0.68              |
| 2:M:109:SER:OG   | 2:M:116:TYR:HB2  | 1.94                     | 0.68              |
| 4:a:118:GLU:N    | 4:b:36:GLY:H     | 1.92                     | 0.68              |
| 6:t:112:LEU:HD13 | 7:y:57:GLY:H     | 1.59                     | 0.68              |
| 4:c:118:GLU:HB3  | 6:u:147:GLY:CA   | 2.22                     | 0.68              |
| 5:l:36:TRP:HB3   | 5:l:53:LEU:HD12  | 1.75                     | 0.68              |
| 1:B:76:ARG:NH2   | 2:C:1:MET:SD     | 2.67                     | 0.68              |
| 2:M:51:VAL:HG23  | 2:M:52:GLU:OE1   | 1.92                     | 0.68              |
| 1:Q:113:ASP:OD1  | 1:Q:114:LEU:N    | 2.27                     | 0.68              |
| 6:u:103:GLY:HA3  | 7:x:114:ARG:CB   | 2.24                     | 0.68              |
| 4:c:158:ASN:HB3  | 6:u:168:GLU:OE2  | 1.93                     | 0.68              |
| 6:v:97:ARG:HD2   | 7:x:49:PRO:C     | 2.18                     | 0.68              |
| 1:B:209:ARG:NH2  | 1:B:260:GLU:OE1  | 2.26                     | 0.68              |
| 7:w:101:ASN:ND2  | 7:w:109:SER:O    | 2.26                     | 0.68              |
| 1:E:113:ASP:OD1  | 1:E:114:LEU:N    | 2.26                     | 0.67              |
| 1:R:59:ARG:HG3   | 5:k:32:THR:HG21  | 1.76                     | 0.67              |
| 4:a:118:GLU:HB3  | 6:t:147:GLY:CA   | 2.24                     | 0.67              |
| 1:F:23:GLU:OE2   | 4:f:135:LYS:HB3  | 1.94                     | 0.67              |
| 1:H:109:ILE:HD11 | 2:J:77:HIS:CE1   | 2.29                     | 0.67              |
| 1:O:132:ASN:ND2  | 1:O:142:ILE:O    | 2.26                     | 0.67              |
| 4:e:118:GLU:N    | 4:f:36:GLY:H     | 1.92                     | 0.67              |
| 4:e:121:THR:HB   | 6:v:166:ASN:HB3  | 1.75                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:159:ALA:HB1  | 4:e:162:LYS:HE3  | 1.76                     | 0.67              |
| 6:t:100:SER:HA   | 7:w:109:SER:HB2  | 1.75                     | 0.67              |
| 6:u:143:THR:N    | 6:u:146:THR:OG1  | 2.27                     | 0.67              |
| 6:v:99:TYR:HD1   | 7:x:52:LYS:HB2   | 1.59                     | 0.67              |
| 4:a:116:ILE:HG22 | 4:b:36:GLY:CA    | 2.23                     | 0.67              |
| 4:e:140:SER:OG   | 4:e:142:ASP:OD1  | 2.11                     | 0.67              |
| 7:w:177:ALA:HB2  | 7:x:215:VAL:HG23 | 1.77                     | 0.67              |
| 2:G:94:TYR:CE2   | 2:G:96:GLY:HA3   | 2.28                     | 0.67              |
| 1:l:59:ARG:HG3   | 5:m:32:THR:HG21  | 1.74                     | 0.67              |
| 6:u:99:TYR:HB2   | 7:w:52:LYS:CD    | 2.21                     | 0.67              |
| 2:D:235:TYR:CE1  | 1:O:108:ARG:HD2  | 2.30                     | 0.67              |
| 2:S:51:VAL:HG23  | 2:S:52:GLU:OE1   | 1.93                     | 0.67              |
| 4:a:84:MET:HE3   | 3:p:76:LEU:HD11  | 1.77                     | 0.67              |
| 6:t:54:SER:HA    | 7:w:111:SER:C    | 2.20                     | 0.67              |
| 4:c:118:GLU:H    | 4:d:36:GLY:CA    | 2.08                     | 0.67              |
| 6:u:56:THR:N     | 7:x:109:SER:O    | 2.27                     | 0.67              |
| 7:y:96:MET:HE3   | 7:y:97:ARG:CG    | 2.25                     | 0.67              |
| 1:A:109:ILE:HD11 | 2:C:77:HIS:HE1   | 1.58                     | 0.67              |
| 6:v:67:VAL:HG23  | 7:x:58:VAL:CG2   | 2.24                     | 0.67              |
| 1:L:257:PRO:O    | 1:Q:246:TYR:OH   | 2.13                     | 0.67              |
| 4:b:117:VAL:H    | 4:c:36:GLY:HA3   | 1.60                     | 0.67              |
| 7:x:189:GLN:NE2  | 7:x:190:ILE:O    | 2.28                     | 0.67              |
| 6:t:56:THR:HA    | 7:w:109:SER:OG   | 1.94                     | 0.66              |
| 6:u:107:ARG:NH2  | 7:x:115:SER:OG   | 2.27                     | 0.66              |
| 1:B:242:ASP:O    | 1:B:244:THR:OG1  | 2.12                     | 0.66              |
| 6:u:104:SER:N    | 7:x:113:SER:O    | 2.27                     | 0.66              |
| 7:w:96:MET:HE3   | 7:w:97:ARG:HG3   | 1.75                     | 0.66              |
| 2:G:177:ARG:N    | 2:G:208:GLN:O    | 2.28                     | 0.66              |
| 2:G:213:GLY:N    | 2:G:218:TRP:HE1  | 1.94                     | 0.66              |
| 1:K:109:ILE:CD1  | 2:M:77:HIS:HE1   | 1.96                     | 0.66              |
| 1:L:201:SER:OG   | 1:L:267:SER:OG   | 2.11                     | 0.66              |
| 2:S:106:PRO:HG2  | 2:S:182:THR:HG22 | 1.77                     | 0.66              |
| 4:b:158:ASN:HA   | 6:u:186:ARG:HH12 | 1.60                     | 0.66              |
| 1:F:76:ARG:CZ    | 2:G:4:LEU:HD11   | 2.26                     | 0.66              |
| 4:d:41:ASP:HB3   | 6:u:6:TYR:HD1    | 1.60                     | 0.66              |
| 4:d:122:ALA:HA   | 4:d:158:ASN:O    | 1.95                     | 0.66              |
| 4:e:115:LYS:CG   | 4:f:34:GLU:HB3   | 2.25                     | 0.66              |
| 4:e:121:THR:HG22 | 6:v:166:ASN:CG   | 2.19                     | 0.66              |
| 4:f:67:VAL:O     | 4:f:71:GLU:OE1   | 2.14                     | 0.66              |
| 6:v:56:THR:CA    | 7:y:109:SER:OG   | 2.44                     | 0.66              |
| 7:y:55:PHE:HD2   | 7:y:60:THR:HG1   | 1.44                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:u:102:CYS:HA   | 7:x:112:ASP:N    | 2.11                     | 0.66              |
| 6:v:109:LEU:HD23 | 6:v:112:LEU:HD11 | 1.78                     | 0.66              |
| 1:K:132:ASN:ND2  | 1:K:142:ILE:O    | 2.27                     | 0.66              |
| 1:P:42:LEU:HD12  | 3:p:9:LEU:HD12   | 1.76                     | 0.66              |
| 4:c:177:LYS:NZ   | 5:j:106:ALA:OXT  | 2.29                     | 0.66              |
| 4:d:67:VAL:O     | 4:d:71:GLU:OE1   | 2.14                     | 0.66              |
| 4:b:162:LYS:HE3  | 6:u:186:ARG:HG2  | 1.76                     | 0.66              |
| 6:t:63:LEU:HD23  | 6:t:90:VAL:HG13  | 1.76                     | 0.66              |
| 1:R:175:GLY:O    | 1:R:191:ARG:NH2  | 2.29                     | 0.66              |
| 4:e:121:THR:OG1  | 6:v:168:GLU:N    | 2.26                     | 0.66              |
| 7:x:47:VAL:HG11  | 7:x:92:LEU:HD21  | 1.77                     | 0.66              |
| 4:a:118:GLU:HB2  | 4:b:35:SER:CA    | 2.22                     | 0.65              |
| 4:d:116:ILE:N    | 4:e:34:GLU:HB2   | 2.10                     | 0.65              |
| 5:j:42:LEU:HD11  | 5:j:65:LEU:HD22  | 1.77                     | 0.65              |
| 6:v:102:CYS:HA   | 7:y:112:ASP:N    | 2.11                     | 0.65              |
| 7:w:125:ILE:HG23 | 7:x:75:MET:HG2   | 1.78                     | 0.65              |
| 7:w:190:ILE:HD11 | 7:x:200:HIS:ND1  | 2.10                     | 0.65              |
| 2:D:51:VAL:HG23  | 2:D:52:GLU:OE2   | 1.96                     | 0.65              |
| 3:X:6:ARG:NH2    | 3:X:118:GLU:OE1  | 2.28                     | 0.65              |
| 4:a:2:ILE:HD11   | 4:f:103:LYS:HA   | 1.76                     | 0.65              |
| 2:D:84:PRO:HD3   | 2:D:185:ARG:NH1  | 2.12                     | 0.65              |
| 4:a:36:GLY:HA3   | 4:f:117:VAL:H    | 1.61                     | 0.65              |
| 4:d:116:ILE:HG22 | 4:d:117:VAL:N    | 2.12                     | 0.65              |
| 6:v:53:ILE:HG23  | 7:y:112:ASP:HA   | 1.78                     | 0.65              |
| 6:v:103:GLY:H    | 7:y:112:ASP:CG   | 2.03                     | 0.65              |
| 2:D:73:PHE:CE1   | 1:O:109:ILE:CD1  | 2.79                     | 0.65              |
| 4:b:141:LYS:HG3  | 4:b:150:ALA:HB1  | 1.77                     | 0.65              |
| 6:t:100:SER:CA   | 7:w:109:SER:HB2  | 2.26                     | 0.65              |
| 6:t:103:GLY:N    | 7:w:113:SER:N    | 2.45                     | 0.65              |
| 4:b:157:VAL:O    | 6:u:186:ARG:NH2  | 2.29                     | 0.65              |
| 6:t:101:MET:O    | 7:w:110:ALA:C    | 2.39                     | 0.65              |
| 6:t:108:GLU:HG3  | 7:w:113:SER:HB2  | 1.78                     | 0.65              |
| 6:v:54:SER:HA    | 7:y:111:SER:CA   | 2.27                     | 0.65              |
| 6:u:103:GLY:N    | 7:x:112:ASP:C    | 2.55                     | 0.65              |
| 6:v:104:SER:O    | 7:y:113:SER:OG   | 2.15                     | 0.65              |
| 2:G:86:VAL:HA    | 2:G:101:ALA:HB3  | 1.78                     | 0.65              |
| 2:M:87:GLY:C     | 2:M:100:LEU:HD12 | 2.21                     | 0.65              |
| 4:a:122:ALA:HB1  | 4:a:157:VAL:HA   | 1.79                     | 0.65              |
| 4:f:162:LYS:HE3  | 6:t:186:ARG:CG   | 2.25                     | 0.65              |
| 6:t:63:LEU:CA    | 7:y:58:VAL:HG11  | 2.27                     | 0.65              |
| 6:u:99:TYR:C     | 7:x:109:SER:HB2  | 2.22                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:u:181:VAL:HG12 | 6:u:185:ASN:OD1  | 1.97                     | 0.65              |
| 7:x:53:PRO:HD3   | 7:x:62:MET:HE3   | 1.78                     | 0.65              |
| 1:B:223:MET:HE3  | 1:B:295:VAL:HG11 | 1.79                     | 0.65              |
| 6:t:24:ARG:N     | 6:t:40:SER:O     | 2.26                     | 0.65              |
| 6:t:55:LYS:N     | 7:w:111:SER:O    | 2.30                     | 0.65              |
| 6:t:102:CYS:HA   | 7:w:112:ASP:N    | 2.12                     | 0.65              |
| 2:J:84:PRO:HA    | 2:J:99:GLN:HG3   | 1.78                     | 0.65              |
| 4:c:118:GLU:HB2  | 4:d:35:SER:CA    | 2.27                     | 0.65              |
| 4:f:162:LYS:HE3  | 6:t:186:ARG:CB   | 2.27                     | 0.65              |
| 5:m:53:LEU:HB3   | 5:m:72:LEU:HD11  | 1.79                     | 0.65              |
| 6:u:24:ARG:N     | 6:u:40:SER:O     | 2.29                     | 0.65              |
| 6:u:99:TYR:HE2   | 6:u:101:MET:HE3  | 1.61                     | 0.64              |
| 3:p:9:LEU:HD21   | 3:p:29:LEU:HD21  | 1.79                     | 0.64              |
| 6:u:109:LEU:HD23 | 6:u:112:LEU:HD11 | 1.79                     | 0.64              |
| 6:t:103:GLY:CA   | 7:w:114:ARG:HG3  | 2.27                     | 0.64              |
| 7:x:101:ASN:ND2  | 7:x:109:SER:O    | 2.30                     | 0.64              |
| 1:B:11:VAL:HG22  | 5:i:49:THR:HG21  | 1.78                     | 0.64              |
| 6:v:108:GLU:HA   | 6:v:111:THR:HG22 | 1.79                     | 0.64              |
| 1:B:56:LEU:HD12  | 2:C:44:SER:CB    | 2.28                     | 0.64              |
| 1:P:11:VAL:HG22  | 5:l:49:THR:HG21  | 1.80                     | 0.64              |
| 7:w:180:MET:CE   | 7:x:215:VAL:HG21 | 2.28                     | 0.64              |
| 2:S:84:PRO:HA    | 2:S:99:GLN:HG3   | 1.80                     | 0.64              |
| 2:S:90:CYS:HB2   | 2:S:94:TYR:HB3   | 1.80                     | 0.64              |
| 6:t:95:LEU:HD21  | 7:y:59:PRO:O     | 1.97                     | 0.64              |
| 6:u:103:GLY:HA3  | 7:x:114:ARG:N    | 2.13                     | 0.64              |
| 6:v:103:GLY:N    | 7:y:112:ASP:C    | 2.56                     | 0.64              |
| 6:v:103:GLY:HA2  | 7:y:114:ARG:HH11 | 1.63                     | 0.64              |
| 2:D:105:GLU:OE2  | 2:D:107:GLY:N    | 2.30                     | 0.64              |
| 2:S:106:PRO:HG2  | 2:S:182:THR:CG2  | 2.28                     | 0.64              |
| 7:w:56:ASN:O     | 7:w:58:VAL:HG23  | 1.98                     | 0.64              |
| 2:D:50:MET:HE2   | 1:O:64:TYR:HB2   | 1.79                     | 0.64              |
| 1:I:164:ARG:HH22 | 2:J:166:THR:HG21 | 1.63                     | 0.64              |
| 6:t:53:ILE:HG23  | 7:w:112:ASP:HA   | 1.80                     | 0.64              |
| 6:t:99:TYR:HA    | 7:y:52:LYS:HB2   | 1.80                     | 0.63              |
| 6:u:99:TYR:CD1   | 7:w:59:PRO:HA    | 2.33                     | 0.63              |
| 1:B:268:GLN:O    | 1:B:271:ALA:N    | 2.31                     | 0.63              |
| 1:I:83:TYR:OH    | 2:J:54:PHE:O     | 2.16                     | 0.63              |
| 2:S:114:SER:OG   | 2:S:115:PRO:HD3  | 1.97                     | 0.63              |
| 2:G:71:LEU:HD22  | 2:G:140:MET:SD   | 2.38                     | 0.63              |
| 6:u:157:ASN:ND2  | 6:u:223:ASP:OD2  | 2.31                     | 0.63              |
| 6:v:108:GLU:HG3  | 7:y:113:SER:HB2  | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:26:MET:HE1   | 2:M:32:LEU:HD12  | 1.80                     | 0.63              |
| 1:O:164:ARG:HB2  | 1:O:190:ILE:HD11 | 1.81                     | 0.63              |
| 6:u:97:ARG:O     | 7:w:52:LYS:CE    | 2.46                     | 0.63              |
| 6:v:70:ILE:HG22  | 6:v:74:MET:HE2   | 1.80                     | 0.63              |
| 1:I:56:LEU:HD12  | 2:J:44:SER:CB    | 2.28                     | 0.63              |
| 2:S:89:ASP:HA    | 2:S:94:TYR:HE2   | 1.64                     | 0.63              |
| 4:e:116:ILE:HG22 | 4:f:36:GLY:HA2   | 1.81                     | 0.63              |
| 7:w:43:ARG:O     | 7:w:70:LEU:N     | 2.30                     | 0.63              |
| 2:G:82:THR:O     | 2:G:82:THR:HG23  | 1.98                     | 0.63              |
| 4:a:119:THR:HG23 | 4:b:39:VAL:HG21  | 1.80                     | 0.63              |
| 4:e:125:SER:HB3  | 6:v:141:LEU:HB2  | 1.81                     | 0.63              |
| 4:a:118:GLU:H    | 4:b:36:GLY:CA    | 2.12                     | 0.62              |
| 4:c:32:PRO:HB2   | 6:t:202:ASN:HB2  | 1.81                     | 0.62              |
| 5:m:15:SER:OG    | 5:m:22:ARG:NE    | 2.27                     | 0.62              |
| 1:F:268:GLN:O    | 1:F:271:ALA:N    | 2.32                     | 0.62              |
| 1:L:95:GLU:OE2   | 1:L:99:ARG:NH2   | 2.32                     | 0.62              |
| 5:h:53:LEU:HB3   | 5:h:72:LEU:HD11  | 1.80                     | 0.62              |
| 6:v:99:TYR:CD1   | 7:x:59:PRO:HA    | 2.34                     | 0.62              |
| 6:v:100:SER:HB2  | 7:x:51:TYR:CZ    | 2.34                     | 0.62              |
| 1:B:99:ARG:NH2   | 4:e:182:GLY:O    | 2.32                     | 0.62              |
| 6:u:56:THR:HA    | 7:x:109:SER:OG   | 1.99                     | 0.62              |
| 6:u:112:LEU:HD21 | 7:w:54:LYS:HG2   | 1.80                     | 0.62              |
| 4:e:121:THR:H    | 6:v:166:ASN:ND2  | 1.97                     | 0.62              |
| 6:v:99:TYR:CE1   | 7:x:53:PRO:O     | 2.53                     | 0.62              |
| 6:v:103:GLY:N    | 7:y:113:SER:N    | 2.46                     | 0.62              |
| 1:F:76:ARG:HH12  | 2:G:4:LEU:HD21   | 1.64                     | 0.62              |
| 4:a:117:VAL:C    | 4:b:37:ALA:HB2   | 2.25                     | 0.62              |
| 4:d:116:ILE:HG22 | 4:e:36:GLY:HA3   | 1.80                     | 0.62              |
| 6:t:56:THR:CA    | 7:w:109:SER:OG   | 2.47                     | 0.62              |
| 6:u:54:SER:HA    | 7:x:111:SER:CA   | 2.30                     | 0.62              |
| 6:u:63:LEU:HA    | 7:w:58:VAL:HG11  | 1.81                     | 0.62              |
| 7:x:52:LYS:HB3   | 7:x:60:THR:O     | 1.99                     | 0.62              |
| 2:C:51:VAL:HG23  | 2:C:52:GLU:OE1   | 1.99                     | 0.62              |
| 1:H:110:ASP:HB3  | 2:J:139:GLN:NE2  | 2.15                     | 0.62              |
| 2:M:211:ILE:HD11 | 2:M:227:LEU:HB2  | 1.81                     | 0.62              |
| 3:n:6:ARG:NH1    | 3:n:89:ASP:OD1   | 2.33                     | 0.62              |
| 7:w:96:MET:HE3   | 7:w:97:ARG:CG    | 2.30                     | 0.62              |
| 2:D:106:PRO:HB3  | 2:D:186:TYR:CZ   | 2.34                     | 0.62              |
| 1:I:216:PRO:HB2  | 2:M:80:CYS:SG    | 2.40                     | 0.62              |
| 4:b:162:LYS:HE3  | 6:u:186:ARG:CG   | 2.30                     | 0.62              |
| 4:c:119:THR:HG22 | 6:u:166:ASN:ND2  | 2.14                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:41:CYS:O     | 7:x:7:LYS:N      | 2.28                     | 0.62              |
| 7:w:102:TYR:O    | 7:y:130:SER:OG   | 2.11                     | 0.62              |
| 2:S:87:GLY:O     | 2:S:100:LEU:HD12 | 2.00                     | 0.61              |
| 6:t:103:GLY:N    | 7:w:112:ASP:C    | 2.58                     | 0.61              |
| 7:x:101:ASN:OD1  | 7:x:109:SER:O    | 2.18                     | 0.61              |
| 2:D:114:SER:OG   | 2:D:115:PRO:HD3  | 1.99                     | 0.61              |
| 1:L:11:VAL:HG22  | 5:j:49:THR:HG21  | 1.82                     | 0.61              |
| 1:P:206:VAL:HG12 | 1:P:261:VAL:HA   | 1.82                     | 0.61              |
| 4:c:117:VAL:H    | 4:d:37:ALA:H     | 1.48                     | 0.61              |
| 6:t:24:ARG:HG3   | 7:y:5:LEU:HB3    | 1.82                     | 0.61              |
| 6:t:54:SER:HA    | 7:w:111:SER:CA   | 2.29                     | 0.61              |
| 6:u:49:ARG:HB2   | 6:u:50:ARG:HD2   | 1.82                     | 0.61              |
| 2:G:90:CYS:HB2   | 2:G:94:TYR:HB3   | 1.83                     | 0.61              |
| 2:S:82:THR:O     | 2:S:99:GLN:NE2   | 2.33                     | 0.61              |
| 6:t:74:MET:HE2   | 6:t:109:LEU:HD11 | 1.81                     | 0.61              |
| 6:t:100:SER:HB2  | 7:y:51:TYR:CE2   | 2.36                     | 0.61              |
| 6:u:67:VAL:HG23  | 7:w:58:VAL:CG2   | 2.30                     | 0.61              |
| 6:v:95:LEU:HD21  | 7:x:59:PRO:O     | 2.01                     | 0.61              |
| 1:A:105:ASP:O    | 1:A:106:ARG:HB2  | 1.99                     | 0.61              |
| 2:J:87:GLY:O     | 2:J:100:LEU:HD12 | 2.00                     | 0.61              |
| 2:M:90:CYS:HB2   | 2:M:94:TYR:HB3   | 1.81                     | 0.61              |
| 6:v:55:LYS:N     | 7:y:111:SER:O    | 2.33                     | 0.61              |
| 7:y:176:ILE:HG22 | 7:y:180:MET:HE2  | 1.81                     | 0.61              |
| 1:B:75:SER:H     | 2:C:1:MET:H2     | 1.49                     | 0.61              |
| 1:I:26:MET:HE2   | 1:I:42:LEU:CD1   | 2.30                     | 0.61              |
| 1:L:268:GLN:O    | 1:L:271:ALA:N    | 2.33                     | 0.61              |
| 4:e:37:ALA:O     | 4:e:38:ASP:OD1   | 2.19                     | 0.61              |
| 2:D:211:ILE:HD11 | 2:D:227:LEU:HB2  | 1.82                     | 0.61              |
| 1:H:108:ARG:HH21 | 1:H:111:LEU:CD1  | 2.14                     | 0.61              |
| 2:S:213:GLY:N    | 2:S:218:TRP:HE1  | 1.99                     | 0.61              |
| 6:u:112:LEU:HD22 | 7:w:57:GLY:H     | 1.64                     | 0.61              |
| 6:v:56:THR:OG1   | 7:y:101:ASN:HB3  | 2.00                     | 0.61              |
| 7:w:105:GLU:O    | 7:y:132:LYS:NZ   | 2.28                     | 0.61              |
| 1:F:164:ARG:HH22 | 2:G:166:THR:HG21 | 1.65                     | 0.61              |
| 1:F:209:ARG:NH2  | 1:F:260:GLU:OE1  | 2.33                     | 0.61              |
| 7:x:98:SER:O     | 7:x:110:ALA:HB2  | 2.01                     | 0.61              |
| 2:C:90:CYS:HB2   | 2:C:94:TYR:HB3   | 1.82                     | 0.61              |
| 4:f:115:LYS:O    | 4:f:116:ILE:HG13 | 2.01                     | 0.61              |
| 4:f:158:ASN:HA   | 6:t:186:ARG:HH12 | 1.65                     | 0.61              |
| 5:i:36:TRP:HB3   | 5:i:53:LEU:HD12  | 1.83                     | 0.61              |
| 6:u:63:LEU:HD13  | 7:w:59:PRO:O     | 2.01                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:y:30:GLU:OE2   | 7:y:91:THR:OG1   | 2.18                     | 0.61              |
| 1:Q:26:MET:HE1   | 2:S:32:LEU:HD12  | 1.82                     | 0.61              |
| 6:u:55:LYS:N     | 7:x:111:SER:O    | 2.34                     | 0.61              |
| 1:H:238:GLY:N    | 1:H:241:GLU:OE1  | 2.32                     | 0.61              |
| 6:u:63:LEU:HD12  | 7:w:58:VAL:HB    | 1.82                     | 0.61              |
| 6:v:100:SER:CA   | 7:y:109:SER:HB2  | 2.31                     | 0.61              |
| 7:y:43:ARG:O     | 7:y:70:LEU:N     | 2.34                     | 0.61              |
| 6:t:99:TYR:CZ    | 7:y:54:LYS:HA    | 2.36                     | 0.60              |
| 6:u:24:ARG:HG3   | 7:w:5:LEU:HB3    | 1.83                     | 0.60              |
| 6:v:95:LEU:HD11  | 7:x:59:PRO:HB2   | 1.83                     | 0.60              |
| 6:v:103:GLY:CA   | 7:y:113:SER:C    | 2.74                     | 0.60              |
| 7:y:60:THR:HG22  | 7:y:61:ASP:N     | 2.16                     | 0.60              |
| 2:D:217:GLY:N    | 1:P:185:GLY:O    | 2.34                     | 0.60              |
| 6:t:108:GLU:O    | 6:t:111:THR:HG22 | 2.00                     | 0.60              |
| 6:u:24:ARG:HB3   | 6:u:40:SER:C     | 2.26                     | 0.60              |
| 4:a:119:THR:OG1  | 4:b:39:VAL:HG23  | 2.02                     | 0.60              |
| 4:a:145:ALA:HB3  | 3:p:54:PHE:HA    | 1.81                     | 0.60              |
| 1:Q:104:VAL:O    | 1:Q:106:ARG:HG3  | 2.02                     | 0.60              |
| 5:m:35:ARG:HH12  | 5:m:79:PRO:HB2   | 1.65                     | 0.60              |
| 6:u:102:CYS:SG   | 7:x:114:ARG:NH1  | 2.74                     | 0.60              |
| 6:v:112:LEU:HD23 | 7:x:54:LYS:C     | 2.26                     | 0.60              |
| 1:A:109:ILE:HD12 | 2:C:73:PHE:HE1   | 1.67                     | 0.60              |
| 1:H:178:THR:OG1  | 1:H:191:ARG:NH1  | 2.30                     | 0.60              |
| 1:L:88:ARG:NH2   | 1:L:94:ASP:OD1   | 2.34                     | 0.60              |
| 4:e:118:GLU:HB2  | 4:f:35:SER:CA    | 2.29                     | 0.60              |
| 6:u:56:THR:CA    | 7:x:109:SER:OG   | 2.50                     | 0.60              |
| 4:d:31:ASN:HB3   | 4:d:32:PRO:HD2   | 1.84                     | 0.60              |
| 6:t:56:THR:OG1   | 7:w:101:ASN:CG   | 2.44                     | 0.60              |
| 2:C:211:ILE:HD11 | 2:C:227:LEU:HB2  | 1.83                     | 0.60              |
| 2:D:56:LEU:O     | 2:D:130:ARG:NH1  | 2.33                     | 0.60              |
| 1:E:84:ARG:HG2   | 2:G:140:MET:HE3  | 1.82                     | 0.60              |
| 1:K:18:HIS:NE2   | 1:K:57:ASP:OD2   | 2.33                     | 0.60              |
| 1:Q:253:GLU:OE1  | 1:Q:253:GLU:N    | 2.35                     | 0.60              |
| 7:w:180:MET:HE1  | 7:x:215:VAL:HG11 | 1.84                     | 0.60              |
| 2:J:212:ALA:C    | 2:J:218:TRP:HE1  | 2.09                     | 0.60              |
| 4:b:32:PRO:HD2   | 6:t:149:ILE:CG2  | 2.31                     | 0.60              |
| 4:b:175:LEU:CD1  | 5:m:1:MET:HE1    | 2.31                     | 0.60              |
| 4:f:39:VAL:HG13  | 6:v:6:TYR:CD1    | 2.37                     | 0.60              |
| 6:t:24:ARG:HB3   | 6:t:40:SER:C     | 2.27                     | 0.60              |
| 6:v:67:VAL:N     | 7:x:58:VAL:HG22  | 2.17                     | 0.60              |
| 1:L:75:SER:H     | 2:M:1:MET:H2     | 1.50                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:159:ALA:HB3  | 6:v:186:ARG:HB2  | 1.84                     | 0.60              |
| 6:t:116:HIS:HB2  | 7:y:55:PHE:CE1   | 2.37                     | 0.60              |
| 1:A:230:GLU:HG2  | 1:A:251:ILE:HG23 | 1.84                     | 0.60              |
| 1:B:23:GLU:OE1   | 4:e:135:LYS:HB3  | 2.02                     | 0.60              |
| 4:f:31:ASN:HB3   | 6:v:149:ILE:HG21 | 1.83                     | 0.60              |
| 6:t:112:LEU:HA   | 7:y:55:PHE:HA    | 1.84                     | 0.60              |
| 7:w:173:LEU:HD21 | 7:x:172:LEU:HD21 | 1.84                     | 0.60              |
| 2:D:71:LEU:HD22  | 2:D:140:MET:SD   | 2.41                     | 0.59              |
| 4:b:51:GLU:OE1   | 4:b:110:ARG:NE   | 2.34                     | 0.59              |
| 6:t:112:LEU:HB3  | 7:y:56:ASN:H     | 1.66                     | 0.59              |
| 6:u:35:ILE:HD11  | 6:v:151:THR:HG21 | 1.84                     | 0.59              |
| 6:u:56:THR:HG23  | 7:x:107:ASP:O    | 2.02                     | 0.59              |
| 1:B:101:ILE:O    | 1:B:102:THR:HG23 | 2.02                     | 0.59              |
| 2:D:87:GLY:C     | 2:D:100:LEU:HD12 | 2.26                     | 0.59              |
| 1:K:230:GLU:HG2  | 1:K:251:ILE:HG23 | 1.83                     | 0.59              |
| 4:a:118:GLU:H    | 4:b:36:GLY:H     | 1.49                     | 0.59              |
| 5:k:53:LEU:HB3   | 5:k:72:LEU:HD11  | 1.83                     | 0.59              |
| 5:m:20:ASP:N     | 6:u:219:ASP:OD2  | 2.34                     | 0.59              |
| 6:u:103:GLY:CA   | 7:x:114:ARG:HB3  | 2.33                     | 0.59              |
| 7:x:60:THR:HG22  | 7:x:61:ASP:N     | 2.17                     | 0.59              |
| 2:C:106:PRO:HG2  | 2:C:182:THR:HB   | 1.83                     | 0.59              |
| 4:d:158:ASN:HA   | 6:v:186:ARG:HH12 | 1.65                     | 0.59              |
| 6:t:181:VAL:HG12 | 6:t:185:ASN:OD1  | 2.03                     | 0.59              |
| 1:A:227:LEU:HD13 | 1:A:252:MET:SD   | 2.43                     | 0.59              |
| 1:B:152:ILE:HD11 | 1:B:285:MET:HE1  | 1.84                     | 0.59              |
| 2:J:114:SER:HB2  | 2:J:115:PRO:HD3  | 1.83                     | 0.59              |
| 2:M:114:SER:OG   | 2:M:115:PRO:HD3  | 2.03                     | 0.59              |
| 1:O:84:ARG:NH1   | 1:O:101:ILE:O    | 2.34                     | 0.59              |
| 4:e:117:VAL:C    | 4:f:37:ALA:HB2   | 2.28                     | 0.59              |
| 6:v:99:TYR:HB2   | 7:x:52:LYS:CD    | 2.32                     | 0.59              |
| 1:E:109:ILE:CD1  | 2:G:73:PHE:CD1   | 2.60                     | 0.59              |
| 1:E:121:ILE:HD11 | 1:E:162:LEU:HD13 | 1.84                     | 0.59              |
| 2:G:84:PRO:HA    | 2:G:99:GLN:HG3   | 1.84                     | 0.59              |
| 2:S:89:ASP:HA    | 2:S:94:TYR:CE2   | 2.38                     | 0.59              |
| 3:p:10:ALA:HB2   | 3:p:32:VAL:HG13  | 1.84                     | 0.59              |
| 2:C:109:SER:OG   | 2:C:116:TYR:HB2  | 2.03                     | 0.59              |
| 4:a:36:GLY:O     | 4:f:119:THR:OG1  | 2.12                     | 0.59              |
| 6:u:67:VAL:N     | 7:w:58:VAL:HG22  | 2.16                     | 0.59              |
| 1:B:201:SER:OG   | 1:B:267:SER:OG   | 2.18                     | 0.59              |
| 1:Q:121:ILE:HD11 | 1:Q:162:LEU:HD13 | 1.84                     | 0.59              |
| 5:l:29:TYR:OH    | 5:l:34:ASP:OD1   | 2.21                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:74:MET:HE1   | 6:v:127:MET:SD   | 2.43                     | 0.59              |
| 2:D:77:HIS:HE1   | 1:O:109:ILE:HD11 | 1.65                     | 0.59              |
| 1:H:117:ALA:CB   | 1:H:162:LEU:HD21 | 2.33                     | 0.59              |
| 4:a:125:SER:HB3  | 6:t:141:LEU:HB2  | 1.85                     | 0.59              |
| 5:j:41:ALA:HB2   | 5:j:46:ASN:HD22  | 1.68                     | 0.59              |
| 6:u:102:CYS:CA   | 7:x:112:ASP:O    | 2.51                     | 0.59              |
| 2:J:106:PRO:HG2  | 2:J:182:THR:HB   | 1.84                     | 0.58              |
| 4:e:160:GLY:HA3  | 6:v:16:GLY:HA3   | 1.85                     | 0.58              |
| 6:t:103:GLY:CA   | 7:w:114:ARG:CG   | 2.81                     | 0.58              |
| 6:t:103:GLY:HA3  | 7:w:114:ARG:CG   | 2.33                     | 0.58              |
| 7:w:190:ILE:HD11 | 7:x:200:HIS:HD1  | 1.67                     | 0.58              |
| 1:I:117:ALA:HB1  | 1:I:162:LEU:HD11 | 1.85                     | 0.58              |
| 1:L:62:ASP:OD1   | 5:j:52:ARG:NH2   | 2.36                     | 0.58              |
| 4:e:121:THR:HG22 | 6:v:166:ASN:OD1  | 2.03                     | 0.58              |
| 6:t:63:LEU:C     | 7:y:58:VAL:HG11  | 2.28                     | 0.58              |
| 6:v:24:ARG:HG3   | 7:x:5:LEU:CB     | 2.34                     | 0.58              |
| 7:w:216:ARG:NH2  | 7:y:181:GLU:OE1  | 2.37                     | 0.58              |
| 2:S:89:ASP:HB3   | 2:S:100:LEU:HG   | 1.85                     | 0.58              |
| 6:v:99:TYR:HE2   | 6:v:101:MET:HE3  | 1.69                     | 0.58              |
| 2:D:89:ASP:HA    | 2:D:94:TYR:CD1   | 2.38                     | 0.58              |
| 7:y:52:LYS:HE3   | 7:y:61:ASP:OD1   | 2.03                     | 0.58              |
| 4:c:173:GLN:CD   | 4:c:177:LYS:HE2  | 2.28                     | 0.58              |
| 4:d:117:VAL:H    | 4:e:36:GLY:HA3   | 1.68                     | 0.58              |
| 6:t:56:THR:N     | 7:w:109:SER:O    | 2.37                     | 0.58              |
| 6:t:102:CYS:HB2  | 7:w:110:ALA:HB3  | 1.86                     | 0.58              |
| 6:t:109:LEU:HA   | 6:t:112:LEU:HG   | 1.86                     | 0.58              |
| 1:F:26:MET:HE2   | 1:F:42:LEU:HD23  | 1.85                     | 0.58              |
| 4:d:162:LYS:HD3  | 6:v:186:ARG:CB   | 2.34                     | 0.58              |
| 3:q:6:ARG:NH1    | 3:q:118:GLU:OE2  | 2.32                     | 0.58              |
| 6:t:63:LEU:HD22  | 6:t:93:THR:HB    | 1.86                     | 0.58              |
| 6:u:95:LEU:HD11  | 7:w:59:PRO:HB2   | 1.85                     | 0.58              |
| 1:H:45:LEU:HD21  | 1:I:26:MET:HE1   | 1.86                     | 0.58              |
| 4:c:118:GLU:H    | 4:d:36:GLY:H     | 1.51                     | 0.58              |
| 6:t:103:GLY:HA3  | 7:w:114:ARG:N    | 2.19                     | 0.58              |
| 6:u:67:VAL:HG23  | 7:w:58:VAL:HG23  | 1.85                     | 0.58              |
| 6:v:103:GLY:HA3  | 7:y:113:SER:C    | 2.29                     | 0.58              |
| 1:L:59:ARG:CG    | 5:j:32:THR:HG21  | 2.34                     | 0.58              |
| 6:u:104:SER:O    | 7:x:113:SER:OG   | 2.21                     | 0.58              |
| 1:B:56:LEU:HD12  | 2:C:44:SER:HB3   | 1.86                     | 0.58              |
| 1:L:101:ILE:O    | 1:L:102:THR:HG23 | 2.04                     | 0.58              |
| 1:O:212:LYS:HD2  | 1:O:212:LYS:O    | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:119:THR:OG1  | 4:f:39:VAL:HG23  | 2.03                     | 0.58              |
| 4:e:119:THR:HG23 | 4:f:39:VAL:CG2   | 2.34                     | 0.58              |
| 3:r:105:ARG:NH2  | 3:r:109:GLU:OE2  | 2.34                     | 0.58              |
| 6:t:43:ASP:N     | 7:y:7:LYS:HG2    | 2.19                     | 0.58              |
| 1:Q:138:ASP:OD1  | 1:Q:142:ILE:N    | 2.37                     | 0.57              |
| 4:a:179:VAL:CG2  | 5:l:73:LEU:HD21  | 2.34                     | 0.57              |
| 4:c:92:GLU:HG2   | 4:d:25:LYS:HD3   | 1.86                     | 0.57              |
| 4:c:29:THR:OG1   | 6:t:34:ASP:OD1   | 2.13                     | 0.57              |
| 4:c:175:LEU:HD12 | 5:j:1:MET:CE     | 2.34                     | 0.57              |
| 4:e:175:LEU:HD12 | 5:i:1:MET:HE1    | 1.87                     | 0.57              |
| 5:i:42:LEU:HD21  | 5:i:67:ILE:HD13  | 1.86                     | 0.57              |
| 1:B:152:ILE:CD1  | 1:B:285:MET:HE1  | 2.34                     | 0.57              |
| 1:O:277:PRO:O    | 1:O:278:LEU:C    | 2.47                     | 0.57              |
| 6:t:49:ARG:HB2   | 6:t:50:ARG:HD2   | 1.86                     | 0.57              |
| 6:u:100:SER:HA   | 7:x:109:SER:HB2  | 1.85                     | 0.57              |
| 1:F:100:ALA:O    | 1:F:103:ASN:ND2  | 2.37                     | 0.57              |
| 2:G:87:GLY:O     | 2:G:100:LEU:HD12 | 2.02                     | 0.57              |
| 1:I:12:LYS:HZ2   | 5:m:28:TRP:CD1   | 2.23                     | 0.57              |
| 2:J:38:SER:O     | 2:J:42:GLU:HG3   | 2.05                     | 0.57              |
| 4:c:140:SER:OG   | 4:c:142:ASP:OD1  | 2.19                     | 0.57              |
| 6:u:66:VAL:HB    | 7:w:58:VAL:HA    | 1.85                     | 0.57              |
| 6:v:154:ILE:HD11 | 6:v:182:LEU:HD23 | 1.87                     | 0.57              |
| 5:l:41:ALA:HB2   | 5:l:46:ASN:HD22  | 1.70                     | 0.57              |
| 5:l:42:LEU:HD21  | 5:l:67:ILE:HD13  | 1.87                     | 0.57              |
| 6:t:70:ILE:HD11  | 7:y:54:LYS:HE3   | 1.85                     | 0.57              |
| 1:B:99:ARG:NH2   | 4:e:179:VAL:O    | 2.38                     | 0.57              |
| 1:B:216:PRO:HB2  | 2:G:80:CYS:SG    | 2.44                     | 0.57              |
| 2:D:47:TYR:O     | 2:D:50:MET:N     | 2.38                     | 0.57              |
| 1:E:84:ARG:CG    | 2:G:140:MET:HE3  | 2.34                     | 0.57              |
| 1:P:101:ILE:O    | 1:P:102:THR:HG23 | 2.03                     | 0.57              |
| 4:e:118:GLU:H    | 4:f:36:GLY:CA    | 2.17                     | 0.57              |
| 6:t:101:MET:O    | 7:w:110:ALA:O    | 2.22                     | 0.57              |
| 6:u:102:CYS:C    | 7:x:113:SER:HA   | 2.30                     | 0.57              |
| 7:w:212:ALA:O    | 7:w:215:VAL:HG22 | 2.05                     | 0.57              |
| 1:I:11:VAL:HG22  | 5:m:49:THR:HG21  | 1.86                     | 0.57              |
| 4:a:37:ALA:H     | 4:f:116:ILE:HG22 | 1.70                     | 0.57              |
| 4:c:119:THR:N    | 4:d:37:ALA:HB3   | 2.20                     | 0.57              |
| 4:d:157:VAL:HG13 | 6:v:186:ARG:HH21 | 1.69                     | 0.57              |
| 1:E:280:MET:HE3  | 1:E:286:MET:CG   | 2.34                     | 0.57              |
| 1:K:70:GLU:O     | 1:K:98:ARG:NH1   | 2.38                     | 0.57              |
| 1:L:59:ARG:HG3   | 5:j:32:THR:HG21  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:1:MET:HE2    | 5:j:52:ARG:HH12  | 1.68                     | 0.57              |
| 2:M:5:CYS:HB2    | 2:M:45:MET:HE1   | 1.86                     | 0.57              |
| 4:b:117:VAL:N    | 4:c:36:GLY:HA3   | 2.19                     | 0.57              |
| 4:d:39:VAL:HG13  | 6:u:6:TYR:CD1    | 2.39                     | 0.57              |
| 4:e:29:THR:HG21  | 6:u:33:GLY:H     | 1.68                     | 0.57              |
| 4:e:118:GLU:H    | 4:f:36:GLY:H     | 1.52                     | 0.57              |
| 1:B:257:PRO:O    | 1:E:246:TYR:OH   | 2.20                     | 0.57              |
| 1:I:175:GLY:O    | 1:I:191:ARG:NH2  | 2.38                     | 0.57              |
| 2:M:85:VAL:O     | 2:M:100:LEU:HA   | 2.05                     | 0.57              |
| 4:e:119:THR:HG23 | 4:f:39:VAL:HG21  | 1.87                     | 0.57              |
| 6:u:99:TYR:HD1   | 7:w:52:LYS:HB2   | 1.70                     | 0.57              |
| 6:u:104:SER:H    | 7:x:113:SER:C    | 2.12                     | 0.57              |
| 6:v:43:ASP:N     | 7:x:7:LYS:HG2    | 2.20                     | 0.57              |
| 7:x:43:ARG:O     | 7:x:70:LEU:N     | 2.38                     | 0.57              |
| 1:B:76:ARG:HH12  | 2:C:4:LEU:HD21   | 1.70                     | 0.56              |
| 1:F:76:ARG:CZ    | 2:G:4:LEU:HD21   | 2.34                     | 0.56              |
| 1:I:76:ARG:NH2   | 2:J:51:VAL:O     | 2.38                     | 0.56              |
| 1:Q:111:LEU:HD21 | 1:Q:131:VAL:HG21 | 1.87                     | 0.56              |
| 4:a:118:GLU:H    | 4:b:36:GLY:N     | 2.03                     | 0.56              |
| 4:c:118:GLU:H    | 4:d:36:GLY:N     | 2.03                     | 0.56              |
| 7:w:215:VAL:HG21 | 7:y:180:MET:CE   | 2.34                     | 0.56              |
| 2:D:85:VAL:HG11  | 2:D:111:ILE:HG23 | 1.87                     | 0.56              |
| 4:c:117:VAL:N    | 4:d:36:GLY:HA3   | 2.20                     | 0.56              |
| 5:h:78:GLU:OE1   | 5:h:78:GLU:N     | 2.36                     | 0.56              |
| 6:u:53:ILE:HG23  | 7:x:112:ASP:HA   | 1.88                     | 0.56              |
| 6:v:97:ARG:HH22  | 7:x:62:MET:C     | 2.09                     | 0.56              |
| 1:E:44:GLN:OE1   | 1:F:29:LEU:HD22  | 2.06                     | 0.56              |
| 1:E:111:LEU:HD11 | 1:E:131:VAL:HG21 | 1.87                     | 0.56              |
| 2:J:80:CYS:SG    | 1:P:216:PRO:HB2  | 2.45                     | 0.56              |
| 4:a:119:THR:HG23 | 4:b:39:VAL:CG2   | 2.36                     | 0.56              |
| 4:a:167:VAL:HG13 | 4:a:171:ARG:HH11 | 1.70                     | 0.56              |
| 4:c:115:LYS:CB   | 4:d:34:GLU:HB3   | 2.35                     | 0.56              |
| 6:t:98:PRO:O     | 7:y:52:LYS:HB2   | 2.05                     | 0.56              |
| 6:u:53:ILE:O     | 7:x:112:ASP:HB3  | 2.05                     | 0.56              |
| 6:v:70:ILE:HD12  | 7:x:57:GLY:CA    | 2.36                     | 0.56              |
| 6:v:103:GLY:HA3  | 7:y:114:ARG:CA   | 2.35                     | 0.56              |
| 2:D:166:THR:HG21 | 1:P:164:ARG:HH22 | 1.70                     | 0.56              |
| 1:E:106:ARG:NH2  | 1:E:115:SER:OG   | 2.38                     | 0.56              |
| 1:O:165:ARG:HB3  | 1:P:106:ARG:HE   | 1.69                     | 0.56              |
| 1:Q:212:LYS:HD2  | 1:Q:212:LYS:O    | 2.05                     | 0.56              |
| 4:e:175:LEU:HD12 | 5:i:1:MET:CE     | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:102:CYS:CB   | 7:w:98:SER:OG    | 2.53                     | 0.56              |
| 6:v:63:LEU:HA    | 7:x:58:VAL:HG11  | 1.86                     | 0.56              |
| 1:R:42:LEU:HD12  | 3:X:9:LEU:HD12   | 1.87                     | 0.56              |
| 4:c:2:ILE:HG23   | 4:c:81:GLY:O     | 2.06                     | 0.56              |
| 4:f:179:VAL:CG2  | 5:h:73:LEU:HD21  | 2.35                     | 0.56              |
| 6:t:53:ILE:CG2   | 7:w:112:ASP:HA   | 2.35                     | 0.56              |
| 6:v:181:VAL:HG12 | 6:v:185:ASN:OD1  | 2.06                     | 0.56              |
| 4:c:33:ILE:HG23  | 4:c:34:GLU:OE1   | 2.05                     | 0.56              |
| 4:c:118:GLU:HG2  | 6:u:144:PRO:O    | 2.06                     | 0.56              |
| 6:t:176:LYS:NZ   | 6:t:189:GLU:OE1  | 2.27                     | 0.56              |
| 7:x:129:GLU:OE1  | 7:x:129:GLU:N    | 2.37                     | 0.56              |
| 7:x:176:ILE:HG22 | 7:x:180:MET:HE3  | 1.88                     | 0.56              |
| 2:C:87:GLY:C     | 2:C:100:LEU:HD12 | 2.31                     | 0.56              |
| 2:D:73:PHE:CE1   | 1:O:109:ILE:HD13 | 2.41                     | 0.56              |
| 1:E:69:PRO:O     | 1:E:98:ARG:NE    | 2.36                     | 0.56              |
| 2:J:8:PRO:HG3    | 2:J:45:MET:HG3   | 1.87                     | 0.56              |
| 4:c:79:MET:HE1   | 4:c:84:MET:HE2   | 1.88                     | 0.56              |
| 5:j:42:LEU:CD1   | 5:j:65:LEU:HD22  | 2.34                     | 0.56              |
| 6:u:100:SER:HB2  | 7:w:51:TYR:CE2   | 2.41                     | 0.56              |
| 7:w:52:LYS:HG2   | 7:w:61:ASP:OD1   | 2.05                     | 0.56              |
| 2:D:54:PHE:O     | 1:P:83:TYR:OH    | 2.22                     | 0.56              |
| 1:E:109:ILE:HD13 | 2:G:73:PHE:HD1   | 1.56                     | 0.56              |
| 4:e:121:THR:OG1  | 6:v:168:GLU:HB2  | 2.05                     | 0.56              |
| 4:f:157:VAL:HG13 | 6:t:186:ARG:HH21 | 1.66                     | 0.56              |
| 6:t:182:LEU:HD22 | 6:t:187:LYS:HB2  | 1.87                     | 0.56              |
| 6:v:102:CYS:CB   | 7:y:98:SER:OG    | 2.54                     | 0.56              |
| 2:D:69:ARG:HG3   | 1:O:102:THR:HG22 | 1.88                     | 0.56              |
| 2:D:142:GLY:O    | 1:P:107:ALA:HB2  | 2.05                     | 0.56              |
| 1:E:203:GLU:OE2  | 1:E:294:LEU:HD22 | 2.05                     | 0.56              |
| 4:c:116:ILE:HA   | 4:d:36:GLY:HA3   | 1.88                     | 0.56              |
| 4:d:34:GLU:H     | 4:d:34:GLU:CD    | 2.10                     | 0.56              |
| 4:e:92:GLU:HG2   | 4:f:25:LYS:HD3   | 1.87                     | 0.56              |
| 6:t:106:THR:HA   | 6:t:109:LEU:HD12 | 1.86                     | 0.56              |
| 1:R:268:GLN:O    | 1:R:271:ALA:N    | 2.39                     | 0.56              |
| 4:f:1:MET:HE2    | 4:f:1:MET:H1     | 1.71                     | 0.56              |
| 6:v:70:ILE:HD12  | 7:x:57:GLY:HA2   | 1.88                     | 0.56              |
| 7:w:138:LEU:HD12 | 7:x:41:ASP:O     | 2.05                     | 0.56              |
| 2:C:80:CYS:SG    | 1:R:216:PRO:HB2  | 2.45                     | 0.55              |
| 1:I:215:CYS:N    | 1:K:107:ALA:HB1  | 2.22                     | 0.55              |
| 1:O:111:LEU:HD21 | 1:O:131:VAL:CG2  | 2.36                     | 0.55              |
| 1:O:200:THR:CG2  | 1:O:278:LEU:HD21 | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:b:142:ASP:OD1  | 4:b:143:LYS:N    | 2.39                     | 0.55              |
| 3:q:9:LEU:HD21   | 3:q:29:LEU:HD21  | 1.88                     | 0.55              |
| 6:t:30:ARG:CG    | 6:u:151:THR:HG23 | 2.36                     | 0.55              |
| 6:t:97:ARG:O     | 7:y:52:LYS:CE    | 2.54                     | 0.55              |
| 6:t:99:TYR:CD1   | 7:y:52:LYS:HD3   | 2.42                     | 0.55              |
| 7:x:45:VAL:HG23  | 7:x:47:VAL:HG23  | 1.87                     | 0.55              |
| 2:D:90:CYS:HB2   | 2:D:94:TYR:HB3   | 1.88                     | 0.55              |
| 1:L:56:LEU:HD23  | 2:M:44:SER:OG    | 2.06                     | 0.55              |
| 4:c:1:MET:HE2    | 4:c:1:MET:HA     | 1.88                     | 0.55              |
| 1:I:185:GLY:O    | 2:J:217:GLY:N    | 2.39                     | 0.55              |
| 2:M:168:VAL:HG23 | 2:M:168:VAL:O    | 2.06                     | 0.55              |
| 1:O:275:THR:O    | 1:O:277:PRO:CD   | 2.52                     | 0.55              |
| 3:r:6:ARG:NH2    | 3:r:89:ASP:OD2   | 2.40                     | 0.55              |
| 6:v:60:GLY:H     | 6:v:95:LEU:HB2   | 1.71                     | 0.55              |
| 1:I:215:CYS:HB2  | 1:I:216:PRO:CD   | 2.36                     | 0.55              |
| 1:L:277:PRO:O    | 1:L:278:LEU:C    | 2.49                     | 0.55              |
| 1:Q:44:GLN:OE1   | 1:R:29:LEU:HD22  | 2.07                     | 0.55              |
| 4:b:39:VAL:HG13  | 6:t:6:TYR:CD2    | 2.41                     | 0.55              |
| 4:d:116:ILE:O    | 4:d:117:VAL:CG1  | 2.47                     | 0.55              |
| 6:u:112:LEU:HD13 | 7:w:57:GLY:H     | 1.70                     | 0.55              |
| 1:F:121:ILE:HD11 | 1:F:162:LEU:HD13 | 1.87                     | 0.55              |
| 1:K:109:ILE:CD1  | 2:M:73:PHE:CD1   | 2.89                     | 0.55              |
| 1:O:252:MET:HB2  | 1:O:261:VAL:HG21 | 1.88                     | 0.55              |
| 1:P:158:GLU:O    | 1:P:162:LEU:HD23 | 2.06                     | 0.55              |
| 4:b:33:ILE:HG12  | 4:b:34:GLU:H     | 1.71                     | 0.55              |
| 4:e:9:ILE:HD12   | 4:e:14:LEU:HD11  | 1.88                     | 0.55              |
| 7:x:88:GLN:HB3   | 7:y:75:MET:HE2   | 1.88                     | 0.55              |
| 7:x:181:GLU:OE1  | 7:y:216:ARG:NH2  | 2.40                     | 0.55              |
| 2:G:170:GLN:NE2  | 2:G:203:MET:SD   | 2.79                     | 0.55              |
| 1:K:105:ASP:O    | 1:K:106:ARG:HB2  | 2.06                     | 0.55              |
| 1:L:198:ILE:HD11 | 1:L:280:MET:HE1  | 1.88                     | 0.55              |
| 4:a:116:ILE:C    | 4:b:36:GLY:HA3   | 2.31                     | 0.55              |
| 4:b:175:LEU:HD12 | 5:m:1:MET:CE     | 2.35                     | 0.55              |
| 4:c:116:ILE:C    | 4:d:36:GLY:HA3   | 2.32                     | 0.55              |
| 4:f:12:VAL:HG11  | 4:f:66:LEU:HD23  | 1.88                     | 0.55              |
| 6:t:99:TYR:CE1   | 7:y:53:PRO:O     | 2.59                     | 0.55              |
| 6:u:103:GLY:N    | 7:x:113:SER:N    | 2.55                     | 0.55              |
| 2:D:94:TYR:CE2   | 2:D:96:GLY:HA3   | 2.41                     | 0.55              |
| 2:D:101:ALA:HB1  | 2:D:105:GLU:HG2  | 1.89                     | 0.55              |
| 1:I:121:ILE:HD11 | 1:I:162:LEU:CD1  | 2.36                     | 0.55              |
| 1:L:23:GLU:OE1   | 4:c:135:LYS:HB3  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:116:ILE:C    | 4:d:117:VAL:HG12 | 2.32                     | 0.55              |
| 4:e:116:ILE:HG22 | 4:f:36:GLY:CA    | 2.36                     | 0.55              |
| 4:e:121:THR:CG2  | 4:e:122:ALA:N    | 2.69                     | 0.55              |
| 6:v:108:GLU:O    | 6:v:112:LEU:HG   | 2.06                     | 0.55              |
| 1:I:75:SER:H     | 2:J:1:MET:H2     | 1.53                     | 0.55              |
| 1:L:278:LEU:CD2  | 1:L:280:MET:HE2  | 2.34                     | 0.55              |
| 1:P:23:GLU:OE1   | 4:a:135:LYS:HB3  | 2.07                     | 0.55              |
| 4:d:116:ILE:HG23 | 4:e:36:GLY:CA    | 2.33                     | 0.55              |
| 6:v:66:VAL:HB    | 7:x:58:VAL:HA    | 1.89                     | 0.55              |
| 4:a:121:THR:CG2  | 6:t:166:ASN:CG   | 2.79                     | 0.55              |
| 7:w:54:LYS:HZ1   | 7:x:113:SER:CB   | 2.19                     | 0.55              |
| 1:L:173:MET:HE1  | 1:L:190:ILE:HG23 | 1.89                     | 0.55              |
| 2:M:99:GLN:C     | 2:M:100:LEU:HD22 | 2.31                     | 0.55              |
| 4:b:31:ASN:HB3   | 6:t:149:ILE:CG2  | 2.37                     | 0.55              |
| 4:c:125:SER:HB3  | 6:u:141:LEU:HD13 | 1.89                     | 0.55              |
| 4:e:32:PRO:HB2   | 6:u:202:ASN:HB2  | 1.89                     | 0.55              |
| 7:y:129:GLU:OE1  | 7:y:129:GLU:N    | 2.40                     | 0.55              |
| 4:c:142:ASP:OD1  | 4:c:143:LYS:N    | 2.40                     | 0.54              |
| 5:j:72:LEU:HD22  | 5:j:90:VAL:HG12  | 1.88                     | 0.54              |
| 6:t:49:ARG:NH2   | 7:y:5:LEU:HA     | 2.22                     | 0.54              |
| 6:t:103:GLY:HA3  | 7:w:114:ARG:CA   | 2.38                     | 0.54              |
| 6:v:24:ARG:HB3   | 6:v:40:SER:C     | 2.32                     | 0.54              |
| 2:D:137:ARG:HG2  | 1:P:85:LEU:HD11  | 1.90                     | 0.54              |
| 1:F:26:MET:SD    | 1:F:46:ASN:ND2   | 2.78                     | 0.54              |
| 1:H:246:TYR:OH   | 1:P:257:PRO:O    | 2.22                     | 0.54              |
| 1:L:242:ASP:O    | 1:L:244:THR:OG1  | 2.20                     | 0.54              |
| 6:t:70:ILE:HD12  | 7:y:57:GLY:CA    | 2.37                     | 0.54              |
| 6:u:30:ARG:NE    | 6:v:151:THR:HG23 | 2.22                     | 0.54              |
| 7:w:129:GLU:O    | 7:x:71:ARG:NH1   | 2.39                     | 0.54              |
| 1:I:73:GLU:O     | 2:J:1:MET:N      | 2.36                     | 0.54              |
| 4:e:125:SER:HB3  | 6:v:141:LEU:HD13 | 1.89                     | 0.54              |
| 4:f:167:VAL:HG12 | 4:f:172:ALA:HB2  | 1.89                     | 0.54              |
| 6:t:112:LEU:HB3  | 7:y:56:ASN:N     | 2.21                     | 0.54              |
| 6:u:100:SER:CA   | 7:x:109:SER:HB2  | 2.37                     | 0.54              |
| 6:u:102:CYS:HB2  | 7:x:110:ALA:CB   | 2.36                     | 0.54              |
| 2:C:115:PRO:HB2  | 2:C:122:CYS:SG   | 2.48                     | 0.54              |
| 1:H:134:ASP:OD1  | 2:J:201:LYS:NZ   | 2.39                     | 0.54              |
| 1:I:26:MET:HE2   | 1:I:42:LEU:HD12  | 1.88                     | 0.54              |
| 1:L:246:TYR:OH   | 1:Q:257:PRO:O    | 2.25                     | 0.54              |
| 4:c:125:SER:HB3  | 6:u:141:LEU:HB2  | 1.90                     | 0.54              |
| 4:f:128:LYS:NZ   | 4:f:136:SER:O    | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:108:GLU:CB   | 7:y:54:LYS:HD3   | 2.36                     | 0.54              |
| 6:v:109:LEU:HA   | 6:v:112:LEU:HG   | 1.89                     | 0.54              |
| 4:a:34:GLU:HG2   | 4:a:34:GLU:O     | 2.06                     | 0.54              |
| 4:a:121:THR:OG1  | 6:t:168:GLU:HB2  | 2.08                     | 0.54              |
| 4:b:12:VAL:HG11  | 4:b:66:LEU:HD23  | 1.90                     | 0.54              |
| 3:o:6:ARG:NH2    | 3:o:118:GLU:OE2  | 2.40                     | 0.54              |
| 6:u:43:ASP:N     | 7:w:7:LYS:HG2    | 2.21                     | 0.54              |
| 4:a:121:THR:CG2  | 6:t:166:ASN:OD1  | 2.56                     | 0.54              |
| 5:l:36:TRP:CB    | 5:l:53:LEU:HD12  | 2.37                     | 0.54              |
| 6:t:102:CYS:HB2  | 7:w:110:ALA:CB   | 2.38                     | 0.54              |
| 6:u:112:LEU:HD23 | 7:w:54:LYS:C     | 2.31                     | 0.54              |
| 1:O:181:THR:HG21 | 1:O:190:ILE:HD12 | 1.89                     | 0.54              |
| 4:b:31:ASN:HB3   | 6:t:149:ILE:HG23 | 1.89                     | 0.54              |
| 4:e:121:THR:HB   | 6:v:166:ASN:CB   | 2.38                     | 0.54              |
| 6:v:98:PRO:C     | 7:x:52:LYS:HG3   | 2.33                     | 0.54              |
| 6:v:100:SER:HA   | 7:y:109:SER:CB   | 2.37                     | 0.54              |
| 1:H:108:ARG:HH21 | 1:H:111:LEU:HD12 | 1.71                     | 0.54              |
| 4:e:117:VAL:HA   | 4:f:37:ALA:HB2   | 1.90                     | 0.54              |
| 4:e:121:THR:CG2  | 6:v:166:ASN:CG   | 2.81                     | 0.54              |
| 6:t:83:GLU:CG    | 6:t:136:LEU:HD22 | 2.37                     | 0.54              |
| 6:v:24:ARG:HG3   | 7:x:5:LEU:HB3    | 1.90                     | 0.54              |
| 7:y:56:ASN:O     | 7:y:58:VAL:HG23  | 2.07                     | 0.54              |
| 1:B:156:ASP:OD1  | 1:B:157:ASP:N    | 2.40                     | 0.54              |
| 1:P:100:ALA:O    | 1:P:103:ASN:ND2  | 2.40                     | 0.54              |
| 4:a:43:ALA:O     | 4:f:73:ARG:NH1   | 2.36                     | 0.54              |
| 4:c:175:LEU:HD12 | 5:j:1:MET:HE1    | 1.88                     | 0.54              |
| 4:f:33:ILE:HD11  | 6:u:30:ARG:HH12  | 1.73                     | 0.54              |
| 6:t:109:LEU:HD13 | 6:t:120:TRP:CZ2  | 2.43                     | 0.54              |
| 6:u:100:SER:HA   | 7:x:109:SER:HA   | 1.89                     | 0.54              |
| 6:u:108:GLU:HG3  | 7:x:113:SER:HB2  | 1.90                     | 0.54              |
| 6:u:165:ILE:HD12 | 6:u:207:TRP:CE3  | 2.34                     | 0.54              |
| 7:y:52:LYS:CE    | 7:y:61:ASP:OD1   | 2.56                     | 0.54              |
| 1:O:248:PHE:HE2  | 1:O:266:LEU:HD11 | 1.71                     | 0.53              |
| 4:f:35:SER:HB3   | 6:v:164:LEU:HD11 | 1.90                     | 0.53              |
| 5:k:78:GLU:OE1   | 5:k:78:GLU:N     | 2.38                     | 0.53              |
| 6:u:101:MET:O    | 7:x:111:SER:N    | 2.41                     | 0.53              |
| 7:y:12:ASP:O     | 7:y:16:VAL:HG23  | 2.08                     | 0.53              |
| 1:A:21:GLU:OE2   | 2:C:39:LYS:NZ    | 2.42                     | 0.53              |
| 4:a:116:ILE:CG2  | 4:b:36:GLY:HA3   | 2.38                     | 0.53              |
| 4:a:125:SER:HB2  | 6:t:176:LYS:HD3  | 1.90                     | 0.53              |
| 4:f:32:PRO:HG2   | 6:v:149:ILE:HG22 | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:164:ARG:HB2  | 1:E:190:ILE:HD11 | 1.90                     | 0.53              |
| 1:L:264:VAL:HG12 | 1:L:276:PRO:HB3  | 1.91                     | 0.53              |
| 4:a:36:GLY:HA3   | 4:f:117:VAL:N    | 2.23                     | 0.53              |
| 6:t:100:SER:HA   | 7:w:109:SER:CB   | 2.38                     | 0.53              |
| 6:u:229:LYS:OXT  | 7:y:1:MET:HE3    | 2.09                     | 0.53              |
| 6:v:112:LEU:CD1  | 7:x:57:GLY:H     | 2.20                     | 0.53              |
| 1:K:110:ASP:O    | 1:K:111:LEU:HG   | 2.09                     | 0.53              |
| 1:R:84:ARG:NH2   | 1:R:103:ASN:OD1  | 2.41                     | 0.53              |
| 6:t:118:PHE:CZ   | 7:y:56:ASN:HA    | 2.43                     | 0.53              |
| 6:u:104:SER:N    | 7:x:113:SER:C    | 2.66                     | 0.53              |
| 6:v:103:GLY:C    | 7:y:113:SER:H    | 2.17                     | 0.53              |
| 7:x:202:MET:N    | 7:x:202:MET:SD   | 2.80                     | 0.53              |
| 2:C:49:ASP:O     | 2:C:53:LYS:HG3   | 2.08                     | 0.53              |
| 1:I:156:ASP:OD1  | 1:I:194:ARG:NH2  | 2.42                     | 0.53              |
| 4:d:142:ASP:OD1  | 4:d:143:LYS:N    | 2.41                     | 0.53              |
| 4:e:115:LYS:HB3  | 4:f:34:GLU:HB3   | 1.90                     | 0.53              |
| 6:t:108:GLU:HB2  | 7:y:54:LYS:HD3   | 1.90                     | 0.53              |
| 6:v:63:LEU:HD13  | 7:x:59:PRO:O     | 2.09                     | 0.53              |
| 2:D:117:GLY:O    | 1:F:256:TYR:OH   | 2.17                     | 0.53              |
| 1:F:164:ARG:NH2  | 2:G:166:THR:HG21 | 2.23                     | 0.53              |
| 1:I:76:ARG:CZ    | 2:J:51:VAL:HA    | 2.38                     | 0.53              |
| 1:L:170:GLY:O    | 2:M:169:GLY:N    | 2.38                     | 0.53              |
| 4:a:32:PRO:HA    | 6:v:203:GLN:CG   | 2.38                     | 0.53              |
| 4:b:32:PRO:HG2   | 6:t:149:ILE:HG22 | 1.91                     | 0.53              |
| 4:b:128:LYS:NZ   | 4:b:136:SER:O    | 2.41                     | 0.53              |
| 4:e:115:LYS:CB   | 4:f:34:GLU:HB3   | 2.39                     | 0.53              |
| 4:e:118:GLU:H    | 4:f:36:GLY:N     | 2.07                     | 0.53              |
| 4:f:33:ILE:HD11  | 6:u:30:ARG:NH1   | 2.23                     | 0.53              |
| 6:u:63:LEU:C     | 7:w:58:VAL:HG11  | 2.33                     | 0.53              |
| 2:C:85:VAL:HG11  | 2:C:111:ILE:HG23 | 1.91                     | 0.53              |
| 1:K:105:ASP:C    | 1:K:107:ALA:H    | 2.16                     | 0.53              |
| 1:P:268:GLN:O    | 1:P:271:ALA:N    | 2.42                     | 0.53              |
| 6:t:165:ILE:HB   | 6:t:207:TRP:HB3  | 1.91                     | 0.53              |
| 6:t:201:ASP:N    | 6:t:205:GLY:O    | 2.41                     | 0.53              |
| 6:v:102:CYS:HB2  | 7:y:110:ALA:CB   | 2.39                     | 0.53              |
| 7:y:31:MET:SD    | 7:y:51:TYR:HB3   | 2.48                     | 0.53              |
| 1:H:181:THR:HG21 | 1:H:190:ILE:HD12 | 1.89                     | 0.53              |
| 1:P:42:LEU:CD1   | 3:p:9:LEU:HD12   | 2.39                     | 0.53              |
| 1:P:175:GLY:O    | 1:P:191:ARG:NH2  | 2.41                     | 0.53              |
| 4:a:161:ASP:HB2  | 6:t:170:ARG:NH2  | 2.24                     | 0.53              |
| 4:b:115:LYS:O    | 4:b:116:ILE:HG23 | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:c:116:ILE:CA   | 4:d:36:GLY:HA3   | 2.38                     | 0.53              |
| 4:e:115:LYS:HB3  | 4:f:34:GLU:CB    | 2.38                     | 0.53              |
| 3:q:61:VAL:HG22  | 3:q:84:GLU:HG2   | 1.91                     | 0.53              |
| 6:t:66:VAL:HB    | 7:y:58:VAL:HA    | 1.90                     | 0.53              |
| 6:t:108:GLU:O    | 6:t:112:LEU:HG   | 2.09                     | 0.53              |
| 6:u:97:ARG:O     | 7:w:52:LYS:CG    | 2.57                     | 0.53              |
| 6:v:109:LEU:O    | 6:v:112:LEU:HB2  | 2.09                     | 0.53              |
| 6:v:112:LEU:HA   | 7:x:55:PHE:HA    | 1.90                     | 0.53              |
| 7:w:33:GLY:HA2   | 7:w:49:PRO:HA    | 1.90                     | 0.53              |
| 1:A:215:CYS:SG   | 1:A:216:PRO:HD2  | 2.48                     | 0.53              |
| 1:H:117:ALA:HB3  | 1:H:162:LEU:HD21 | 1.90                     | 0.53              |
| 1:O:266:LEU:CB   | 1:O:278:LEU:HD13 | 2.39                     | 0.53              |
| 2:S:177:ARG:N    | 2:S:208:GLN:O    | 2.42                     | 0.53              |
| 7:y:60:THR:HG22  | 7:y:61:ASP:H     | 1.72                     | 0.53              |
| 1:H:111:LEU:HD11 | 1:H:131:VAL:HG21 | 1.90                     | 0.53              |
| 2:M:89:ASP:HA    | 2:M:94:TYR:CD1   | 2.44                     | 0.53              |
| 1:P:52:LEU:O     | 1:P:56:LEU:HD13  | 2.09                     | 0.53              |
| 4:a:115:LYS:CB   | 4:b:34:GLU:HB3   | 2.39                     | 0.53              |
| 6:t:142:ILE:HG21 | 6:t:161:VAL:HG11 | 1.90                     | 0.53              |
| 6:u:97:ARG:NH2   | 7:w:51:TYR:O     | 2.41                     | 0.53              |
| 6:v:99:TYR:O     | 7:y:109:SER:CB   | 2.56                     | 0.53              |
| 7:w:101:ASN:OD1  | 7:w:109:SER:O    | 2.27                     | 0.53              |
| 7:x:52:LYS:NZ    | 7:x:59:PRO:HB3   | 2.24                     | 0.53              |
| 1:A:106:ARG:C    | 1:A:108:ARG:H    | 2.16                     | 0.52              |
| 1:P:51:ASP:OD2   | 3:p:54:PHE:CE2   | 2.62                     | 0.52              |
| 1:Q:212:LYS:O    | 1:Q:213:ASN:OD1  | 2.27                     | 0.52              |
| 4:a:2:ILE:HG23   | 4:a:81:GLY:CA    | 2.39                     | 0.52              |
| 6:t:30:ARG:HE    | 6:u:151:THR:HG23 | 1.74                     | 0.52              |
| 6:t:103:GLY:C    | 7:w:113:SER:H    | 2.17                     | 0.52              |
| 1:I:206:VAL:O    | 1:I:298:VAL:N    | 2.36                     | 0.52              |
| 2:J:157:TRP:O    | 2:J:177:ARG:NH2  | 2.36                     | 0.52              |
| 1:P:156:ASP:HA   | 1:P:159:VAL:HG12 | 1.91                     | 0.52              |
| 4:a:2:ILE:HG23   | 4:a:81:GLY:O     | 2.09                     | 0.52              |
| 4:a:115:LYS:HB3  | 4:b:34:GLU:HB3   | 1.91                     | 0.52              |
| 4:c:125:SER:HB2  | 6:u:176:LYS:HD3  | 1.92                     | 0.52              |
| 5:l:72:LEU:O     | 5:l:73:LEU:HD23  | 2.09                     | 0.52              |
| 1:H:109:ILE:HD11 | 2:J:73:PHE:CE1   | 2.36                     | 0.52              |
| 4:a:2:ILE:HD11   | 4:f:102:SER:O    | 2.09                     | 0.52              |
| 4:b:173:GLN:HG2  | 4:b:177:LYS:NZ   | 2.25                     | 0.52              |
| 4:c:122:ALA:HA   | 6:u:168:GLU:OE2  | 2.09                     | 0.52              |
| 4:c:159:ALA:HB1  | 4:c:162:LYS:HE3  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:e:116:ILE:C    | 4:f:36:GLY:HA3   | 2.34                     | 0.52              |
| 5:h:29:TYR:OH    | 5:h:34:ASP:OD1   | 2.18                     | 0.52              |
| 6:t:24:ARG:HG3   | 7:y:5:LEU:CB     | 2.40                     | 0.52              |
| 6:v:54:SER:HA    | 7:y:111:SER:HA   | 1.91                     | 0.52              |
| 1:A:132:ASN:ND2  | 1:A:142:ILE:O    | 2.38                     | 0.52              |
| 1:B:169:PRO:O    | 2:C:200:ILE:HD13 | 2.09                     | 0.52              |
| 4:a:118:GLU:CB   | 4:b:35:SER:HA    | 2.32                     | 0.52              |
| 4:b:116:ILE:HG22 | 4:c:36:GLY:HA3   | 1.90                     | 0.52              |
| 6:u:98:PRO:O     | 7:w:52:LYS:N     | 2.42                     | 0.52              |
| 7:x:101:ASN:CG   | 7:x:109:SER:O    | 2.52                     | 0.52              |
| 1:P:205:ASP:O    | 1:P:262:VAL:N    | 2.34                     | 0.52              |
| 1:R:76:ARG:HD3   | 2:S:51:VAL:HB    | 1.92                     | 0.52              |
| 4:a:158:ASN:ND2  | 6:t:168:GLU:OE2  | 2.42                     | 0.52              |
| 4:e:2:ILE:HG23   | 4:e:81:GLY:O     | 2.08                     | 0.52              |
| 7:w:95:GLN:HG2   | 7:y:30:GLU:OE1   | 2.10                     | 0.52              |
| 1:B:185:GLY:O    | 2:C:217:GLY:N    | 2.40                     | 0.52              |
| 2:C:89:ASP:HA    | 2:C:94:TYR:CD1   | 2.45                     | 0.52              |
| 2:D:44:SER:OG    | 1:P:56:LEU:HD23  | 2.09                     | 0.52              |
| 1:E:105:ASP:O    | 1:E:106:ARG:HB2  | 2.09                     | 0.52              |
| 2:J:90:CYS:CB    | 2:J:94:TYR:HB3   | 2.34                     | 0.52              |
| 1:L:76:ARG:CZ    | 2:M:4:LEU:HD21   | 2.38                     | 0.52              |
| 4:a:116:ILE:CA   | 4:b:36:GLY:CA    | 2.86                     | 0.52              |
| 4:f:116:ILE:O    | 4:f:117:VAL:CG1  | 2.50                     | 0.52              |
| 5:k:81:THR:HG22  | 5:k:82:ARG:N     | 2.24                     | 0.52              |
| 6:u:109:LEU:HA   | 6:u:112:LEU:HG   | 1.91                     | 0.52              |
| 6:v:53:ILE:CG2   | 7:y:112:ASP:HA   | 2.38                     | 0.52              |
| 6:v:99:TYR:O     | 7:y:109:SER:HB2  | 2.09                     | 0.52              |
| 6:v:102:CYS:C    | 7:y:114:ARG:N    | 2.66                     | 0.52              |
| 7:y:15:VAL:O     | 7:y:15:VAL:HG12  | 2.10                     | 0.52              |
| 1:B:114:LEU:HD13 | 1:B:166:TYR:HB2  | 1.90                     | 0.52              |
| 4:d:159:ALA:HB3  | 6:v:186:ARG:HD2  | 1.92                     | 0.52              |
| 4:e:121:THR:HG23 | 4:e:122:ALA:N    | 2.25                     | 0.52              |
| 4:f:31:ASN:CB    | 4:f:32:PRO:HD2   | 2.38                     | 0.52              |
| 4:f:142:ASP:OD1  | 4:f:143:LYS:N    | 2.43                     | 0.52              |
| 3:r:24:ASP:OD1   | 3:r:26:SER:OG    | 2.27                     | 0.52              |
| 6:t:99:TYR:HD1   | 7:y:52:LYS:HD3   | 1.75                     | 0.52              |
| 6:v:57:ILE:HD13  | 6:v:66:VAL:HG11  | 1.91                     | 0.52              |
| 6:v:98:PRO:O     | 7:x:52:LYS:N     | 2.43                     | 0.52              |
| 1:E:109:ILE:HD11 | 2:G:77:HIS:HE1   | 1.73                     | 0.52              |
| 1:I:173:MET:HE1  | 1:I:190:ILE:HG23 | 1.90                     | 0.52              |
| 1:O:266:LEU:HB2  | 1:O:278:LEU:HD13 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:f:132:ASP:OD2  | 4:f:135:LYS:HE3  | 2.10                     | 0.52              |
| 6:t:94:GLN:C     | 6:t:95:LEU:HD23  | 2.35                     | 0.52              |
| 6:t:103:GLY:H    | 7:w:112:ASP:C    | 2.18                     | 0.52              |
| 6:v:99:TYR:OH    | 7:x:54:LYS:HG2   | 2.10                     | 0.52              |
| 2:C:58:THR:O     | 2:C:58:THR:HG22  | 2.10                     | 0.52              |
| 1:f:23:GLU:OE2   | 4:f:135:LYS:HD3  | 2.10                     | 0.52              |
| 1:I:23:GLU:OE1   | 4:b:128:LYS:HE2  | 2.10                     | 0.52              |
| 1:I:215:CYS:HB2  | 1:I:216:PRO:HD2  | 1.91                     | 0.52              |
| 1:O:248:PHE:CE2  | 1:O:266:LEU:HD11 | 2.45                     | 0.52              |
| 1:P:176:ASN:OD1  | 1:P:177:THR:N    | 2.43                     | 0.52              |
| 4:b:116:ILE:HG22 | 4:c:36:GLY:CA    | 2.40                     | 0.52              |
| 6:u:70:ILE:HD12  | 7:w:57:GLY:CA    | 2.40                     | 0.52              |
| 6:u:109:LEU:O    | 6:u:112:LEU:HB2  | 2.09                     | 0.52              |
| 7:w:15:VAL:O     | 7:w:15:VAL:HG12  | 2.10                     | 0.52              |
| 7:w:97:ARG:HG3   | 7:y:51:TYR:CE2   | 2.45                     | 0.52              |
| 2:J:106:PRO:HD2  | 2:J:185:ARG:HH22 | 1.75                     | 0.52              |
| 1:K:249:ARG:O    | 1:K:253:GLU:OE1  | 2.28                     | 0.52              |
| 2:S:94:TYR:OH    | 2:S:100:LEU:HD21 | 2.10                     | 0.52              |
| 6:u:57:ILE:N     | 7:x:109:SER:OG   | 2.42                     | 0.52              |
| 6:v:53:ILE:O     | 7:y:112:ASP:HB3  | 2.10                     | 0.52              |
| 7:x:51:TYR:OH    | 7:y:97:ARG:HG3   | 2.09                     | 0.52              |
| 4:d:117:VAL:H    | 4:e:36:GLY:CA    | 2.24                     | 0.51              |
| 4:f:41:ASP:HB3   | 6:v:6:TYR:HD1    | 1.75                     | 0.51              |
| 6:v:63:LEU:C     | 7:x:58:VAL:HG11  | 2.36                     | 0.51              |
| 7:x:190:ILE:HD11 | 7:y:200:HIS:NE2  | 2.25                     | 0.51              |
| 6:t:109:LEU:HD13 | 6:t:120:TRP:CH2  | 2.45                     | 0.51              |
| 6:u:102:CYS:C    | 7:x:112:ASP:C    | 2.78                     | 0.51              |
| 6:v:99:TYR:CD1   | 7:x:52:LYS:HB2   | 2.42                     | 0.51              |
| 7:y:48:GLN:CD    | 7:y:64:VAL:HG22  | 2.35                     | 0.51              |
| 1:O:12:LYS:NZ    | 1:O:61:GLU:OE1   | 2.43                     | 0.51              |
| 4:c:32:PRO:HA    | 6:t:203:GLN:CD   | 2.35                     | 0.51              |
| 4:c:115:LYS:CG   | 4:d:34:GLU:CB    | 2.71                     | 0.51              |
| 6:u:142:ILE:HG21 | 6:u:161:VAL:HG11 | 1.92                     | 0.51              |
| 6:v:57:ILE:HD12  | 6:v:99:TYR:HD2   | 1.75                     | 0.51              |
| 7:w:215:VAL:HG23 | 7:y:177:ALA:HB2  | 1.91                     | 0.51              |
| 7:x:164:GLU:HG2  | 7:x:171:ASN:OD1  | 2.10                     | 0.51              |
| 2:D:87:GLY:CA    | 2:D:100:LEU:HD12 | 2.40                     | 0.51              |
| 1:I:52:LEU:O     | 1:I:56:LEU:HD23  | 2.10                     | 0.51              |
| 5:l:100:ILE:O    | 5:l:104:ILE:HG12 | 2.10                     | 0.51              |
| 3:r:10:ALA:HB2   | 3:r:32:VAL:HG13  | 1.93                     | 0.51              |
| 6:t:99:TYR:O     | 7:w:109:SER:CB   | 2.59                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:85:VAL:O     | 2:C:100:LEU:HA   | 2.10                     | 0.51              |
| 2:D:85:VAL:O     | 2:D:100:LEU:HA   | 2.11                     | 0.51              |
| 2:G:90:CYS:SG    | 2:G:94:TYR:HB3   | 2.51                     | 0.51              |
| 2:G:106:PRO:CG   | 2:G:182:THR:HG23 | 2.39                     | 0.51              |
| 4:a:115:LYS:HB3  | 4:b:34:GLU:CB    | 2.40                     | 0.51              |
| 4:b:132:ASP:OD2  | 4:b:135:LYS:HE3  | 2.10                     | 0.51              |
| 6:v:104:SER:N    | 7:y:113:SER:C    | 2.69                     | 0.51              |
| 1:F:117:ALA:HB1  | 1:F:162:LEU:HD11 | 1.91                     | 0.51              |
| 1:L:230:GLU:OE2  | 1:L:254:ARG:NH2  | 2.38                     | 0.51              |
| 4:a:116:ILE:CG2  | 4:b:36:GLY:CA    | 2.89                     | 0.51              |
| 4:b:116:ILE:O    | 4:c:34:GLU:CG    | 2.59                     | 0.51              |
| 6:u:53:ILE:HG12  | 6:u:55:LYS:HG2   | 1.91                     | 0.51              |
| 6:u:108:GLU:O    | 6:u:112:LEU:HG   | 2.10                     | 0.51              |
| 1:I:256:TYR:OH   | 2:M:117:GLY:O    | 2.15                     | 0.51              |
| 2:M:73:PHE:O     | 2:M:129:TYR:OH   | 2.24                     | 0.51              |
| 1:Q:227:LEU:HD21 | 1:Q:231:LEU:HD11 | 1.93                     | 0.51              |
| 5:j:100:ILE:O    | 5:j:104:ILE:HG12 | 2.11                     | 0.51              |
| 6:t:63:LEU:HA    | 7:y:58:VAL:CG1   | 2.37                     | 0.51              |
| 6:u:182:LEU:HD22 | 6:u:187:LYS:HB2  | 1.91                     | 0.51              |
| 6:v:103:GLY:C    | 7:y:113:SER:N    | 2.69                     | 0.51              |
| 7:x:177:ALA:HB2  | 7:y:215:VAL:HG23 | 1.91                     | 0.51              |
| 2:D:51:VAL:HG23  | 2:D:52:GLU:H     | 1.76                     | 0.51              |
| 2:D:78:CYS:O     | 2:D:192:ARG:NH2  | 2.39                     | 0.51              |
| 1:H:106:ARG:HG3  | 1:H:106:ARG:HH11 | 1.76                     | 0.51              |
| 1:H:128:ARG:NH2  | 1:P:213:ASN:OD1  | 2.43                     | 0.51              |
| 4:b:173:GLN:HG2  | 4:b:177:LYS:HZ3  | 1.75                     | 0.51              |
| 6:v:107:ARG:HG3  | 7:x:21:GLN:OE1   | 2.10                     | 0.51              |
| 7:x:173:LEU:HD21 | 7:y:172:LEU:HD21 | 1.93                     | 0.51              |
| 1:H:54:TYR:CE2   | 1:H:58:GLU:OE2   | 2.64                     | 0.51              |
| 4:d:162:LYS:HG2  | 5:k:14:PHE:HB2   | 1.93                     | 0.51              |
| 6:u:49:ARG:NH2   | 7:w:5:LEU:HA     | 2.25                     | 0.51              |
| 6:u:108:GLU:O    | 6:u:111:THR:HG22 | 2.11                     | 0.51              |
| 6:v:24:ARG:HB2   | 7:x:6:GLY:HA3    | 1.93                     | 0.51              |
| 1:A:187:CYS:SG   | 1:E:215:CYS:N    | 2.83                     | 0.51              |
| 1:B:19:LEU:O     | 1:B:22:ILE:HG22  | 2.11                     | 0.51              |
| 2:C:106:PRO:CD   | 2:C:182:THR:HG22 | 2.41                     | 0.51              |
| 1:E:18:HIS:NE2   | 1:E:57:ASP:OD2   | 2.40                     | 0.51              |
| 1:H:55:ASP:HA    | 1:H:58:GLU:OE1   | 2.10                     | 0.51              |
| 1:L:216:PRO:HB2  | 2:S:80:CYS:SG    | 2.51                     | 0.51              |
| 2:M:106:PRO:HB3  | 2:M:186:TYR:CZ   | 2.46                     | 0.51              |
| 1:Q:70:GLU:HA    | 1:Q:98:ARG:HD3   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:205:ASP:O    | 1:R:262:VAL:N    | 2.41                     | 0.51              |
| 4:b:115:LYS:C    | 4:b:116:ILE:HG13 | 2.36                     | 0.51              |
| 5:k:1:MET:HE3    | 5:k:93:TYR:CD1   | 2.46                     | 0.51              |
| 6:t:151:THR:HG21 | 6:v:35:ILE:HD11  | 1.93                     | 0.51              |
| 6:u:21:GLY:HA2   | 7:w:7:LYS:HE2    | 1.91                     | 0.51              |
| 6:u:67:VAL:H     | 7:w:58:VAL:HG22  | 1.76                     | 0.51              |
| 7:w:200:HIS:CE1  | 7:y:190:ILE:HD11 | 2.46                     | 0.51              |
| 7:x:101:ASN:OD1  | 7:x:109:SER:C    | 2.54                     | 0.51              |
| 2:M:147:GLU:O    | 2:M:151:GLU:OE1  | 2.30                     | 0.50              |
| 4:e:116:ILE:CG2  | 4:f:36:GLY:HA3   | 2.41                     | 0.50              |
| 5:h:19:ASN:N     | 6:t:219:ASP:OD2  | 2.45                     | 0.50              |
| 6:t:64:THR:HA    | 7:y:58:VAL:HG21  | 1.93                     | 0.50              |
| 7:w:181:GLU:OE1  | 7:x:216:ARG:NH2  | 2.44                     | 0.50              |
| 7:x:146:ARG:NE   | 7:y:77:GLY:O     | 2.38                     | 0.50              |
| 2:D:137:ARG:HG2  | 1:P:85:LEU:CD1   | 2.41                     | 0.50              |
| 1:E:1:MET:O      | 1:E:6:GLN:NE2    | 2.45                     | 0.50              |
| 2:M:27:PRO:O     | 2:M:31:ASN:ND2   | 2.43                     | 0.50              |
| 2:M:180:THR:HG22 | 2:M:181:ALA:N    | 2.27                     | 0.50              |
| 5:m:81:THR:HG22  | 5:m:82:ARG:N     | 2.25                     | 0.50              |
| 6:u:54:SER:CA    | 7:x:111:SER:O    | 2.59                     | 0.50              |
| 6:u:95:LEU:HD13  | 7:w:52:LYS:HZ3   | 1.76                     | 0.50              |
| 1:H:170:GLY:N    | 1:I:133:GLU:OE2  | 2.44                     | 0.50              |
| 4:b:117:VAL:O    | 4:b:117:VAL:HG22 | 2.11                     | 0.50              |
| 3:n:10:ALA:HB2   | 3:n:32:VAL:HG13  | 1.93                     | 0.50              |
| 6:u:97:ARG:CZ    | 7:w:51:TYR:O     | 2.58                     | 0.50              |
| 6:v:102:CYS:CA   | 7:y:112:ASP:O    | 2.58                     | 0.50              |
| 6:v:195:GLU:OE1  | 6:v:212:THR:HB   | 2.11                     | 0.50              |
| 7:y:39:SER:OG    | 7:y:41:ASP:OD1   | 2.25                     | 0.50              |
| 7:y:212:ALA:O    | 7:y:215:VAL:HG22 | 2.11                     | 0.50              |
| 2:C:117:GLY:O    | 1:R:256:TYR:OH   | 2.20                     | 0.50              |
| 2:D:73:PHE:CD1   | 1:O:109:ILE:CD1  | 2.89                     | 0.50              |
| 4:b:162:LYS:HE3  | 6:u:186:ARG:HB3  | 1.93                     | 0.50              |
| 4:e:34:GLU:O     | 4:e:34:GLU:HG2   | 2.09                     | 0.50              |
| 6:t:99:TYR:O     | 7:w:109:SER:HB2  | 2.12                     | 0.50              |
| 6:u:112:LEU:CD2  | 7:w:54:LYS:HG2   | 2.41                     | 0.50              |
| 1:A:215:CYS:SG   | 1:Q:187:CYS:SG   | 3.08                     | 0.50              |
| 1:B:52:LEU:O     | 1:B:56:LEU:HD23  | 2.11                     | 0.50              |
| 2:C:99:GLN:C     | 2:C:100:LEU:HD22 | 2.37                     | 0.50              |
| 1:H:86:LEU:HD22  | 1:H:116:THR:HG21 | 1.94                     | 0.50              |
| 2:M:106:PRO:HB3  | 2:M:186:TYR:OH   | 2.11                     | 0.50              |
| 4:b:91:THR:HG22  | 4:c:28:LEU:HD13  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:32:PRO:HG2   | 6:u:149:ILE:CG2  | 2.42                     | 0.50              |
| 4:d:91:THR:HG22  | 4:e:28:LEU:HD13  | 1.93                     | 0.50              |
| 6:t:41:CYS:C     | 7:y:7:LYS:HG3    | 2.37                     | 0.50              |
| 1:H:84:ARG:HG2   | 2:J:140:MET:HE3  | 1.94                     | 0.50              |
| 4:a:37:ALA:H     | 4:f:116:ILE:CG2  | 2.24                     | 0.50              |
| 6:u:63:LEU:HA    | 7:w:58:VAL:CG1   | 2.41                     | 0.50              |
| 2:D:85:VAL:O     | 2:D:100:LEU:HD13 | 2.11                     | 0.50              |
| 2:D:137:ARG:HE   | 1:P:85:LEU:HD12  | 1.77                     | 0.50              |
| 1:F:206:VAL:HG21 | 1:F:223:MET:HE1  | 1.93                     | 0.50              |
| 1:I:62:ASP:OD2   | 2:J:1:MET:HE1    | 2.12                     | 0.50              |
| 1:I:227:LEU:CD1  | 1:I:252:MET:HE3  | 2.35                     | 0.50              |
| 4:d:33:ILE:HD11  | 6:t:30:ARG:NH1   | 2.25                     | 0.50              |
| 4:e:121:THR:CG2  | 6:v:166:ASN:OD1  | 2.60                     | 0.50              |
| 6:v:64:THR:HA    | 7:x:58:VAL:HG21  | 1.94                     | 0.50              |
| 6:v:97:ARG:HD2   | 7:x:49:PRO:O     | 2.11                     | 0.50              |
| 7:x:98:SER:HA    | 7:x:120:ASP:OD1  | 2.12                     | 0.50              |
| 2:D:180:THR:HG22 | 2:D:181:ALA:N    | 2.27                     | 0.50              |
| 1:E:178:THR:OG1  | 1:E:191:ARG:NE   | 2.45                     | 0.50              |
| 1:H:109:ILE:HD13 | 2:J:73:PHE:HE1   | 1.01                     | 0.50              |
| 3:o:20:ASP:OD1   | 3:o:21:ILE:N     | 2.44                     | 0.50              |
| 6:t:21:GLY:HA2   | 7:y:7:LYS:HE2    | 1.93                     | 0.50              |
| 6:u:103:GLY:O    | 7:x:112:ASP:CG   | 2.55                     | 0.50              |
| 6:u:115:SER:HB3  | 7:w:55:PHE:CE1   | 2.47                     | 0.50              |
| 6:v:165:ILE:HD12 | 6:v:207:TRP:CE3  | 2.47                     | 0.50              |
| 2:J:177:ARG:N    | 2:J:208:GLN:O    | 2.45                     | 0.50              |
| 4:a:142:ASP:O    | 3:p:57:LYS:NZ    | 2.44                     | 0.50              |
| 4:c:173:GLN:NE2  | 4:c:177:LYS:HE2  | 2.27                     | 0.50              |
| 5:j:36:TRP:HB3   | 5:j:53:LEU:HD12  | 1.93                     | 0.50              |
| 6:u:95:LEU:HD21  | 7:w:59:PRO:O     | 2.10                     | 0.50              |
| 6:v:46:LYS:HE2   | 6:v:50:ARG:HH21  | 1.77                     | 0.50              |
| 6:v:55:LYS:C     | 7:y:110:ALA:O    | 2.55                     | 0.50              |
| 6:v:83:GLU:CG    | 6:v:136:LEU:HD22 | 2.42                     | 0.50              |
| 1:A:111:LEU:HD11 | 1:A:131:VAL:CG2  | 2.41                     | 0.49              |
| 1:F:42:LEU:HD12  | 3:o:9:LEU:HD12   | 1.93                     | 0.49              |
| 1:F:88:ARG:NH2   | 1:F:94:ASP:OD1   | 2.42                     | 0.49              |
| 4:c:115:LYS:HB3  | 4:d:34:GLU:CB    | 2.41                     | 0.49              |
| 4:d:116:ILE:O    | 4:e:34:GLU:CG    | 2.59                     | 0.49              |
| 4:d:131:THR:O    | 4:d:131:THR:HG22 | 2.11                     | 0.49              |
| 5:m:78:GLU:OE1   | 5:m:78:GLU:N     | 2.41                     | 0.49              |
| 3:r:96:SER:OG    | 3:r:112:ASP:O    | 2.25                     | 0.49              |
| 6:t:104:SER:N    | 7:w:113:SER:C    | 2.70                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:116:HIS:HB2  | 7:y:55:PHE:CZ    | 2.47                     | 0.49              |
| 6:u:45:ASP:OD2   | 6:u:49:ARG:NH2   | 2.45                     | 0.49              |
| 6:u:56:THR:OG1   | 7:x:101:ASN:CG   | 2.55                     | 0.49              |
| 6:v:54:SER:O     | 6:v:55:LYS:HD3   | 2.12                     | 0.49              |
| 1:B:75:SER:N     | 2:C:1:MET:H2     | 2.09                     | 0.49              |
| 1:F:62:ASP:OD2   | 5:h:33:ASN:ND2   | 2.44                     | 0.49              |
| 1:I:268:GLN:O    | 1:I:271:ALA:N    | 2.45                     | 0.49              |
| 2:J:2:SER:O      | 2:J:4:LEU:HD12   | 2.12                     | 0.49              |
| 1:K:110:ASP:OD1  | 1:K:111:LEU:N    | 2.44                     | 0.49              |
| 1:P:19:LEU:O     | 1:P:22:ILE:HG22  | 2.12                     | 0.49              |
| 4:c:115:LYS:CB   | 4:d:34:GLU:CB    | 2.90                     | 0.49              |
| 4:f:31:ASN:HB3   | 6:v:149:ILE:CG2  | 2.42                     | 0.49              |
| 1:E:109:ILE:HD11 | 2:G:73:PHE:CE1   | 2.37                     | 0.49              |
| 6:u:57:ILE:HD13  | 6:u:66:VAL:HG11  | 1.94                     | 0.49              |
| 6:u:99:TYR:C     | 7:x:109:SER:CB   | 2.86                     | 0.49              |
| 6:u:103:GLY:C    | 7:x:113:SER:H    | 2.20                     | 0.49              |
| 6:v:45:ASP:O     | 6:v:49:ARG:HG2   | 2.11                     | 0.49              |
| 6:v:55:LYS:N     | 7:y:110:ALA:O    | 2.45                     | 0.49              |
| 6:v:103:GLY:H    | 7:y:112:ASP:C    | 2.20                     | 0.49              |
| 7:x:131:LEU:HD23 | 7:y:43:ARG:HD3   | 1.94                     | 0.49              |
| 1:H:76:ARG:NE    | 1:I:64:TYR:OH    | 2.45                     | 0.49              |
| 1:I:158:GLU:HA   | 1:I:158:GLU:OE2  | 2.12                     | 0.49              |
| 1:L:52:LEU:O     | 1:L:56:LEU:HD13  | 2.12                     | 0.49              |
| 1:L:76:ARG:HH12  | 2:M:4:LEU:HD21   | 1.76                     | 0.49              |
| 1:O:279:VAL:HG23 | 1:O:279:VAL:O    | 2.12                     | 0.49              |
| 3:X:32:VAL:HB    | 3:X:36:GLU:HG2   | 1.93                     | 0.49              |
| 4:e:32:PRO:HA    | 6:u:203:GLN:CD   | 2.37                     | 0.49              |
| 4:f:117:VAL:HG22 | 4:f:117:VAL:O    | 2.12                     | 0.49              |
| 5:l:53:LEU:HB3   | 5:l:72:LEU:HD11  | 1.94                     | 0.49              |
| 6:v:57:ILE:HD12  | 6:v:99:TYR:CD2   | 2.47                     | 0.49              |
| 7:x:95:GLN:HB3   | 7:x:120:ASP:HB3  | 1.94                     | 0.49              |
| 1:A:232:THR:O    | 1:A:232:THR:HG22 | 2.11                     | 0.49              |
| 2:G:8:PRO:HG3    | 2:G:45:MET:HG3   | 1.93                     | 0.49              |
| 1:H:54:TYR:O     | 1:H:58:GLU:OE1   | 2.30                     | 0.49              |
| 1:L:55:ASP:OD2   | 2:M:15:ARG:NH2   | 2.45                     | 0.49              |
| 1:L:131:VAL:HG23 | 1:L:147:VAL:HG12 | 1.95                     | 0.49              |
| 1:R:23:GLU:OE1   | 4:d:135:LYS:HB3  | 2.12                     | 0.49              |
| 4:a:121:THR:CG2  | 4:a:122:ALA:N    | 2.76                     | 0.49              |
| 4:d:133:LYS:O    | 4:d:133:LYS:HG2  | 2.12                     | 0.49              |
| 4:e:12:VAL:HG11  | 4:e:66:LEU:HD23  | 1.95                     | 0.49              |
| 4:e:118:GLU:HG2  | 6:v:144:PRO:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:102:CYS:C    | 7:w:113:SER:HA   | 2.38                     | 0.49              |
| 7:w:60:THR:HG22  | 7:w:61:ASP:H     | 1.77                     | 0.49              |
| 1:K:104:VAL:O    | 1:K:106:ARG:N    | 2.45                     | 0.49              |
| 1:O:249:ARG:O    | 1:O:253:GLU:OE1  | 2.31                     | 0.49              |
| 1:R:117:ALA:HB1  | 1:R:162:LEU:HD11 | 1.93                     | 0.49              |
| 4:a:37:ALA:O     | 4:a:38:ASP:CG    | 2.56                     | 0.49              |
| 4:a:39:VAL:HG23  | 4:f:119:THR:OG1  | 2.12                     | 0.49              |
| 4:a:121:THR:HG21 | 6:t:167:PRO:HD2  | 1.94                     | 0.49              |
| 6:v:67:VAL:H     | 7:x:58:VAL:HG22  | 1.77                     | 0.49              |
| 6:v:102:CYS:C    | 7:y:113:SER:HA   | 2.36                     | 0.49              |
| 6:v:112:LEU:HD13 | 7:x:57:GLY:H     | 1.77                     | 0.49              |
| 7:w:190:ILE:HD12 | 7:x:198:THR:H    | 1.78                     | 0.49              |
| 7:y:68:VAL:HG13  | 7:y:121:MET:O    | 2.13                     | 0.49              |
| 2:C:87:GLY:CA    | 2:C:100:LEU:HD12 | 2.42                     | 0.49              |
| 2:D:52:GLU:OE2   | 2:D:52:GLU:N     | 2.46                     | 0.49              |
| 1:I:56:LEU:HD12  | 2:J:44:SER:HB3   | 1.94                     | 0.49              |
| 1:Q:60:GLY:HA3   | 2:S:47:TYR:CE1   | 2.47                     | 0.49              |
| 6:t:99:TYR:HA    | 7:y:52:LYS:CB    | 2.43                     | 0.49              |
| 6:t:112:LEU:HD13 | 7:y:57:GLY:N     | 2.26                     | 0.49              |
| 7:w:183:VAL:O    | 7:x:202:MET:HE2  | 2.13                     | 0.49              |
| 1:B:170:GLY:O    | 2:C:169:GLY:N    | 2.39                     | 0.49              |
| 2:D:49:ASP:O     | 2:D:53:LYS:HG3   | 2.12                     | 0.49              |
| 1:H:109:ILE:HD12 | 2:J:192:ARG:HB3  | 1.94                     | 0.49              |
| 1:O:121:ILE:HD11 | 1:O:162:LEU:HD23 | 1.95                     | 0.49              |
| 1:P:59:ARG:CG    | 5:l:32:THR:HG21  | 2.42                     | 0.49              |
| 1:R:76:ARG:HG2   | 1:R:79:ILE:HD12  | 1.94                     | 0.49              |
| 2:S:56:LEU:HD13  | 2:S:67:ILE:HG21  | 1.95                     | 0.49              |
| 2:S:201:LYS:HG2  | 2:S:203:MET:HE2  | 1.95                     | 0.49              |
| 4:e:121:THR:HG21 | 6:v:167:PRO:CD   | 2.42                     | 0.49              |
| 4:e:122:ALA:CB   | 4:e:158:ASN:H    | 2.26                     | 0.49              |
| 5:k:55:THR:HG23  | 5:k:80:PRO:HD3   | 1.94                     | 0.49              |
| 6:t:56:THR:HG21  | 7:w:107:ASP:HB3  | 1.95                     | 0.49              |
| 6:u:63:LEU:CA    | 7:w:58:VAL:HG11  | 2.42                     | 0.49              |
| 6:u:99:TYR:CD1   | 7:w:52:LYS:HB2   | 2.47                     | 0.49              |
| 6:u:99:TYR:OH    | 7:w:54:LYS:HG2   | 2.13                     | 0.49              |
| 6:u:103:GLY:C    | 7:x:113:SER:N    | 2.70                     | 0.49              |
| 7:y:98:SER:CB    | 7:y:120:ASP:OD1  | 2.61                     | 0.49              |
| 1:B:164:ARG:HH21 | 2:C:146:ILE:HD12 | 1.78                     | 0.49              |
| 2:D:50:MET:O     | 2:D:50:MET:HG2   | 2.13                     | 0.49              |
| 1:I:107:ALA:HB2  | 2:J:142:GLY:O    | 2.12                     | 0.49              |
| 1:K:109:ILE:CD1  | 2:M:73:PHE:CE1   | 2.96                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:212:LYS:O    | 1:O:213:ASN:OD1  | 2.31                     | 0.49              |
| 1:R:169:PRO:O    | 2:S:200:ILE:HD13 | 2.13                     | 0.49              |
| 6:t:67:VAL:H     | 7:y:58:VAL:HG22  | 1.77                     | 0.49              |
| 6:t:118:PHE:CE1  | 7:y:56:ASN:HA    | 2.47                     | 0.49              |
| 6:t:153:THR:HG23 | 6:v:28:HIS:O     | 2.12                     | 0.49              |
| 6:t:155:THR:HG1  | 6:t:158:GLY:C    | 2.20                     | 0.49              |
| 1:F:185:GLY:O    | 2:G:217:GLY:N    | 2.44                     | 0.49              |
| 2:M:49:ASP:O     | 2:M:53:LYS:HG3   | 2.13                     | 0.49              |
| 1:O:121:ILE:HD11 | 1:O:162:LEU:CD2  | 2.42                     | 0.49              |
| 4:c:32:PRO:HA    | 6:t:203:GLN:HG3  | 1.94                     | 0.49              |
| 4:c:121:THR:HG23 | 4:c:122:ALA:N    | 2.27                     | 0.49              |
| 6:t:83:GLU:HG2   | 6:t:136:LEU:HD22 | 1.95                     | 0.49              |
| 6:u:54:SER:HA    | 7:x:111:SER:O    | 2.13                     | 0.49              |
| 6:u:101:MET:O    | 7:x:110:ALA:O    | 2.30                     | 0.49              |
| 6:v:41:CYS:C     | 7:x:7:LYS:HG3    | 2.38                     | 0.49              |
| 7:w:16:VAL:HG12  | 7:x:19:VAL:HG21  | 1.94                     | 0.49              |
| 1:A:26:MET:CE    | 2:C:32:LEU:HD12  | 2.41                     | 0.48              |
| 1:L:19:LEU:O     | 1:L:22:ILE:HG22  | 2.13                     | 0.48              |
| 4:d:162:LYS:HD2  | 6:v:186:ARG:O    | 2.13                     | 0.48              |
| 4:f:18:ILE:N     | 4:f:53:GLU:O     | 2.39                     | 0.48              |
| 6:t:102:CYS:CA   | 7:w:112:ASP:C    | 2.86                     | 0.48              |
| 1:B:211:LEU:O    | 1:B:212:LYS:C    | 2.56                     | 0.48              |
| 1:E:26:MET:HE1   | 2:G:32:LEU:HD12  | 1.94                     | 0.48              |
| 1:H:105:ASP:O    | 1:H:106:ARG:HB2  | 2.12                     | 0.48              |
| 1:K:52:LEU:HD13  | 1:L:49:TYR:CE1   | 2.48                     | 0.48              |
| 1:O:52:LEU:HD13  | 1:P:49:TYR:CZ    | 2.48                     | 0.48              |
| 1:Q:85:LEU:HD12  | 1:R:105:ASP:OD2  | 2.13                     | 0.48              |
| 4:a:145:ALA:HB2  | 3:p:57:LYS:HB3   | 1.95                     | 0.48              |
| 4:d:115:LYS:CG   | 4:e:34:GLU:HB3   | 2.43                     | 0.48              |
| 6:t:63:LEU:CD1   | 7:y:59:PRO:O     | 2.60                     | 0.48              |
| 6:t:97:ARG:CG    | 7:y:52:LYS:HG3   | 2.41                     | 0.48              |
| 6:u:55:LYS:C     | 7:x:109:SER:O    | 2.56                     | 0.48              |
| 6:v:46:LYS:HG2   | 6:v:77:GLU:OE1   | 2.14                     | 0.48              |
| 7:w:173:LEU:HD21 | 7:x:172:LEU:CD2  | 2.42                     | 0.48              |
| 2:C:83:ILE:H     | 2:C:83:ILE:HD12  | 1.78                     | 0.48              |
| 1:E:86:LEU:HD22  | 1:E:116:THR:HG21 | 1.94                     | 0.48              |
| 1:H:126:TRP:CZ2  | 1:H:128:ARG:HG3  | 2.47                     | 0.48              |
| 2:M:84:PRO:HG2   | 2:M:107:GLY:HA3  | 1.96                     | 0.48              |
| 1:P:51:ASP:OD2   | 3:p:54:PHE:CZ    | 2.67                     | 0.48              |
| 4:c:128:LYS:HG2  | 4:c:129:ASP:N    | 2.29                     | 0.48              |
| 6:t:13:ASN:OD1   | 6:t:15:ILE:HG13  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:103:GLY:C    | 7:w:113:SER:N    | 2.72                     | 0.48              |
| 6:v:165:ILE:HG23 | 6:v:198:PHE:CD1  | 2.48                     | 0.48              |
| 7:x:97:ARG:CD    | 7:x:114:ARG:O    | 2.61                     | 0.48              |
| 1:A:52:LEU:HD13  | 1:B:49:TYR:CZ    | 2.48                     | 0.48              |
| 2:C:5:CYS:HB2    | 2:C:45:MET:HE1   | 1.96                     | 0.48              |
| 1:F:26:MET:CE    | 1:F:42:LEU:HD23  | 2.42                     | 0.48              |
| 1:K:60:GLY:HA3   | 2:M:47:TYR:CE1   | 2.47                     | 0.48              |
| 2:S:90:CYS:CB    | 2:S:94:TYR:HB3   | 2.42                     | 0.48              |
| 4:d:159:ALA:H    | 6:v:186:ARG:CD   | 2.26                     | 0.48              |
| 4:f:34:GLU:H     | 4:f:34:GLU:CD    | 2.18                     | 0.48              |
| 4:f:162:LYS:HD3  | 6:t:186:ARG:O    | 2.13                     | 0.48              |
| 6:t:24:ARG:HA    | 7:y:5:LEU:O      | 2.14                     | 0.48              |
| 6:t:53:ILE:O     | 7:w:112:ASP:HB3  | 2.13                     | 0.48              |
| 6:u:176:LYS:HA   | 6:u:189:GLU:O    | 2.13                     | 0.48              |
| 6:v:55:LYS:C     | 7:y:109:SER:OG   | 2.57                     | 0.48              |
| 7:w:41:ASP:O     | 7:y:138:LEU:HD12 | 2.14                     | 0.48              |
| 7:x:125:ILE:HG22 | 7:y:75:MET:SD    | 2.53                     | 0.48              |
| 1:I:75:SER:N     | 2:J:1:MET:N      | 2.62                     | 0.48              |
| 6:t:30:ARG:HA    | 6:t:34:ASP:O     | 2.13                     | 0.48              |
| 6:t:54:SER:HA    | 7:w:111:SER:HA   | 1.95                     | 0.48              |
| 6:t:102:CYS:SG   | 7:w:114:ARG:NH2  | 2.86                     | 0.48              |
| 6:u:57:ILE:HG21  | 7:w:59:PRO:CG    | 2.43                     | 0.48              |
| 1:B:215:CYS:N    | 1:E:107:ALA:HB1  | 2.28                     | 0.48              |
| 2:G:29:LEU:HB2   | 3:o:21:ILE:HG12  | 1.96                     | 0.48              |
| 4:a:117:VAL:N    | 4:b:36:GLY:HA3   | 2.29                     | 0.48              |
| 4:f:41:ASP:HB3   | 6:v:6:TYR:CD1    | 2.48                     | 0.48              |
| 4:f:140:SER:OG   | 4:f:143:LYS:HG2  | 2.14                     | 0.48              |
| 3:r:23:LEU:HD23  | 3:r:23:LEU:H     | 1.77                     | 0.48              |
| 6:t:140:LEU:HD13 | 6:t:168:GLU:OE1  | 2.13                     | 0.48              |
| 6:u:41:CYS:C     | 7:w:7:LYS:HG3    | 2.38                     | 0.48              |
| 6:u:108:GLU:HA   | 6:u:111:THR:HG22 | 1.95                     | 0.48              |
| 6:v:101:MET:O    | 7:y:111:SER:N    | 2.46                     | 0.48              |
| 7:x:32:PRO:HG3   | 7:y:102:TYR:CE2  | 2.49                     | 0.48              |
| 7:x:51:TYR:CE1   | 7:x:52:LYS:O     | 2.66                     | 0.48              |
| 1:E:52:LEU:HD13  | 1:F:49:TYR:CE1   | 2.49                     | 0.48              |
| 1:L:176:ASN:OD1  | 1:L:177:THR:N    | 2.47                     | 0.48              |
| 2:S:47:TYR:C     | 2:S:49:ASP:H     | 2.22                     | 0.48              |
| 5:j:42:LEU:HD21  | 5:j:67:ILE:HD13  | 1.96                     | 0.48              |
| 6:t:54:SER:CA    | 7:w:111:SER:O    | 2.61                     | 0.48              |
| 6:u:97:ARG:HB2   | 7:w:49:PRO:O     | 2.14                     | 0.48              |
| 6:u:112:LEU:CD2  | 7:w:57:GLY:H     | 2.26                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:43:ASP:HB2   | 7:x:7:LYS:HG2    | 1.96                     | 0.48              |
| 7:y:66:GLN:OE1   | 7:y:66:GLN:HA    | 2.14                     | 0.48              |
| 1:A:171:VAL:N    | 1:B:133:GLU:OE1  | 2.47                     | 0.48              |
| 1:L:169:PRO:HG3  | 2:M:146:ILE:HG13 | 1.96                     | 0.48              |
| 1:Q:166:TYR:CD2  | 1:R:106:ARG:HD3  | 2.49                     | 0.48              |
| 4:b:175:LEU:HD22 | 5:m:73:LEU:HD13  | 1.96                     | 0.48              |
| 5:m:81:THR:HG22  | 5:m:82:ARG:H     | 1.78                     | 0.48              |
| 6:u:24:ARG:HG3   | 7:w:5:LEU:CB     | 2.44                     | 0.48              |
| 6:u:97:ARG:O     | 7:w:52:LYS:HG3   | 2.14                     | 0.48              |
| 6:v:53:ILE:HG12  | 6:v:55:LYS:HG2   | 1.95                     | 0.48              |
| 6:v:56:THR:OG1   | 7:y:101:ASN:CB   | 2.62                     | 0.48              |
| 6:v:100:SER:HB2  | 7:x:51:TYR:CE2   | 2.49                     | 0.48              |
| 7:w:55:PHE:O     | 7:w:58:VAL:O     | 2.32                     | 0.48              |
| 7:w:95:GLN:OE1   | 7:w:99:MET:HG2   | 2.14                     | 0.48              |
| 7:x:190:ILE:HG21 | 7:y:195:SER:HA   | 1.95                     | 0.48              |
| 1:B:156:ASP:HA   | 1:B:159:VAL:HG12 | 1.96                     | 0.48              |
| 2:D:51:VAL:CG2   | 2:D:52:GLU:OE2   | 2.61                     | 0.48              |
| 2:D:106:PRO:HB3  | 2:D:186:TYR:CE2  | 2.49                     | 0.48              |
| 2:G:211:ILE:HD13 | 2:G:227:LEU:HD13 | 1.95                     | 0.48              |
| 4:b:89:ILE:HD12  | 4:b:114:VAL:CG2  | 2.44                     | 0.48              |
| 4:c:119:THR:OG1  | 4:d:39:VAL:HG23  | 2.14                     | 0.48              |
| 4:e:165:THR:HG22 | 5:i:3:GLU:HB3    | 1.95                     | 0.48              |
| 4:f:159:ALA:H    | 6:t:186:ARG:HD2  | 1.77                     | 0.48              |
| 6:t:103:GLY:HA3  | 7:w:113:SER:C    | 2.39                     | 0.48              |
| 6:v:113:GLY:O    | 6:v:117:GLY:N    | 2.44                     | 0.48              |
| 6:v:116:HIS:HB2  | 7:x:55:PHE:CE1   | 2.48                     | 0.48              |
| 7:w:1:MET:HB3    | 7:w:4:TYR:HE1    | 1.79                     | 0.48              |
| 2:C:73:PHE:O     | 2:C:129:TYR:OH   | 2.29                     | 0.48              |
| 2:C:97:SER:O     | 1:R:221:ASN:ND2  | 2.45                     | 0.48              |
| 1:E:105:ASP:C    | 1:E:107:ALA:H    | 2.22                     | 0.48              |
| 3:X:102:ASP:OD1  | 3:X:104:GLY:N    | 2.47                     | 0.48              |
| 4:a:21:LYS:HB3   | 4:a:51:GLU:HB2   | 1.96                     | 0.48              |
| 6:t:55:LYS:C     | 7:w:109:SER:HG   | 2.19                     | 0.48              |
| 6:u:64:THR:HA    | 7:w:58:VAL:HG21  | 1.96                     | 0.48              |
| 6:u:99:TYR:O     | 7:x:109:SER:CB   | 2.60                     | 0.48              |
| 1:A:60:GLY:HA3   | 2:C:47:TYR:CE1   | 2.49                     | 0.47              |
| 1:B:99:ARG:HD3   | 5:i:56:GLY:O     | 2.14                     | 0.47              |
| 2:D:99:GLN:C     | 2:D:100:LEU:HD22 | 2.39                     | 0.47              |
| 1:E:104:VAL:O    | 1:E:106:ARG:N    | 2.47                     | 0.47              |
| 1:E:198:ILE:HG13 | 1:E:198:ILE:O    | 2.14                     | 0.47              |
| 4:c:34:GLU:HG2   | 4:c:34:GLU:O     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:c:117:VAL:N    | 4:d:37:ALA:H     | 2.12                     | 0.47              |
| 4:d:33:ILE:CG2   | 4:d:34:GLU:N     | 2.77                     | 0.47              |
| 4:f:179:VAL:HG21 | 5:h:73:LEU:HD21  | 1.94                     | 0.47              |
| 6:t:101:MET:HE2  | 7:y:54:LYS:HG3   | 1.96                     | 0.47              |
| 6:u:112:LEU:CD1  | 7:w:57:GLY:H     | 2.26                     | 0.47              |
| 6:u:152:PRO:HB3  | 6:u:177:VAL:HG11 | 1.96                     | 0.47              |
| 6:v:66:VAL:HG12  | 7:x:57:GLY:O     | 2.14                     | 0.47              |
| 2:C:106:PRO:HG2  | 2:C:182:THR:CB   | 2.44                     | 0.47              |
| 1:K:52:LEU:HD13  | 1:L:49:TYR:CZ    | 2.49                     | 0.47              |
| 1:P:88:ARG:NH2   | 1:P:94:ASP:OD1   | 2.47                     | 0.47              |
| 4:d:117:VAL:N    | 4:e:36:GLY:HA3   | 2.27                     | 0.47              |
| 4:e:116:ILE:CB   | 4:f:36:GLY:CA    | 2.74                     | 0.47              |
| 6:u:55:LYS:C     | 7:x:110:ALA:O    | 2.57                     | 0.47              |
| 1:B:169:PRO:HG3  | 2:C:146:ILE:HG13 | 1.96                     | 0.47              |
| 2:D:73:PHE:HD1   | 1:O:109:ILE:HD13 | 1.75                     | 0.47              |
| 1:H:138:ASP:OD1  | 1:H:142:ILE:N    | 2.46                     | 0.47              |
| 1:P:211:LEU:HD23 | 1:P:211:LEU:H    | 1.79                     | 0.47              |
| 1:Q:109:ILE:HG21 | 2:S:73:PHE:HD1   | 1.78                     | 0.47              |
| 4:c:121:THR:CG2  | 4:c:122:ALA:N    | 2.76                     | 0.47              |
| 4:c:128:LYS:HG2  | 4:c:129:ASP:H    | 1.78                     | 0.47              |
| 4:e:115:LYS:C    | 4:f:34:GLU:HB2   | 2.39                     | 0.47              |
| 4:e:116:ILE:CA   | 4:f:36:GLY:CA    | 2.88                     | 0.47              |
| 4:f:31:ASN:HD22  | 6:v:149:ILE:HD13 | 1.79                     | 0.47              |
| 5:h:12:GLN:HB2   | 6:t:186:ARG:NH2  | 2.29                     | 0.47              |
| 5:j:36:TRP:CB    | 5:j:53:LEU:HD12  | 2.44                     | 0.47              |
| 6:t:30:ARG:NE    | 6:u:151:THR:HG23 | 2.29                     | 0.47              |
| 6:v:21:GLY:HA2   | 7:x:7:LYS:HE2    | 1.96                     | 0.47              |
| 7:w:58:VAL:HG12  | 7:w:59:PRO:N     | 2.30                     | 0.47              |
| 7:w:164:GLU:HB2  | 7:x:221:ILE:HD12 | 1.95                     | 0.47              |
| 2:D:106:PRO:CG   | 2:D:182:THR:HG22 | 2.43                     | 0.47              |
| 2:J:49:ASP:O     | 2:J:53:LYS:CG    | 2.63                     | 0.47              |
| 2:M:106:PRO:HD3  | 2:M:182:THR:HG22 | 1.96                     | 0.47              |
| 1:P:85:LEU:O     | 1:P:86:LEU:HD22  | 2.14                     | 0.47              |
| 4:b:157:VAL:O    | 6:u:186:ARG:NH1  | 2.47                     | 0.47              |
| 4:c:179:VAL:CG2  | 5:j:73:LEU:HD21  | 2.44                     | 0.47              |
| 4:e:158:ASN:HD22 | 6:v:168:GLU:HG3  | 1.79                     | 0.47              |
| 6:t:112:LEU:CD1  | 7:y:57:GLY:H     | 2.25                     | 0.47              |
| 7:w:190:ILE:HG21 | 7:x:195:SER:HA   | 1.95                     | 0.47              |
| 1:A:106:ARG:O    | 1:A:108:ARG:N    | 2.47                     | 0.47              |
| 1:F:175:GLY:O    | 1:F:191:ARG:NH2  | 2.48                     | 0.47              |
| 1:H:210:PRO:HB2  | 1:H:213:ASN:HA   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:2:ILE:HB     | 4:d:81:GLY:O     | 2.13                     | 0.47              |
| 4:d:34:GLU:N     | 4:d:34:GLU:OE1   | 2.35                     | 0.47              |
| 5:h:27:LEU:HD22  | 5:h:53:LEU:HD11  | 1.96                     | 0.47              |
| 6:t:102:CYS:C    | 7:w:114:ARG:N    | 2.69                     | 0.47              |
| 6:t:103:GLY:CA   | 7:w:113:SER:C    | 2.87                     | 0.47              |
| 6:u:112:LEU:HD13 | 7:w:57:GLY:N     | 2.30                     | 0.47              |
| 7:x:125:ILE:HB   | 7:y:75:MET:HG3   | 1.97                     | 0.47              |
| 7:y:22:SER:O     | 7:y:25:GLU:HB2   | 2.14                     | 0.47              |
| 1:E:30:PHE:CD1   | 3:o:23:LEU:HD11  | 2.49                     | 0.47              |
| 1:Q:252:MET:HA   | 1:Q:252:MET:HE3  | 1.96                     | 0.47              |
| 4:c:173:GLN:HE21 | 5:j:103:ALA:HA   | 1.80                     | 0.47              |
| 4:e:37:ALA:O     | 4:e:38:ASP:CG    | 2.58                     | 0.47              |
| 4:f:116:ILE:C    | 4:f:117:VAL:HG12 | 2.35                     | 0.47              |
| 5:k:81:THR:HG22  | 5:k:82:ARG:H     | 1.78                     | 0.47              |
| 5:l:81:THR:HG22  | 5:l:82:ARG:N     | 2.29                     | 0.47              |
| 3:o:71:GLY:O     | 3:o:72:TYR:C     | 2.57                     | 0.47              |
| 6:u:70:ILE:HD12  | 7:w:57:GLY:HA2   | 1.97                     | 0.47              |
| 6:v:42:GLY:C     | 7:x:7:LYS:HG2    | 2.40                     | 0.47              |
| 7:x:188:LEU:HD22 | 7:y:188:LEU:HD22 | 1.96                     | 0.47              |
| 2:D:102:GLY:O    | 2:D:103:TYR:HB2  | 2.14                     | 0.47              |
| 2:G:87:GLY:CA    | 2:G:100:LEU:HD12 | 2.44                     | 0.47              |
| 1:K:76:ARG:HH22  | 1:L:67:PHE:HB2   | 1.79                     | 0.47              |
| 2:S:212:ALA:O    | 2:S:218:TRP:HZ2  | 1.97                     | 0.47              |
| 4:a:115:LYS:O    | 4:a:116:ILE:HG23 | 2.15                     | 0.47              |
| 4:b:33:ILE:HG22  | 6:t:149:ILE:HA   | 1.96                     | 0.47              |
| 4:b:157:VAL:HG13 | 6:u:186:ARG:HH21 | 1.72                     | 0.47              |
| 4:c:115:LYS:C    | 4:c:116:ILE:HG12 | 2.39                     | 0.47              |
| 4:c:173:GLN:HE22 | 4:c:177:LYS:HE2  | 1.79                     | 0.47              |
| 4:d:117:VAL:HG22 | 4:d:117:VAL:O    | 2.14                     | 0.47              |
| 4:e:49:GLU:HG2   | 4:e:112:ARG:HG2  | 1.96                     | 0.47              |
| 4:e:142:ASP:OD1  | 4:e:143:LYS:N    | 2.48                     | 0.47              |
| 4:f:33:ILE:CG2   | 4:f:34:GLU:N     | 2.77                     | 0.47              |
| 6:t:43:ASP:HB2   | 7:y:7:LYS:HG2    | 1.97                     | 0.47              |
| 6:u:103:GLY:HA3  | 7:x:113:SER:C    | 2.39                     | 0.47              |
| 6:v:13:ASN:OD1   | 6:v:15:ILE:HG13  | 2.15                     | 0.47              |
| 6:v:24:ARG:HA    | 7:x:5:LEU:O      | 2.15                     | 0.47              |
| 6:v:54:SER:CA    | 7:y:111:SER:O    | 2.63                     | 0.47              |
| 6:v:102:CYS:CA   | 7:y:112:ASP:C    | 2.88                     | 0.47              |
| 7:w:43:ARG:NH1   | 7:y:133:ASP:O    | 2.48                     | 0.47              |
| 1:Q:67:PHE:CD1   | 1:Q:67:PHE:O     | 2.68                     | 0.47              |
| 2:S:18:GLU:OE1   | 2:S:18:GLU:HA    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:55:LYS:C     | 7:w:109:SER:OG   | 2.57                     | 0.47              |
| 7:w:101:ASN:CG   | 7:w:109:SER:O    | 2.58                     | 0.47              |
| 1:R:23:GLU:OE2   | 4:d:128:LYS:NZ   | 2.40                     | 0.47              |
| 3:X:24:ASP:OD1   | 3:X:24:ASP:N     | 2.46                     | 0.47              |
| 4:b:39:VAL:HG13  | 6:t:6:TYR:CE2    | 2.49                     | 0.47              |
| 5:i:36:TRP:CB    | 5:i:53:LEU:HD12  | 2.45                     | 0.47              |
| 5:l:16:VAL:HG13  | 5:l:18:LEU:HG    | 1.97                     | 0.47              |
| 5:l:27:LEU:HD22  | 5:l:53:LEU:HD11  | 1.97                     | 0.47              |
| 6:u:43:ASP:HB2   | 7:w:7:LYS:HG2    | 1.97                     | 0.47              |
| 6:v:63:LEU:CA    | 7:x:58:VAL:HG11  | 2.45                     | 0.47              |
| 7:w:221:ILE:HD12 | 7:y:164:GLU:HB2  | 1.97                     | 0.47              |
| 1:F:238:GLY:N    | 1:F:241:GLU:OE1  | 2.48                     | 0.47              |
| 1:I:12:LYS:HZ2   | 5:m:28:TRP:HD1   | 1.62                     | 0.47              |
| 1:I:162:LEU:HD23 | 1:I:162:LEU:C    | 2.40                     | 0.47              |
| 1:Q:12:LYS:HD2   | 1:Q:61:GLU:OE1   | 2.15                     | 0.47              |
| 3:X:71:GLY:O     | 3:X:72:TYR:C     | 2.57                     | 0.47              |
| 4:b:33:ILE:HG12  | 4:b:34:GLU:N     | 2.30                     | 0.47              |
| 4:c:37:ALA:O     | 4:c:38:ASP:CG    | 2.58                     | 0.47              |
| 3:q:71:GLY:O     | 3:q:72:TYR:C     | 2.57                     | 0.47              |
| 6:t:107:ARG:HG3  | 7:y:25:GLU:OE2   | 2.15                     | 0.47              |
| 6:t:113:GLY:O    | 6:t:117:GLY:N    | 2.47                     | 0.47              |
| 6:u:109:LEU:HD23 | 6:u:112:LEU:CD1  | 2.43                     | 0.47              |
| 6:v:102:CYS:SG   | 7:y:98:SER:OG    | 2.71                     | 0.47              |
| 6:v:102:CYS:SG   | 7:y:114:ARG:HD3  | 2.55                     | 0.47              |
| 7:w:99:MET:HE3   | 7:w:102:TYR:CB   | 2.45                     | 0.47              |
| 7:y:47:VAL:HG11  | 7:y:92:LEU:HD11  | 1.97                     | 0.47              |
| 2:D:76:CYS:HB2   | 2:D:121:LEU:O    | 2.15                     | 0.46              |
| 2:D:169:GLY:N    | 1:P:170:GLY:O    | 2.45                     | 0.46              |
| 1:E:168:VAL:HG12 | 1:F:109:ILE:HD11 | 1.97                     | 0.46              |
| 1:H:84:ARG:NH2   | 1:H:101:ILE:O    | 2.48                     | 0.46              |
| 1:O:167:VAL:HG11 | 1:O:173:MET:SD   | 2.56                     | 0.46              |
| 1:R:121:ILE:HD11 | 1:R:162:LEU:HD13 | 1.96                     | 0.46              |
| 4:e:128:LYS:HG2  | 4:e:129:ASP:H    | 1.81                     | 0.46              |
| 5:l:97:GLN:O     | 5:l:101:ASP:OD2  | 2.34                     | 0.46              |
| 6:v:49:ARG:HG3   | 6:v:50:ARG:CG    | 2.41                     | 0.46              |
| 6:v:63:LEU:HA    | 7:x:58:VAL:CG1   | 2.46                     | 0.46              |
| 6:v:83:GLU:HG2   | 6:v:136:LEU:HD22 | 1.97                     | 0.46              |
| 6:v:101:MET:O    | 7:y:110:ALA:O    | 2.33                     | 0.46              |
| 1:F:278:LEU:CD2  | 1:F:280:MET:HE2  | 2.45                     | 0.46              |
| 1:H:109:ILE:HD12 | 2:J:73:PHE:HE1   | 1.67                     | 0.46              |
| 1:I:202:VAL:HG12 | 1:I:266:LEU:HD23 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:j:81:THR:HG22  | 5:j:82:ARG:N     | 2.30                     | 0.46              |
| 6:t:109:LEU:HA   | 6:t:112:LEU:CD1  | 2.46                     | 0.46              |
| 6:t:153:THR:CG2  | 6:v:28:HIS:O     | 2.64                     | 0.46              |
| 6:u:112:LEU:HD22 | 7:w:57:GLY:N     | 2.28                     | 0.46              |
| 6:v:57:ILE:CD1   | 6:v:66:VAL:HG11  | 2.45                     | 0.46              |
| 6:v:116:HIS:HB2  | 7:x:55:PHE:CZ    | 2.50                     | 0.46              |
| 4:e:175:LEU:CD1  | 5:i:1:MET:HE1    | 2.45                     | 0.46              |
| 6:t:55:LYS:C     | 7:w:109:SER:O    | 2.59                     | 0.46              |
| 6:u:90:VAL:HG21  | 7:w:56:ASN:ND2   | 2.30                     | 0.46              |
| 6:u:101:MET:O    | 7:x:111:SER:O    | 2.33                     | 0.46              |
| 6:v:53:ILE:O     | 7:y:112:ASP:CA   | 2.64                     | 0.46              |
| 6:v:103:GLY:N    | 7:y:114:ARG:HD2  | 2.29                     | 0.46              |
| 7:y:1:MET:HB3    | 7:y:4:TYR:HE1    | 1.80                     | 0.46              |
| 2:D:50:MET:HE1   | 1:O:60:GLY:O     | 2.16                     | 0.46              |
| 1:I:75:SER:N     | 2:J:1:MET:H2     | 2.14                     | 0.46              |
| 1:I:216:PRO:CB   | 2:M:80:CYS:SG    | 3.03                     | 0.46              |
| 1:L:49:TYR:O     | 1:L:50:ALA:C     | 2.57                     | 0.46              |
| 1:P:19:LEU:O     | 1:P:23:GLU:HG3   | 2.16                     | 0.46              |
| 2:S:104:CYS:O    | 2:S:105:GLU:HG3  | 2.16                     | 0.46              |
| 2:S:109:SER:HB2  | 2:S:116:TYR:HB2  | 1.97                     | 0.46              |
| 5:i:81:THR:HG22  | 5:i:82:ARG:N     | 2.29                     | 0.46              |
| 6:t:109:LEU:HA   | 6:t:112:LEU:CG   | 2.46                     | 0.46              |
| 6:u:118:PHE:CD1  | 7:w:56:ASN:OD1   | 2.68                     | 0.46              |
| 6:v:97:ARG:O     | 7:x:52:LYS:CG    | 2.63                     | 0.46              |
| 7:w:52:LYS:NZ    | 7:w:59:PRO:HB3   | 2.30                     | 0.46              |
| 1:B:211:LEU:O    | 1:B:214:GLY:N    | 2.48                     | 0.46              |
| 1:I:169:PRO:O    | 2:J:200:ILE:HD13 | 2.16                     | 0.46              |
| 1:I:289:ASN:OD1  | 1:I:290:ALA:N    | 2.48                     | 0.46              |
| 4:b:179:VAL:CG2  | 5:m:73:LEU:HD21  | 2.46                     | 0.46              |
| 4:c:119:THR:OG1  | 4:d:36:GLY:O     | 2.33                     | 0.46              |
| 4:e:122:ALA:HA   | 4:e:158:ASN:HB2  | 1.96                     | 0.46              |
| 6:u:24:ARG:HA    | 7:w:5:LEU:O      | 2.16                     | 0.46              |
| 6:u:60:GLY:H     | 6:u:95:LEU:HB2   | 1.81                     | 0.46              |
| 6:u:97:ARG:NH2   | 7:w:49:PRO:HB2   | 2.30                     | 0.46              |
| 6:v:53:ILE:O     | 7:y:112:ASP:N    | 2.48                     | 0.46              |
| 6:v:99:TYR:HE2   | 6:v:101:MET:CE   | 2.28                     | 0.46              |
| 6:v:112:LEU:HD22 | 7:x:57:GLY:H     | 1.80                     | 0.46              |
| 2:M:106:PRO:HB3  | 2:M:186:TYR:CE2  | 2.50                     | 0.46              |
| 1:Q:45:LEU:HD21  | 1:R:26:MET:HE1   | 1.98                     | 0.46              |
| 1:R:131:VAL:HG23 | 1:R:147:VAL:HG22 | 1.98                     | 0.46              |
| 1:R:289:ASN:OD1  | 1:R:290:ALA:N    | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:42:GLY:C     | 7:y:7:LYS:HG2    | 2.41                     | 0.46              |
| 6:u:100:SER:HA   | 7:x:109:SER:CA   | 2.46                     | 0.46              |
| 6:v:99:TYR:CZ    | 7:x:54:LYS:HA    | 2.51                     | 0.46              |
| 7:x:58:VAL:HG12  | 7:x:59:PRO:N     | 2.31                     | 0.46              |
| 1:E:197:LEU:HD12 | 1:E:287:SER:HB2  | 1.97                     | 0.46              |
| 1:H:164:ARG:HB2  | 1:H:190:ILE:HD11 | 1.97                     | 0.46              |
| 4:b:79:MET:HE2   | 4:b:84:MET:HG3   | 1.98                     | 0.46              |
| 4:d:175:LEU:HD12 | 5:k:1:MET:HE1    | 1.98                     | 0.46              |
| 3:q:78:GLU:OE2   | 3:q:82:LYS:HD2   | 2.16                     | 0.46              |
| 6:u:143:THR:HG22 | 6:u:178:LYS:HB2  | 1.96                     | 0.46              |
| 6:v:67:VAL:HG12  | 6:v:84:TRP:CZ3   | 2.50                     | 0.46              |
| 7:y:52:LYS:HG2   | 7:y:60:THR:O     | 2.16                     | 0.46              |
| 1:E:170:GLY:N    | 1:F:133:GLU:OE2  | 2.49                     | 0.46              |
| 1:K:232:THR:O    | 1:K:232:THR:HG22 | 2.15                     | 0.46              |
| 1:L:242:ASP:OD1  | 1:L:280:MET:N    | 2.45                     | 0.46              |
| 2:M:8:PRO:HG3    | 2:M:45:MET:CG    | 2.45                     | 0.46              |
| 2:S:201:LYS:CG   | 2:S:203:MET:HE2  | 2.46                     | 0.46              |
| 4:b:73:ARG:HD2   | 4:c:45:VAL:HG23  | 1.97                     | 0.46              |
| 4:b:117:VAL:H    | 4:c:36:GLY:CA    | 2.27                     | 0.46              |
| 4:f:9:ILE:HD13   | 4:f:109:VAL:HG11 | 1.98                     | 0.46              |
| 6:u:56:THR:CA    | 7:x:109:SER:O    | 2.63                     | 0.46              |
| 6:v:108:GLU:O    | 6:v:111:THR:HG22 | 2.16                     | 0.46              |
| 7:w:180:MET:HG2  | 7:x:179:PHE:CE2  | 2.50                     | 0.46              |
| 7:x:131:LEU:HD23 | 7:y:43:ARG:CD    | 2.45                     | 0.46              |
| 1:E:70:GLU:HA    | 1:E:98:ARG:HD3   | 1.98                     | 0.46              |
| 1:F:73:GLU:OE1   | 5:h:52:ARG:NH1   | 2.49                     | 0.46              |
| 1:R:238:GLY:N    | 1:R:241:GLU:OE1  | 2.43                     | 0.46              |
| 3:o:72:TYR:CE1   | 3:o:101:PHE:HB2  | 2.51                     | 0.46              |
| 1:A:110:ASP:O    | 1:A:111:LEU:HB2  | 2.16                     | 0.46              |
| 1:B:1:MET:HE3    | 1:B:3:TYR:O      | 2.16                     | 0.46              |
| 2:D:180:THR:HG22 | 2:D:181:ALA:H    | 1.81                     | 0.46              |
| 1:L:217:PRO:HG2  | 2:S:237:CYS:SG   | 2.56                     | 0.46              |
| 4:a:118:GLU:HG2  | 6:t:144:PRO:O    | 2.16                     | 0.46              |
| 4:a:118:GLU:OE1  | 6:t:148:LEU:O    | 2.34                     | 0.46              |
| 4:b:116:ILE:C    | 4:b:117:VAL:HG12 | 2.37                     | 0.46              |
| 4:c:32:PRO:O     | 6:t:203:GLN:CG   | 2.64                     | 0.46              |
| 6:t:66:VAL:HG22  | 6:t:69:GLU:OE2   | 2.16                     | 0.46              |
| 6:t:102:CYS:O    | 7:w:114:ARG:CB   | 2.64                     | 0.46              |
| 6:u:13:ASN:OD1   | 6:u:15:ILE:HG13  | 2.15                     | 0.46              |
| 6:u:28:HIS:O     | 6:v:153:THR:CG2  | 2.64                     | 0.46              |
| 6:u:53:ILE:O     | 7:x:112:ASP:N    | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:w:180:MET:HE3  | 7:x:215:VAL:HG21 | 1.98                     | 0.46              |
| 7:x:18:ALA:O     | 7:x:21:GLN:NE2   | 2.48                     | 0.46              |
| 1:E:109:ILE:HG21 | 2:G:73:PHE:HD1   | 1.80                     | 0.45              |
| 1:E:181:THR:HG21 | 1:E:190:ILE:HD12 | 1.98                     | 0.45              |
| 1:I:189:ARG:NH1  | 1:I:191:ARG:HD3  | 2.31                     | 0.45              |
| 2:M:106:PRO:HG2  | 2:M:182:THR:HB   | 1.98                     | 0.45              |
| 1:P:156:ASP:OD1  | 1:P:157:ASP:N    | 2.49                     | 0.45              |
| 4:a:114:VAL:HG12 | 4:a:115:LYS:H    | 1.81                     | 0.45              |
| 4:b:117:VAL:N    | 4:c:36:GLY:CA    | 2.79                     | 0.45              |
| 4:d:117:VAL:H    | 4:e:37:ALA:N     | 2.13                     | 0.45              |
| 4:f:157:VAL:O    | 6:t:186:ARG:NH1  | 2.50                     | 0.45              |
| 3:r:63:TRP:CE3   | 3:r:67:LEU:HD12  | 2.51                     | 0.45              |
| 6:u:24:ARG:NE    | 7:w:5:LEU:HB2    | 2.31                     | 0.45              |
| 6:u:28:HIS:O     | 6:v:153:THR:HG23 | 2.15                     | 0.45              |
| 6:u:54:SER:HA    | 7:x:111:SER:HA   | 1.98                     | 0.45              |
| 6:u:112:LEU:HD22 | 7:w:55:PHE:C     | 2.41                     | 0.45              |
| 6:v:63:LEU:HD12  | 7:x:58:VAL:HB    | 1.98                     | 0.45              |
| 7:y:96:MET:C     | 7:y:97:ARG:HG2   | 2.40                     | 0.45              |
| 2:G:51:VAL:HG23  | 2:G:52:GLU:CD    | 2.39                     | 0.45              |
| 1:I:196:VAL:O    | 1:I:198:ILE:HD12 | 2.16                     | 0.45              |
| 2:S:211:ILE:HD13 | 2:S:227:LEU:HD13 | 1.98                     | 0.45              |
| 4:a:175:LEU:HD22 | 5:l:73:LEU:HD13  | 1.98                     | 0.45              |
| 4:c:160:GLY:H    | 6:u:16:GLY:HA3   | 1.80                     | 0.45              |
| 4:f:34:GLU:N     | 4:f:34:GLU:OE1   | 2.42                     | 0.45              |
| 6:v:67:VAL:HG12  | 6:v:84:TRP:CH2   | 2.51                     | 0.45              |
| 6:v:99:TYR:CB    | 7:x:52:LYS:HD2   | 2.39                     | 0.45              |
| 1:I:208:SER:OG   | 1:I:217:PRO:HB3  | 2.16                     | 0.45              |
| 2:M:87:GLY:CA    | 2:M:100:LEU:HD12 | 2.46                     | 0.45              |
| 1:P:163:VAL:HG11 | 1:P:173:MET:HE3  | 1.98                     | 0.45              |
| 1:Q:109:ILE:HD12 | 2:S:192:ARG:HB3  | 1.97                     | 0.45              |
| 1:Q:132:ASN:ND2  | 1:Q:142:ILE:O    | 2.49                     | 0.45              |
| 1:Q:202:VAL:CG1  | 1:Q:293:ILE:HG12 | 2.46                     | 0.45              |
| 4:b:34:GLU:N     | 4:b:34:GLU:OE1   | 2.50                     | 0.45              |
| 5:i:43:ASP:HB3   | 6:v:83:GLU:HB2   | 1.98                     | 0.45              |
| 6:u:99:TYR:CZ    | 7:w:54:LYS:HA    | 2.50                     | 0.45              |
| 6:v:112:LEU:CD2  | 7:x:57:GLY:H     | 2.29                     | 0.45              |
| 1:B:114:LEU:HD12 | 1:B:162:LEU:CD2  | 2.46                     | 0.45              |
| 1:R:38:GLU:O     | 1:R:44:GLN:NE2   | 2.47                     | 0.45              |
| 4:c:26:VAL:HG22  | 4:c:45:VAL:HG22  | 1.99                     | 0.45              |
| 4:c:143:LYS:HA   | 3:r:57:LYS:NZ    | 2.31                     | 0.45              |
| 5:l:29:TYR:CZ    | 5:l:82:ARG:HB2   | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:n:23:LEU:HD23  | 3:n:23:LEU:H     | 1.81                     | 0.45              |
| 6:t:196:VAL:HG22 | 6:t:211:LEU:CD2  | 2.47                     | 0.45              |
| 6:u:42:GLY:C     | 7:w:7:LYS:HG2    | 2.42                     | 0.45              |
| 6:u:56:THR:HA    | 7:x:109:SER:O    | 2.17                     | 0.45              |
| 7:w:30:GLU:HA    | 7:w:92:LEU:O     | 2.17                     | 0.45              |
| 7:w:73:ALA:HA    | 7:y:126:ALA:HB2  | 1.99                     | 0.45              |
| 7:w:132:LYS:NZ   | 7:x:105:GLU:O    | 2.26                     | 0.45              |
| 7:y:28:TRP:CE3   | 7:y:31:MET:HE1   | 2.52                     | 0.45              |
| 2:G:90:CYS:CB    | 2:G:94:TYR:HB3   | 2.47                     | 0.45              |
| 1:H:212:LYS:O    | 1:H:212:LYS:HD2  | 2.16                     | 0.45              |
| 1:K:265:ARG:NH2  | 1:K:273:PRO:O    | 2.50                     | 0.45              |
| 4:e:145:ALA:HB3  | 3:n:54:PHE:HA    | 1.98                     | 0.45              |
| 4:f:39:VAL:HG13  | 6:v:6:TYR:CE1    | 2.52                     | 0.45              |
| 6:t:46:LYS:HG2   | 6:t:77:GLU:OE2   | 2.17                     | 0.45              |
| 6:u:99:TYR:CD2   | 7:w:59:PRO:HD3   | 2.52                     | 0.45              |
| 6:u:99:TYR:HA    | 7:w:52:LYS:HB2   | 1.99                     | 0.45              |
| 6:u:102:CYS:CA   | 7:x:112:ASP:C    | 2.89                     | 0.45              |
| 6:v:143:THR:HG22 | 6:v:178:LYS:HB2  | 1.98                     | 0.45              |
| 7:x:18:ALA:O     | 7:x:21:GLN:HG3   | 2.17                     | 0.45              |
| 7:x:212:ALA:O    | 7:x:215:VAL:HG22 | 2.16                     | 0.45              |
| 1:A:182:THR:HG22 | 1:E:215:CYS:SG   | 2.56                     | 0.45              |
| 2:D:211:ILE:HD11 | 2:D:227:LEU:CA   | 2.47                     | 0.45              |
| 1:H:52:LEU:HD13  | 1:I:49:TYR:CE1   | 2.52                     | 0.45              |
| 1:K:26:MET:CE    | 2:M:32:LEU:HD12  | 2.46                     | 0.45              |
| 1:Q:164:ARG:HB2  | 1:Q:190:ILE:HD11 | 1.98                     | 0.45              |
| 4:a:36:GLY:CA    | 4:f:117:VAL:H    | 2.26                     | 0.45              |
| 4:b:9:ILE:CD1    | 4:b:14:LEU:HD11  | 2.46                     | 0.45              |
| 4:e:117:VAL:N    | 4:f:36:GLY:HA3   | 2.31                     | 0.45              |
| 6:t:67:VAL:HG12  | 6:t:84:TRP:CH2   | 2.52                     | 0.45              |
| 6:u:53:ILE:CG2   | 7:x:112:ASP:HA   | 2.46                     | 0.45              |
| 6:u:102:CYS:O    | 7:x:114:ARG:HG2  | 2.16                     | 0.45              |
| 6:v:118:PHE:CZ   | 7:x:56:ASN:HA    | 2.52                     | 0.45              |
| 7:w:71:ARG:NH1   | 7:y:129:GLU:O    | 2.44                     | 0.45              |
| 7:x:60:THR:HG22  | 7:x:61:ASP:H     | 1.81                     | 0.45              |
| 1:F:54:TYR:HE2   | 4:f:152:LYS:HG2  | 1.82                     | 0.45              |
| 1:F:213:ASN:OD1  | 1:F:214:GLY:N    | 2.50                     | 0.45              |
| 1:H:44:GLN:HB3   | 1:I:29:LEU:HD22  | 1.98                     | 0.45              |
| 2:J:136:ARG:O    | 2:J:136:ARG:HD2  | 2.17                     | 0.45              |
| 4:b:159:ALA:H    | 6:u:186:ARG:HD2  | 1.82                     | 0.45              |
| 5:h:1:MET:HE3    | 5:h:93:TYR:CD1   | 2.51                     | 0.45              |
| 6:u:53:ILE:O     | 7:x:111:SER:C    | 2.60                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:w:75:MET:SD    | 7:y:125:ILE:HG22 | 2.57                     | 0.45              |
| 7:x:164:GLU:CG   | 7:y:221:ILE:HD12 | 2.47                     | 0.45              |
| 2:C:76:CYS:HB2   | 2:C:121:LEU:O    | 2.16                     | 0.45              |
| 2:D:73:PHE:O     | 2:D:129:TYR:OH   | 2.31                     | 0.45              |
| 1:E:212:LYS:O    | 1:E:213:ASN:OD1  | 2.35                     | 0.45              |
| 1:I:68:ASP:HB3   | 1:I:71:GLN:HB2   | 1.98                     | 0.45              |
| 4:a:12:VAL:O     | 4:a:12:VAL:HG13  | 2.16                     | 0.45              |
| 4:c:115:LYS:HB3  | 4:d:34:GLU:HA    | 1.97                     | 0.45              |
| 4:d:35:SER:HB3   | 6:u:164:LEU:HD11 | 1.98                     | 0.45              |
| 4:e:12:VAL:HG13  | 4:e:12:VAL:O     | 2.17                     | 0.45              |
| 4:e:116:ILE:HB   | 4:f:36:GLY:CA    | 2.24                     | 0.45              |
| 3:o:78:GLU:OE2   | 3:o:82:LYS:HD3   | 2.17                     | 0.45              |
| 3:q:72:TYR:CE1   | 3:q:101:PHE:HB2  | 2.52                     | 0.45              |
| 6:t:28:HIS:O     | 6:u:153:THR:HG23 | 2.17                     | 0.45              |
| 7:w:51:TYR:CE2   | 7:x:97:ARG:HG3   | 2.52                     | 0.45              |
| 7:y:45:VAL:HG23  | 7:y:47:VAL:HG23  | 1.98                     | 0.45              |
| 2:D:83:ILE:H     | 2:D:83:ILE:HD12  | 1.81                     | 0.45              |
| 1:O:155:ASP:OD1  | 1:O:158:GLU:HB3  | 2.17                     | 0.45              |
| 1:Q:104:VAL:O    | 1:Q:105:ASP:C    | 2.60                     | 0.45              |
| 1:Q:227:LEU:HD12 | 1:Q:252:MET:SD   | 2.57                     | 0.45              |
| 4:a:33:ILE:HG21  | 4:f:118:GLU:OE2  | 2.17                     | 0.45              |
| 4:a:84:MET:HE1   | 3:p:66:ASP:CG    | 2.42                     | 0.45              |
| 4:d:118:GLU:O    | 4:e:36:GLY:N     | 2.50                     | 0.45              |
| 4:e:116:ILE:CG2  | 4:f:36:GLY:CA    | 2.95                     | 0.45              |
| 4:e:161:ASP:HB3  | 6:v:17:ILE:HB    | 1.99                     | 0.45              |
| 6:u:99:TYR:OH    | 7:w:54:LYS:CG    | 2.65                     | 0.45              |
| 1:F:73:GLU:O     | 2:G:1:MET:HG2    | 2.17                     | 0.45              |
| 1:I:221:ASN:ND2  | 2:M:97:SER:O     | 2.47                     | 0.45              |
| 1:K:212:LYS:O    | 1:K:213:ASN:OD1  | 2.35                     | 0.45              |
| 2:M:106:PRO:CD   | 2:M:182:THR:HG22 | 2.47                     | 0.45              |
| 2:S:90:CYS:SG    | 2:S:94:TYR:HB3   | 2.57                     | 0.45              |
| 6:t:53:ILE:O     | 7:w:112:ASP:CA   | 2.66                     | 0.45              |
| 6:v:108:GLU:OE1  | 6:v:111:THR:HG21 | 2.17                     | 0.45              |
| 7:x:177:ALA:O    | 7:x:181:GLU:HG3  | 2.16                     | 0.45              |
| 1:B:209:ARG:HG3  | 1:B:209:ARG:O    | 2.17                     | 0.44              |
| 2:J:104:CYS:O    | 2:J:105:GLU:HG2  | 2.16                     | 0.44              |
| 2:J:154:GLN:OE1  | 2:J:159:GLU:HA   | 2.17                     | 0.44              |
| 1:L:156:ASP:OD1  | 1:L:157:ASP:N    | 2.50                     | 0.44              |
| 4:a:121:THR:HG23 | 4:a:122:ALA:N    | 2.31                     | 0.44              |
| 4:b:116:ILE:O    | 4:b:117:VAL:CG1  | 2.53                     | 0.44              |
| 6:v:98:PRO:CA    | 7:x:52:LYS:HE3   | 2.42                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:99:TYR:CD1   | 7:x:52:LYS:HD2   | 2.51                     | 0.44              |
| 6:v:109:LEU:HB3  | 6:v:120:TRP:CE2  | 2.52                     | 0.44              |
| 7:w:195:SER:HA   | 7:y:190:ILE:HG21 | 1.98                     | 0.44              |
| 7:w:197:GLY:HA2  | 7:y:190:ILE:H    | 1.82                     | 0.44              |
| 7:x:56:ASN:O     | 7:x:58:VAL:N     | 2.50                     | 0.44              |
| 7:x:158:SER:OG   | 7:x:162:LYS:N    | 2.50                     | 0.44              |
| 7:x:176:ILE:HG22 | 7:x:180:MET:CE   | 2.47                     | 0.44              |
| 1:A:155:ASP:OD1  | 1:A:155:ASP:N    | 2.50                     | 0.44              |
| 1:A:230:GLU:OE2  | 1:A:254:ARG:NH2  | 2.50                     | 0.44              |
| 2:D:73:PHE:CE1   | 1:O:109:ILE:HD12 | 2.52                     | 0.44              |
| 1:I:66:SER:OG    | 1:I:76:ARG:HD3   | 2.17                     | 0.44              |
| 2:J:47:TYR:C     | 2:J:49:ASP:H     | 2.26                     | 0.44              |
| 1:K:165:ARG:HE   | 1:L:106:ARG:HH21 | 1.64                     | 0.44              |
| 1:L:19:LEU:O     | 1:L:23:GLU:HG3   | 2.17                     | 0.44              |
| 1:R:74:GLY:HA3   | 2:S:1:MET:N      | 2.32                     | 0.44              |
| 1:R:156:ASP:HA   | 1:R:159:VAL:HG12 | 2.00                     | 0.44              |
| 4:a:29:THR:HG21  | 6:v:33:GLY:H     | 1.82                     | 0.44              |
| 4:d:41:ASP:HB3   | 6:u:6:TYR:CD1    | 2.46                     | 0.44              |
| 4:e:118:GLU:CB   | 4:f:35:SER:HA    | 2.41                     | 0.44              |
| 5:i:27:LEU:HD22  | 5:i:53:LEU:HD11  | 1.99                     | 0.44              |
| 3:p:23:LEU:HD23  | 3:p:23:LEU:H     | 1.82                     | 0.44              |
| 6:t:176:LYS:HA   | 6:t:189:GLU:O    | 2.16                     | 0.44              |
| 6:u:53:ILE:O     | 7:x:112:ASP:CA   | 2.65                     | 0.44              |
| 6:v:67:VAL:H     | 7:x:58:VAL:CG2   | 2.30                     | 0.44              |
| 6:v:102:CYS:CB   | 7:y:98:SER:HG    | 2.30                     | 0.44              |
| 7:w:188:LEU:HD12 | 7:w:201:ALA:O    | 2.17                     | 0.44              |
| 2:D:138:TYR:CE1  | 1:P:85:LEU:HD21  | 2.52                     | 0.44              |
| 1:E:111:LEU:CD1  | 1:E:131:VAL:HG21 | 2.46                     | 0.44              |
| 2:J:8:PRO:HG3    | 2:J:45:MET:CG    | 2.47                     | 0.44              |
| 1:Q:111:LEU:HD21 | 1:Q:131:VAL:CG2  | 2.47                     | 0.44              |
| 6:u:22:LYS:HE3   | 6:u:46:LYS:HB2   | 1.98                     | 0.44              |
| 6:u:99:TYR:CE1   | 7:w:54:LYS:HA    | 2.52                     | 0.44              |
| 6:v:55:LYS:O     | 7:y:109:SER:CB   | 2.65                     | 0.44              |
| 6:v:66:VAL:HG13  | 6:v:69:GLU:HB2   | 1.99                     | 0.44              |
| 6:v:101:MET:O    | 7:y:111:SER:O    | 2.35                     | 0.44              |
| 1:B:55:ASP:OD2   | 1:B:59:ARG:NE    | 2.50                     | 0.44              |
| 1:H:60:GLY:CA    | 2:J:47:TYR:CE1   | 3.00                     | 0.44              |
| 1:K:84:ARG:NH1   | 1:K:101:ILE:O    | 2.47                     | 0.44              |
| 4:a:121:THR:HB   | 6:t:166:ASN:HB3  | 1.99                     | 0.44              |
| 4:b:159:ALA:HB1  | 6:u:185:ASN:C    | 2.42                     | 0.44              |
| 4:c:143:LYS:HA   | 3:r:57:LYS:HZ3   | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:140:SER:OG   | 4:d:143:LYS:HG2  | 2.17                     | 0.44              |
| 4:d:157:VAL:O    | 6:v:186:ARG:CZ   | 2.65                     | 0.44              |
| 4:e:125:SER:HB2  | 6:v:176:LYS:HD2  | 2.00                     | 0.44              |
| 6:t:22:LYS:HE3   | 6:t:46:LYS:HB2   | 1.98                     | 0.44              |
| 6:t:229:LYS:OXT  | 7:x:1:MET:HE3    | 2.18                     | 0.44              |
| 6:u:66:VAL:HB    | 7:w:58:VAL:HG13  | 1.99                     | 0.44              |
| 6:v:30:ARG:HA    | 6:v:34:ASP:O     | 2.18                     | 0.44              |
| 6:v:54:SER:HA    | 7:y:111:SER:O    | 2.17                     | 0.44              |
| 6:v:97:ARG:HD3   | 7:x:48:GLN:OE1   | 2.18                     | 0.44              |
| 2:D:205:HIS:O    | 2:D:208:GLN:NE2  | 2.50                     | 0.44              |
| 2:G:83:ILE:HB    | 2:G:116:TYR:HE1  | 1.83                     | 0.44              |
| 2:S:8:PRO:HG3    | 2:S:45:MET:CG    | 2.48                     | 0.44              |
| 4:b:9:ILE:HD13   | 4:b:14:LEU:HD11  | 2.00                     | 0.44              |
| 4:c:117:VAL:O    | 4:c:117:VAL:HG13 | 2.16                     | 0.44              |
| 4:e:129:ASP:OD1  | 4:e:129:ASP:N    | 2.47                     | 0.44              |
| 4:f:128:LYS:HG2  | 4:f:129:ASP:N    | 2.32                     | 0.44              |
| 5:i:43:ASP:O     | 6:v:83:GLU:OE2   | 2.35                     | 0.44              |
| 5:m:12:GLN:HB2   | 6:u:186:ARG:NH2  | 2.32                     | 0.44              |
| 3:o:24:ASP:N     | 3:o:24:ASP:OD1   | 2.49                     | 0.44              |
| 6:u:118:PHE:CZ   | 7:w:56:ASN:HA    | 2.53                     | 0.44              |
| 7:w:98:SER:HA    | 7:w:120:ASP:CG   | 2.42                     | 0.44              |
| 1:A:168:VAL:HG12 | 1:B:109:ILE:HD11 | 1.98                     | 0.44              |
| 1:K:121:ILE:HD11 | 1:K:162:LEU:CD2  | 2.48                     | 0.44              |
| 1:Q:110:ASP:O    | 1:Q:111:LEU:HB2  | 2.16                     | 0.44              |
| 4:d:117:VAL:N    | 4:e:36:GLY:CA    | 2.80                     | 0.44              |
| 4:e:117:VAL:O    | 4:e:117:VAL:HG22 | 2.17                     | 0.44              |
| 5:i:35:ARG:HH12  | 5:i:79:PRO:HB2   | 1.82                     | 0.44              |
| 6:t:67:VAL:N     | 7:y:58:VAL:HG22  | 2.32                     | 0.44              |
| 6:t:102:CYS:CA   | 7:w:112:ASP:O    | 2.66                     | 0.44              |
| 6:v:98:PRO:O     | 7:x:52:LYS:HG3   | 2.18                     | 0.44              |
| 6:v:154:ILE:HD11 | 6:v:182:LEU:CD2  | 2.47                     | 0.44              |
| 7:w:49:PRO:HG3   | 7:w:92:LEU:HD11  | 1.99                     | 0.44              |
| 2:D:147:GLU:O    | 2:D:151:GLU:HG2  | 2.18                     | 0.44              |
| 1:E:108:ARG:HG2  | 2:G:235:TYR:CE1  | 2.52                     | 0.44              |
| 1:I:164:ARG:HH21 | 2:J:146:ILE:HG21 | 1.83                     | 0.44              |
| 1:K:66:SER:O     | 1:K:76:ARG:NE    | 2.45                     | 0.44              |
| 1:O:110:ASP:O    | 1:O:111:LEU:HB2  | 2.18                     | 0.44              |
| 1:Q:227:LEU:C    | 1:Q:227:LEU:HD23 | 2.43                     | 0.44              |
| 2:S:154:GLN:OE1  | 2:S:159:GLU:HA   | 2.17                     | 0.44              |
| 4:b:59:ALA:HA    | 4:b:105:LEU:HB2  | 1.99                     | 0.44              |
| 4:c:175:LEU:CD1  | 5:j:1:MET:HE1    | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:20:GLU:OE1   | 4:d:22:HIS:NE2   | 2.39                     | 0.44              |
| 5:h:23:VAL:HG22  | 5:h:42:LEU:CD2   | 2.47                     | 0.44              |
| 6:t:53:ILE:O     | 7:w:112:ASP:N    | 2.51                     | 0.44              |
| 7:w:5:LEU:HD12   | 7:w:11:GLN:OE1   | 2.16                     | 0.44              |
| 7:x:190:ILE:H    | 7:y:197:GLY:HA2  | 1.83                     | 0.44              |
| 1:E:110:ASP:HB3  | 2:G:139:GLN:NE2  | 2.33                     | 0.44              |
| 1:H:121:ILE:HD11 | 1:H:162:LEU:HD22 | 1.99                     | 0.44              |
| 1:H:181:THR:CG2  | 1:H:190:ILE:HD12 | 2.47                     | 0.44              |
| 1:K:252:MET:HB2  | 1:K:261:VAL:HG21 | 2.00                     | 0.44              |
| 2:M:86:VAL:HA    | 2:M:101:ALA:HB3  | 1.98                     | 0.44              |
| 4:a:2:ILE:HG22   | 4:a:3:ILE:N      | 2.32                     | 0.44              |
| 4:b:31:ASN:HB3   | 4:b:32:PRO:CD    | 2.38                     | 0.44              |
| 4:d:12:VAL:HG11  | 4:d:66:LEU:HD23  | 2.00                     | 0.44              |
| 5:l:20:ASP:OD2   | 6:t:75:LYS:HE2   | 2.17                     | 0.44              |
| 6:t:24:ARG:NE    | 7:y:5:LEU:HB2    | 2.33                     | 0.44              |
| 6:t:28:HIS:O     | 6:u:153:THR:CG2  | 2.66                     | 0.44              |
| 6:t:67:VAL:HG21  | 6:t:86:PHE:CE2   | 2.53                     | 0.44              |
| 6:t:70:ILE:CD1   | 7:y:57:GLY:HA2   | 2.48                     | 0.44              |
| 6:u:54:SER:O     | 6:u:55:LYS:HD3   | 2.18                     | 0.44              |
| 7:y:51:TYR:CE1   | 7:y:52:LYS:O     | 2.70                     | 0.44              |
| 1:B:230:GLU:OE2  | 1:B:254:ARG:NH2  | 2.40                     | 0.44              |
| 1:H:60:GLY:HA3   | 2:J:47:TYR:CE1   | 2.52                     | 0.44              |
| 1:O:83:TYR:O     | 1:P:84:ARG:NH1   | 2.49                     | 0.44              |
| 1:Q:52:LEU:HD13  | 1:R:49:TYR:CE1   | 2.53                     | 0.44              |
| 1:Q:85:LEU:HD12  | 1:R:105:ASP:CG   | 2.43                     | 0.44              |
| 4:b:179:VAL:HG21 | 5:m:73:LEU:HD21  | 1.99                     | 0.44              |
| 4:d:18:ILE:N     | 4:d:53:GLU:O     | 2.40                     | 0.44              |
| 4:d:33:ILE:HG22  | 4:d:34:GLU:N     | 2.32                     | 0.44              |
| 4:d:179:VAL:CG2  | 5:k:73:LEU:HD21  | 2.48                     | 0.44              |
| 4:e:125:SER:CB   | 6:v:176:LYS:HD2  | 2.47                     | 0.44              |
| 4:e:128:LYS:HG2  | 4:e:129:ASP:N    | 2.33                     | 0.44              |
| 4:f:162:LYS:HE2  | 6:t:186:ARG:HA   | 1.99                     | 0.44              |
| 5:i:35:ARG:NH1   | 5:i:79:PRO:HB2   | 2.33                     | 0.44              |
| 6:t:95:LEU:CD1   | 7:y:59:PRO:HB2   | 2.48                     | 0.44              |
| 6:v:22:LYS:HE3   | 6:v:46:LYS:HB2   | 2.00                     | 0.44              |
| 7:x:1:MET:HB3    | 7:x:4:TYR:HE1    | 1.82                     | 0.44              |
| 7:x:24:ARG:NH1   | 7:y:23:GLU:HB3   | 2.33                     | 0.44              |
| 1:A:215:CYS:HB2  | 1:Q:187:CYS:HB3  | 1.99                     | 0.43              |
| 1:H:95:GLU:OE1   | 1:H:95:GLU:N     | 2.45                     | 0.43              |
| 2:M:76:CYS:HB2   | 2:M:121:LEU:O    | 2.18                     | 0.43              |
| 4:a:39:VAL:CG2   | 4:f:119:THR:OG1  | 2.66                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:c:86:ARG:HG2   | 4:c:86:ARG:HH11  | 1.83                     | 0.43              |
| 4:d:9:ILE:HD12   | 4:d:14:LEU:CD1   | 2.35                     | 0.43              |
| 4:e:120:GLY:H    | 4:e:123:GLU:CD   | 2.26                     | 0.43              |
| 4:f:32:PRO:HD2   | 6:v:149:ILE:CG2  | 2.47                     | 0.43              |
| 5:k:12:GLN:HB2   | 6:v:186:ARG:NH2  | 2.33                     | 0.43              |
| 6:v:24:ARG:HB3   | 6:v:40:SER:O     | 2.18                     | 0.43              |
| 7:x:38:VAL:O     | 7:x:38:VAL:HG13  | 2.17                     | 0.43              |
| 7:x:52:LYS:CE    | 7:x:59:PRO:HB3   | 2.48                     | 0.43              |
| 2:D:8:PRO:HG3    | 2:D:45:MET:HG3   | 2.00                     | 0.43              |
| 1:F:280:MET:HE3  | 1:F:286:MET:HG2  | 1.99                     | 0.43              |
| 1:O:106:ARG:C    | 1:O:108:ARG:H    | 2.23                     | 0.43              |
| 1:R:73:GLU:O     | 2:S:1:MET:HG3    | 2.17                     | 0.43              |
| 4:c:2:ILE:HG22   | 4:c:3:ILE:N      | 2.32                     | 0.43              |
| 4:f:33:ILE:HG22  | 4:f:34:GLU:N     | 2.33                     | 0.43              |
| 3:o:78:GLU:OE2   | 3:o:82:LYS:CD    | 2.67                     | 0.43              |
| 6:t:95:LEU:HD11  | 7:y:59:PRO:HB2   | 2.00                     | 0.43              |
| 6:t:206:ASP:O    | 6:t:208:ILE:HD12 | 2.18                     | 0.43              |
| 6:u:30:ARG:HA    | 6:u:34:ASP:O     | 2.18                     | 0.43              |
| 6:u:55:LYS:C     | 7:x:109:SER:HG   | 2.18                     | 0.43              |
| 6:v:176:LYS:HA   | 6:v:189:GLU:O    | 2.18                     | 0.43              |
| 7:w:60:THR:HG22  | 7:w:61:ASP:N     | 2.33                     | 0.43              |
| 7:w:81:THR:O     | 7:y:143:VAL:HG23 | 2.18                     | 0.43              |
| 2:C:102:GLY:O    | 2:C:103:TYR:HB2  | 2.19                     | 0.43              |
| 1:P:70:GLU:O     | 5:l:54:VAL:HG21  | 2.18                     | 0.43              |
| 1:Q:76:ARG:NE    | 1:R:64:TYR:OH    | 2.47                     | 0.43              |
| 1:Q:109:ILE:HG21 | 2:S:73:PHE:CD1   | 2.54                     | 0.43              |
| 4:a:67:VAL:O     | 4:a:71:GLU:HG3   | 2.19                     | 0.43              |
| 4:c:121:THR:OG1  | 6:u:168:GLU:HB2  | 2.18                     | 0.43              |
| 4:c:145:ALA:HB3  | 3:r:54:PHE:HA    | 1.99                     | 0.43              |
| 6:t:95:LEU:HD13  | 7:y:52:LYS:HZ1   | 1.83                     | 0.43              |
| 6:u:103:GLY:HA3  | 7:x:114:ARG:CA   | 2.48                     | 0.43              |
| 6:v:108:GLU:OE2  | 7:y:97:ARG:NH1   | 2.52                     | 0.43              |
| 7:w:30:GLU:C     | 7:x:95:GLN:OE1   | 2.61                     | 0.43              |
| 7:w:52:LYS:CD    | 7:w:61:ASP:OD1   | 2.67                     | 0.43              |
| 1:A:81:ALA:HB2   | 1:A:101:ILE:HD11 | 2.00                     | 0.43              |
| 1:I:78:ASP:OD1   | 1:I:88:ARG:HB2   | 2.19                     | 0.43              |
| 1:I:161:GLN:O    | 1:I:165:ARG:HG3  | 2.19                     | 0.43              |
| 1:I:169:PRO:HG3  | 2:J:146:ILE:CG2  | 2.49                     | 0.43              |
| 1:K:155:ASP:OD1  | 1:K:158:GLU:HB3  | 2.18                     | 0.43              |
| 1:O:156:ASP:OD1  | 1:O:194:ARG:NH2  | 2.44                     | 0.43              |
| 1:O:274:THR:O    | 1:O:275:THR:C    | 2.58                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:26:MET:HE2   | 1:P:42:LEU:HD23  | 2.01                     | 0.43              |
| 1:P:220:VAL:HG13 | 1:P:221:ASN:N    | 2.33                     | 0.43              |
| 4:a:32:PRO:O     | 6:v:203:GLN:HG3  | 2.17                     | 0.43              |
| 4:a:116:ILE:HA   | 4:b:36:GLY:N     | 2.33                     | 0.43              |
| 4:b:12:VAL:HG13  | 4:b:12:VAL:O     | 2.18                     | 0.43              |
| 4:f:122:ALA:HA   | 4:f:158:ASN:O    | 2.18                     | 0.43              |
| 5:m:26:GLU:OE1   | 5:m:28:TRP:CE3   | 2.71                     | 0.43              |
| 6:t:24:ARG:HB3   | 6:t:40:SER:O     | 2.18                     | 0.43              |
| 6:t:99:TYR:C     | 7:w:109:SER:CB   | 2.91                     | 0.43              |
| 6:t:101:MET:O    | 7:w:111:SER:O    | 2.34                     | 0.43              |
| 6:t:103:GLY:O    | 7:w:112:ASP:HB2  | 2.18                     | 0.43              |
| 6:v:63:LEU:HD11  | 7:x:60:THR:OG1   | 2.18                     | 0.43              |
| 7:w:30:GLU:O     | 7:x:95:GLN:OE1   | 2.36                     | 0.43              |
| 7:w:55:PHE:O     | 7:w:56:ASN:C     | 2.62                     | 0.43              |
| 1:A:156:ASP:OD1  | 1:A:194:ARG:NH2  | 2.44                     | 0.43              |
| 1:E:173:MET:HE1  | 1:E:190:ILE:HG23 | 2.01                     | 0.43              |
| 1:L:75:SER:N     | 2:M:1:MET:H2     | 2.14                     | 0.43              |
| 1:R:74:GLY:HA3   | 2:S:1:MET:H2     | 1.83                     | 0.43              |
| 4:c:158:ASN:ND2  | 6:u:168:GLU:HG2  | 2.33                     | 0.43              |
| 5:j:53:LEU:HB3   | 5:j:72:LEU:CD1   | 2.48                     | 0.43              |
| 5:k:29:TYR:CZ    | 5:k:82:ARG:HB2   | 2.54                     | 0.43              |
| 3:p:71:GLY:O     | 3:p:72:TYR:C     | 2.62                     | 0.43              |
| 6:t:108:GLU:HB3  | 7:y:54:LYS:HD3   | 2.01                     | 0.43              |
| 6:u:107:ARG:HG2  | 7:w:25:GLU:OE2   | 2.19                     | 0.43              |
| 6:v:42:GLY:HA2   | 7:x:7:LYS:N      | 2.34                     | 0.43              |
| 6:v:53:ILE:O     | 7:y:111:SER:C    | 2.60                     | 0.43              |
| 6:v:102:CYS:HB2  | 7:y:110:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:211:LEU:O    | 1:A:212:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:73:GLU:HG2   | 1:B:98:ARG:NH2   | 2.33                     | 0.43              |
| 1:K:186:PHE:CZ   | 1:L:111:LEU:HD12 | 2.53                     | 0.43              |
| 1:L:211:LEU:HG   | 1:L:258:ASN:HB3  | 2.01                     | 0.43              |
| 1:Q:197:LEU:HD12 | 1:Q:287:SER:HB2  | 2.00                     | 0.43              |
| 1:R:106:ARG:NH2  | 2:S:144:TYR:OH   | 2.51                     | 0.43              |
| 4:c:118:GLU:HB3  | 6:u:147:GLY:N    | 2.34                     | 0.43              |
| 5:l:34:ASP:O     | 5:l:34:ASP:OD2   | 2.36                     | 0.43              |
| 6:t:53:ILE:CG1   | 6:t:54:SER:H     | 2.32                     | 0.43              |
| 6:u:99:TYR:CD1   | 7:w:52:LYS:HD2   | 2.54                     | 0.43              |
| 6:v:102:CYS:HB3  | 7:y:98:SER:OG    | 2.18                     | 0.43              |
| 1:A:105:ASP:C    | 1:A:107:ALA:H    | 2.26                     | 0.43              |
| 1:B:108:ARG:NE   | 1:B:113:ASP:OD2  | 2.52                     | 0.43              |
| 2:D:1:MET:N      | 1:P:74:GLY:HA3   | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:155:ASP:OD1  | 1:F:156:ASP:N    | 2.51                     | 0.43              |
| 2:J:87:GLY:CA    | 2:J:100:LEU:HD12 | 2.49                     | 0.43              |
| 1:R:26:MET:HB2   | 1:R:36:GLN:NE2   | 2.33                     | 0.43              |
| 1:R:155:ASP:OD1  | 1:R:156:ASP:N    | 2.52                     | 0.43              |
| 4:d:119:THR:OG1  | 4:e:39:VAL:CG2   | 2.66                     | 0.43              |
| 4:e:2:ILE:HG22   | 4:e:4:ALA:H      | 1.84                     | 0.43              |
| 5:m:28:TRP:HZ3   | 5:m:39:SER:HG    | 1.63                     | 0.43              |
| 5:m:88:GLY:O     | 5:m:91:LYS:HE3   | 2.18                     | 0.43              |
| 6:u:66:VAL:HG21  | 7:w:59:PRO:HD2   | 1.99                     | 0.43              |
| 7:w:172:LEU:HD21 | 7:y:173:LEU:HD21 | 2.01                     | 0.43              |
| 7:y:48:GLN:OE1   | 7:y:64:VAL:HG22  | 2.18                     | 0.43              |
| 7:y:55:PHE:HD2   | 7:y:60:THR:OG1   | 2.00                     | 0.43              |
| 7:y:146:ARG:HG2  | 7:y:151:GLY:HA2  | 2.00                     | 0.43              |
| 1:B:164:ARG:CD   | 1:B:173:MET:HE1  | 2.49                     | 0.43              |
| 1:B:245:VAL:HG13 | 1:B:276:PRO:HG2  | 2.00                     | 0.43              |
| 1:B:246:TYR:HD2  | 1:E:260:GLU:HG3  | 1.83                     | 0.43              |
| 1:E:241:GLU:O    | 1:E:280:MET:HE2  | 2.19                     | 0.43              |
| 1:E:294:LEU:HD23 | 1:E:294:LEU:C    | 2.43                     | 0.43              |
| 1:P:244:THR:HG22 | 1:P:245:VAL:N    | 2.34                     | 0.43              |
| 4:d:37:ALA:O     | 4:d:38:ASP:CG    | 2.61                     | 0.43              |
| 4:d:59:ALA:HA    | 4:d:105:LEU:HB2  | 2.00                     | 0.43              |
| 4:d:175:LEU:HD12 | 5:k:1:MET:CE     | 2.49                     | 0.43              |
| 6:t:24:ARG:HB2   | 7:y:6:GLY:HA3    | 1.99                     | 0.43              |
| 6:t:107:ARG:CG   | 7:y:21:GLN:HE22  | 2.31                     | 0.43              |
| 6:u:24:ARG:HB3   | 6:u:40:SER:O     | 2.19                     | 0.43              |
| 6:u:67:VAL:CG2   | 7:w:58:VAL:HG23  | 2.48                     | 0.43              |
| 6:v:56:THR:HA    | 7:y:109:SER:CB   | 2.49                     | 0.43              |
| 6:v:108:GLU:CA   | 6:v:111:THR:HG22 | 2.48                     | 0.43              |
| 7:x:98:SER:HA    | 7:x:120:ASP:CG   | 2.44                     | 0.43              |
| 1:B:76:ARG:O     | 1:B:80:LEU:HD13  | 2.18                     | 0.43              |
| 1:B:118:LEU:CD1  | 1:B:159:VAL:HG23 | 2.49                     | 0.43              |
| 1:K:267:SER:HB2  | 1:K:273:PRO:HA   | 2.01                     | 0.43              |
| 4:e:92:GLU:OE2   | 4:f:23:THR:HG23  | 2.19                     | 0.43              |
| 5:i:100:ILE:O    | 5:i:104:ILE:HG13 | 2.19                     | 0.43              |
| 6:t:53:ILE:O     | 7:w:111:SER:C    | 2.61                     | 0.43              |
| 1:Q:213:ASN:OD1  | 1:Q:213:ASN:O    | 2.37                     | 0.43              |
| 2:S:150:HIS:O    | 2:S:154:GLN:HG2  | 2.19                     | 0.43              |
| 4:b:128:LYS:HG2  | 4:b:129:ASP:N    | 2.34                     | 0.43              |
| 6:t:53:ILE:CG1   | 6:t:54:SER:N     | 2.82                     | 0.43              |
| 6:u:41:CYS:O     | 7:w:7:LYS:N      | 2.34                     | 0.43              |
| 6:u:56:THR:C     | 7:x:109:SER:OG   | 2.62                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:112:LEU:HD22 | 7:x:55:PHE:C     | 2.44                     | 0.43              |
| 7:w:68:VAL:HG13  | 7:w:121:MET:O    | 2.18                     | 0.43              |
| 7:w:96:MET:C     | 7:w:97:ARG:HG2   | 2.43                     | 0.43              |
| 7:y:213:ALA:O    | 7:y:217:THR:HG23 | 2.19                     | 0.43              |
| 2:D:1:MET:H2     | 1:P:74:GLY:HA3   | 1.84                     | 0.42              |
| 1:E:75:SER:HB3   | 1:F:7:PRO:O      | 2.19                     | 0.42              |
| 1:I:243:GLY:N    | 1:I:278:LEU:O    | 2.52                     | 0.42              |
| 1:L:246:TYR:HD2  | 1:Q:260:GLU:HG3  | 1.84                     | 0.42              |
| 2:M:7:ASP:OD2    | 2:M:9:GLU:HB2    | 2.19                     | 0.42              |
| 2:M:172:VAL:HA   | 2:M:203:MET:HB2  | 2.01                     | 0.42              |
| 1:Q:207:GLN:OE1  | 1:Q:209:ARG:NH2  | 2.52                     | 0.42              |
| 3:X:102:ASP:OD1  | 3:X:102:ASP:C    | 2.61                     | 0.42              |
| 4:c:121:THR:HG22 | 6:u:166:ASN:ND2  | 2.31                     | 0.42              |
| 6:t:56:THR:O     | 6:t:57:ILE:HD13  | 2.19                     | 0.42              |
| 6:v:66:VAL:HA    | 6:v:69:GLU:HB2   | 2.01                     | 0.42              |
| 6:v:67:VAL:N     | 7:x:58:VAL:CG2   | 2.81                     | 0.42              |
| 6:v:194:SER:HB2  | 6:v:195:GLU:OE1  | 2.19                     | 0.42              |
| 2:D:211:ILE:HD11 | 2:D:227:LEU:CB   | 2.49                     | 0.42              |
| 1:F:156:ASP:OD1  | 1:F:157:ASP:N    | 2.52                     | 0.42              |
| 1:I:26:MET:HB2   | 1:I:36:GLN:NE2   | 2.33                     | 0.42              |
| 1:I:211:LEU:O    | 1:I:212:LYS:C    | 2.61                     | 0.42              |
| 1:O:108:ARG:HH22 | 1:O:133:GLU:CD   | 2.27                     | 0.42              |
| 1:R:71:GLN:O     | 5:k:52:ARG:NH1   | 2.52                     | 0.42              |
| 1:R:76:ARG:NH2   | 2:S:1:MET:SD     | 2.92                     | 0.42              |
| 3:X:20:ASP:OD1   | 3:X:21:ILE:N     | 2.52                     | 0.42              |
| 4:a:23:THR:HG22  | 4:a:25:LYS:HD3   | 2.00                     | 0.42              |
| 4:c:121:THR:HG22 | 6:u:166:ASN:OD1  | 2.16                     | 0.42              |
| 4:f:157:VAL:O    | 6:t:186:ARG:CZ   | 2.66                     | 0.42              |
| 5:m:29:TYR:CZ    | 5:m:82:ARG:HB2   | 2.54                     | 0.42              |
| 6:t:108:GLU:HA   | 6:t:111:THR:HG22 | 2.00                     | 0.42              |
| 6:t:150:GLY:HA2  | 6:v:30:ARG:NH1   | 2.35                     | 0.42              |
| 6:u:42:GLY:N     | 7:w:7:LYS:HG3    | 2.34                     | 0.42              |
| 6:u:109:LEU:HD13 | 6:u:120:TRP:CZ2  | 2.54                     | 0.42              |
| 7:x:21:GLN:O     | 7:x:25:GLU:HG3   | 2.20                     | 0.42              |
| 7:y:158:SER:OG   | 7:y:162:LYS:N    | 2.51                     | 0.42              |
| 1:E:165:ARG:HD3  | 1:F:106:ARG:NH2  | 2.34                     | 0.42              |
| 1:H:249:ARG:HD2  | 1:H:249:ARG:O    | 2.19                     | 0.42              |
| 2:J:150:HIS:O    | 2:J:154:GLN:HG2  | 2.19                     | 0.42              |
| 1:L:211:LEU:CG   | 1:L:258:ASN:HB3  | 2.50                     | 0.42              |
| 1:R:63:LEU:HD11  | 2:S:47:TYR:O     | 2.19                     | 0.42              |
| 4:a:118:GLU:N    | 4:b:36:GLY:C     | 2.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:b:118:GLU:H    | 4:c:36:GLY:CA    | 2.32                     | 0.42              |
| 4:b:162:LYS:N    | 5:m:15:SER:O     | 2.45                     | 0.42              |
| 4:b:162:LYS:HE2  | 6:u:186:ARG:HA   | 2.01                     | 0.42              |
| 4:e:32:PRO:O     | 6:u:203:GLN:CG   | 2.68                     | 0.42              |
| 4:e:32:PRO:HA    | 6:u:203:GLN:HG3  | 1.99                     | 0.42              |
| 6:t:97:ARG:HD2   | 7:y:49:PRO:O     | 2.19                     | 0.42              |
| 6:u:67:VAL:HG22  | 7:w:56:ASN:O     | 2.20                     | 0.42              |
| 6:u:98:PRO:HD2   | 7:w:50:LEU:O     | 2.19                     | 0.42              |
| 6:u:144:PRO:HG3  | 6:u:148:LEU:HD23 | 2.01                     | 0.42              |
| 6:v:24:ARG:NH1   | 7:x:6:GLY:O      | 2.52                     | 0.42              |
| 6:v:112:LEU:CD2  | 7:x:54:LYS:HG2   | 2.50                     | 0.42              |
| 7:x:101:ASN:HB2  | 7:x:105:GLU:OE1  | 2.18                     | 0.42              |
| 7:x:173:LEU:HD13 | 7:y:219:GLY:HA2  | 2.01                     | 0.42              |
| 7:x:190:ILE:HD11 | 7:y:200:HIS:CE1  | 2.53                     | 0.42              |
| 1:A:212:LYS:HD2  | 1:A:212:LYS:O    | 2.18                     | 0.42              |
| 2:D:12:VAL:O     | 2:D:16:ILE:HG12  | 2.19                     | 0.42              |
| 2:G:145:ASP:OD1  | 2:G:148:SER:OG   | 2.33                     | 0.42              |
| 1:H:106:ARG:HG3  | 1:H:106:ARG:NH1  | 2.34                     | 0.42              |
| 1:L:211:LEU:HD21 | 1:L:258:ASN:HB3  | 2.01                     | 0.42              |
| 1:P:206:VAL:O    | 1:P:298:VAL:N    | 2.42                     | 0.42              |
| 4:b:89:ILE:HD12  | 4:b:114:VAL:HG21 | 2.02                     | 0.42              |
| 5:m:34:ASP:OD1   | 5:m:34:ASP:O     | 2.37                     | 0.42              |
| 6:u:83:GLU:CG    | 6:u:136:LEU:HD22 | 2.49                     | 0.42              |
| 6:v:143:THR:N    | 6:v:146:THR:OG1  | 2.52                     | 0.42              |
| 7:w:101:ASN:HA   | 7:w:104:VAL:HB   | 2.02                     | 0.42              |
| 7:x:60:THR:CG2   | 7:x:61:ASP:N     | 2.82                     | 0.42              |
| 1:B:176:ASN:OD1  | 1:B:177:THR:N    | 2.53                     | 0.42              |
| 1:E:67:PHE:CD2   | 1:E:67:PHE:O     | 2.72                     | 0.42              |
| 1:F:73:GLU:O     | 2:G:1:MET:HA     | 2.18                     | 0.42              |
| 1:I:42:LEU:HD22  | 3:q:9:LEU:HD12   | 2.01                     | 0.42              |
| 1:I:202:VAL:HG12 | 1:I:266:LEU:CD2  | 2.50                     | 0.42              |
| 1:K:89:ARG:NH2   | 1:K:92:GLU:OE2   | 2.53                     | 0.42              |
| 4:f:32:PRO:HG2   | 6:v:149:ILE:CG2  | 2.50                     | 0.42              |
| 6:t:100:SER:CB   | 7:y:51:TYR:CE2   | 3.01                     | 0.42              |
| 6:u:42:GLY:HA2   | 7:w:7:LYS:N      | 2.35                     | 0.42              |
| 7:w:28:TRP:HH2   | 7:w:62:MET:HE1   | 1.85                     | 0.42              |
| 7:x:51:TYR:CZ    | 7:y:97:ARG:HG3   | 2.54                     | 0.42              |
| 7:x:99:MET:HE3   | 7:x:102:TYR:CG   | 2.55                     | 0.42              |
| 7:x:130:SER:O    | 7:y:43:ARG:NH1   | 2.52                     | 0.42              |
| 2:G:206:ILE:HG13 | 2:G:207:ASP:N    | 2.35                     | 0.42              |
| 1:H:106:ARG:C    | 1:H:108:ARG:H    | 2.27                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:73:GLU:OE1   | 5:m:35:ARG:NH2   | 2.53                     | 0.42              |
| 1:K:109:ILE:HD12 | 2:M:73:PHE:CE1   | 2.54                     | 0.42              |
| 1:L:244:THR:HG22 | 1:L:245:VAL:N    | 2.34                     | 0.42              |
| 1:Q:64:TYR:OH    | 2:S:62:ASP:OD2   | 2.28                     | 0.42              |
| 2:S:132:LEU:HD21 | 2:S:190:VAL:HG22 | 2.02                     | 0.42              |
| 4:c:118:GLU:CA   | 4:d:36:GLY:H     | 2.32                     | 0.42              |
| 4:d:117:VAL:HA   | 4:e:37:ALA:HB2   | 2.01                     | 0.42              |
| 4:f:79:MET:HG3   | 4:f:84:MET:HE1   | 2.00                     | 0.42              |
| 4:f:167:VAL:CG1  | 4:f:172:ALA:HB2  | 2.50                     | 0.42              |
| 3:q:20:ASP:OD1   | 3:q:21:ILE:N     | 2.52                     | 0.42              |
| 6:t:99:TYR:CZ    | 7:y:58:VAL:O     | 2.72                     | 0.42              |
| 6:u:24:ARG:HB2   | 7:w:6:GLY:HA3    | 2.00                     | 0.42              |
| 6:u:102:CYS:CB   | 7:x:98:SER:OG    | 2.68                     | 0.42              |
| 7:x:179:PHE:CE1  | 7:x:208:MET:HG2  | 2.55                     | 0.42              |
| 1:B:131:VAL:HG21 | 1:B:133:GLU:OE2  | 2.20                     | 0.42              |
| 1:B:146:THR:HG22 | 1:B:147:VAL:N    | 2.35                     | 0.42              |
| 2:C:19:VAL:HG12  | 2:C:20:LEU:N     | 2.35                     | 0.42              |
| 2:D:86:VAL:HG13  | 2:D:86:VAL:O     | 2.20                     | 0.42              |
| 2:D:125:GLU:OE1  | 2:D:128:ILE:HG13 | 2.20                     | 0.42              |
| 1:F:212:LYS:NZ   | 1:O:238:GLY:HA3  | 2.34                     | 0.42              |
| 1:H:263:ASP:OD1  | 1:H:264:VAL:N    | 2.52                     | 0.42              |
| 1:I:42:LEU:CD2   | 3:q:9:LEU:HD12   | 2.50                     | 0.42              |
| 1:I:137:THR:HG22 | 1:I:138:ASP:N    | 2.34                     | 0.42              |
| 2:J:47:TYR:HA    | 2:J:50:MET:HE3   | 2.01                     | 0.42              |
| 1:K:82:ARG:NE    | 1:L:70:GLU:OE2   | 2.50                     | 0.42              |
| 1:K:203:GLU:HG3  | 1:K:273:PRO:HG2  | 2.02                     | 0.42              |
| 1:O:242:ASP:OD1  | 1:O:242:ASP:N    | 2.50                     | 0.42              |
| 2:S:41:ALA:O     | 2:S:45:MET:HG2   | 2.20                     | 0.42              |
| 4:b:162:LYS:CE   | 6:u:186:ARG:HA   | 2.49                     | 0.42              |
| 4:d:128:LYS:NZ   | 4:d:136:SER:O    | 2.51                     | 0.42              |
| 4:d:128:LYS:HG2  | 4:d:129:ASP:N    | 2.34                     | 0.42              |
| 4:e:3:ILE:O      | 4:e:4:ALA:HB3    | 2.20                     | 0.42              |
| 4:e:121:THR:HG1  | 6:v:168:GLU:N    | 2.18                     | 0.42              |
| 5:i:29:TYR:CZ    | 5:i:82:ARG:HB2   | 2.54                     | 0.42              |
| 5:j:20:ASP:OD2   | 6:u:75:LYS:HE2   | 2.19                     | 0.42              |
| 5:l:72:LEU:HD23  | 5:l:92:LEU:HA    | 2.02                     | 0.42              |
| 6:t:95:LEU:CD2   | 7:y:59:PRO:O     | 2.65                     | 0.42              |
| 6:t:99:TYR:C     | 7:w:109:SER:HB3  | 2.45                     | 0.42              |
| 6:t:112:LEU:HD23 | 7:y:54:LYS:C     | 2.44                     | 0.42              |
| 6:u:99:TYR:CE2   | 7:w:59:PRO:HD3   | 2.55                     | 0.42              |
| 6:v:207:TRP:CE3  | 6:v:207:TRP:HA   | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:w:197:GLY:N    | 7:y:190:ILE:HB   | 2.35                     | 0.42              |
| 1:I:121:ILE:CD1  | 1:I:162:LEU:HD13 | 2.47                     | 0.42              |
| 1:O:26:MET:HB2   | 1:O:36:GLN:NE2   | 2.34                     | 0.42              |
| 1:O:104:VAL:O    | 1:O:105:ASP:C    | 2.62                     | 0.42              |
| 1:O:181:THR:CG2  | 1:O:190:ILE:HD12 | 2.50                     | 0.42              |
| 4:a:3:ILE:HG23   | 3:p:76:LEU:HB2   | 2.01                     | 0.42              |
| 4:a:158:ASN:ND2  | 6:t:168:GLU:HG2  | 2.35                     | 0.42              |
| 4:d:12:VAL:O     | 4:d:12:VAL:HG13  | 2.19                     | 0.42              |
| 4:e:33:ILE:HG23  | 4:e:34:GLU:OE1   | 2.20                     | 0.42              |
| 4:f:115:LYS:C    | 4:f:116:ILE:HG13 | 2.45                     | 0.42              |
| 5:j:54:VAL:HG23  | 5:j:57:VAL:HG12  | 2.00                     | 0.42              |
| 3:q:32:VAL:HB    | 3:q:36:GLU:HG2   | 2.02                     | 0.42              |
| 6:t:107:ARG:CZ   | 7:w:115:SER:OG   | 2.67                     | 0.42              |
| 6:v:52:THR:O     | 6:v:73:GLU:CD    | 2.63                     | 0.42              |
| 6:v:55:LYS:C     | 7:y:109:SER:HG   | 2.25                     | 0.42              |
| 7:x:190:ILE:HB   | 7:y:197:GLY:N    | 2.34                     | 0.42              |
| 1:E:248:PHE:CE1  | 1:E:266:LEU:HD11 | 2.54                     | 0.42              |
| 1:L:280:MET:HE3  | 1:L:286:MET:CG   | 2.47                     | 0.42              |
| 3:X:72:TYR:CE1   | 3:X:101:PHE:HB2  | 2.55                     | 0.42              |
| 4:b:162:LYS:HA   | 6:u:186:ARG:O    | 2.19                     | 0.42              |
| 4:d:89:ILE:HD12  | 4:d:114:VAL:CG2  | 2.50                     | 0.42              |
| 4:d:119:THR:OG1  | 4:e:39:VAL:HG23  | 2.20                     | 0.42              |
| 4:e:118:GLU:C    | 4:f:36:GLY:O     | 2.63                     | 0.42              |
| 6:t:82:GLY:N     | 6:t:127:MET:O    | 2.49                     | 0.42              |
| 6:t:102:CYS:HA   | 7:w:112:ASP:C    | 2.45                     | 0.42              |
| 6:u:101:MET:O    | 7:x:111:SER:CA   | 2.68                     | 0.42              |
| 6:v:115:SER:O    | 6:v:116:HIS:CG   | 2.73                     | 0.42              |
| 7:w:62:MET:SD    | 7:w:118:LEU:HD21 | 2.59                     | 0.42              |
| 7:x:173:LEU:HD21 | 7:y:172:LEU:CD2  | 2.50                     | 0.42              |
| 1:B:19:LEU:O     | 1:B:23:GLU:HG3   | 2.20                     | 0.42              |
| 2:C:211:ILE:HD11 | 2:C:227:LEU:CA   | 2.50                     | 0.42              |
| 2:D:97:SER:O     | 1:F:221:ASN:ND2  | 2.51                     | 0.42              |
| 2:D:146:ILE:HD13 | 1:P:164:ARG:HE   | 1.85                     | 0.42              |
| 2:G:132:LEU:HD21 | 2:G:190:VAL:HG22 | 2.01                     | 0.42              |
| 1:H:108:ARG:HH21 | 1:H:111:LEU:HD11 | 1.85                     | 0.42              |
| 4:c:169:ALA:N    | 4:c:170:PRO:HD2  | 2.35                     | 0.42              |
| 6:u:99:TYR:O     | 6:u:100:SER:C    | 2.63                     | 0.42              |
| 7:w:99:MET:CE    | 7:w:102:TYR:CB   | 2.98                     | 0.42              |
| 1:B:73:GLU:O     | 2:C:1:MET:CA     | 2.68                     | 0.41              |
| 1:B:132:ASN:OD1  | 1:B:144:PRO:HA   | 2.19                     | 0.41              |
| 1:E:111:LEU:HD11 | 1:E:131:VAL:CG2  | 2.49                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:243:GLY:H    | 1:E:280:MET:HE1  | 1.85                     | 0.41              |
| 2:G:114:SER:HB2  | 2:G:115:PRO:HD3  | 2.02                     | 0.41              |
| 1:Q:105:ASP:OD2  | 2:S:120:GLU:OE1  | 2.38                     | 0.41              |
| 1:Q:227:LEU:HD21 | 1:Q:231:LEU:CD1  | 2.50                     | 0.41              |
| 4:a:117:VAL:O    | 4:a:117:VAL:HG13 | 2.20                     | 0.41              |
| 4:c:118:GLU:CB   | 4:d:35:SER:HA    | 2.41                     | 0.41              |
| 4:e:117:VAL:CA   | 4:f:37:ALA:HB2   | 2.49                     | 0.41              |
| 4:e:143:LYS:HA   | 3:n:57:LYS:NZ    | 2.35                     | 0.41              |
| 4:f:25:LYS:HB2   | 4:f:46:LYS:HB2   | 2.01                     | 0.41              |
| 4:f:115:LYS:C    | 4:f:116:ILE:CG1  | 2.93                     | 0.41              |
| 5:i:53:LEU:HB3   | 5:i:72:LEU:HD11  | 2.01                     | 0.41              |
| 5:m:42:LEU:HD21  | 5:m:67:ILE:HD13  | 2.02                     | 0.41              |
| 6:t:109:LEU:CA   | 6:t:112:LEU:HG   | 2.49                     | 0.41              |
| 1:A:106:ARG:C    | 1:A:108:ARG:N    | 2.78                     | 0.41              |
| 2:C:8:PRO:HG3    | 2:C:45:MET:HG3   | 2.02                     | 0.41              |
| 2:D:82:THR:HG23  | 1:F:221:ASN:OD1  | 2.20                     | 0.41              |
| 1:I:176:ASN:HB3  | 1:I:283:PHE:CD2  | 2.55                     | 0.41              |
| 2:J:78:CYS:O     | 2:J:192:ARG:NH1  | 2.53                     | 0.41              |
| 1:L:76:ARG:NH2   | 2:M:4:LEU:HG     | 2.35                     | 0.41              |
| 2:M:211:ILE:HD11 | 2:M:227:LEU:CA   | 2.50                     | 0.41              |
| 1:R:76:ARG:HA    | 1:R:79:ILE:HD12  | 2.02                     | 0.41              |
| 1:R:247:LEU:HD23 | 1:R:251:ILE:HD12 | 2.02                     | 0.41              |
| 4:a:36:GLY:HA3   | 4:f:116:ILE:CA   | 2.49                     | 0.41              |
| 4:c:121:THR:HB   | 6:u:166:ASN:HB3  | 2.02                     | 0.41              |
| 4:d:21:LYS:HB3   | 4:d:51:GLU:HB3   | 2.02                     | 0.41              |
| 5:h:85:LEU:HB3   | 5:h:86:PRO:HD3   | 2.02                     | 0.41              |
| 6:t:67:VAL:H     | 7:y:58:VAL:CG2   | 2.34                     | 0.41              |
| 6:u:155:THR:HG1  | 6:u:158:GLY:C    | 2.28                     | 0.41              |
| 2:D:110:TRP:CD1  | 2:D:110:TRP:N    | 2.89                     | 0.41              |
| 1:E:64:TYR:HB2   | 2:G:50:MET:HE2   | 2.02                     | 0.41              |
| 2:J:94:TYR:HE2   | 2:J:96:GLY:HA3   | 1.82                     | 0.41              |
| 2:J:102:GLY:O    | 2:J:103:TYR:HB2  | 2.21                     | 0.41              |
| 2:S:1:MET:HB3    | 2:S:2:SER:H      | 1.66                     | 0.41              |
| 2:S:211:ILE:HD13 | 2:S:227:LEU:CD1  | 2.50                     | 0.41              |
| 4:d:157:VAL:O    | 6:v:186:ARG:NH1  | 2.53                     | 0.41              |
| 4:e:116:ILE:HA   | 4:f:36:GLY:N     | 2.36                     | 0.41              |
| 4:e:179:VAL:CG2  | 5:i:73:LEU:HD21  | 2.50                     | 0.41              |
| 5:j:29:TYR:CZ    | 5:j:82:ARG:HB2   | 2.54                     | 0.41              |
| 3:p:11:LEU:HD12  | 3:p:44:GLN:HE21  | 1.85                     | 0.41              |
| 6:t:30:ARG:NH1   | 6:u:150:GLY:HA2  | 2.35                     | 0.41              |
| 6:t:102:CYS:C    | 7:w:113:SER:CA   | 2.93                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:v:112:LEU:HD23 | 7:x:54:LYS:O     | 2.21                     | 0.41              |
| 6:v:144:PRO:HG3  | 6:v:148:LEU:HD23 | 2.02                     | 0.41              |
| 6:v:182:LEU:HA   | 6:v:185:ASN:HB2  | 2.03                     | 0.41              |
| 7:w:177:ALA:O    | 7:w:181:GLU:HG3  | 2.20                     | 0.41              |
| 7:x:15:VAL:HG12  | 7:x:15:VAL:O     | 2.20                     | 0.41              |
| 7:y:28:TRP:HE3   | 7:y:31:MET:HE1   | 1.85                     | 0.41              |
| 2:J:94:TYR:CE1   | 2:J:100:LEU:HD21 | 2.56                     | 0.41              |
| 1:Q:86:LEU:HD22  | 1:Q:116:THR:HG21 | 2.03                     | 0.41              |
| 4:d:158:ASN:CA   | 6:v:186:ARG:NH1  | 2.67                     | 0.41              |
| 5:i:85:LEU:HB3   | 5:i:86:PRO:HD3   | 2.02                     | 0.41              |
| 5:k:29:TYR:OH    | 5:k:34:ASP:OD1   | 2.34                     | 0.41              |
| 6:t:5:GLY:HA3    | 6:t:15:ILE:HA    | 2.01                     | 0.41              |
| 6:v:99:TYR:C     | 7:y:109:SER:HB3  | 2.45                     | 0.41              |
| 6:v:102:CYS:HB2  | 7:y:110:ALA:HB1  | 2.00                     | 0.41              |
| 7:w:48:GLN:OE1   | 7:w:64:VAL:HG22  | 2.20                     | 0.41              |
| 7:w:117:SER:HB3  | 7:w:120:ASP:OD2  | 2.21                     | 0.41              |
| 7:y:60:THR:CG2   | 7:y:61:ASP:N     | 2.81                     | 0.41              |
| 2:D:52:GLU:N     | 2:D:52:GLU:CD    | 2.79                     | 0.41              |
| 1:E:110:ASP:N    | 1:E:110:ASP:OD1  | 2.50                     | 0.41              |
| 2:G:102:GLY:O    | 2:G:103:TYR:HB2  | 2.20                     | 0.41              |
| 2:J:211:ILE:HD13 | 2:J:227:LEU:HD13 | 2.01                     | 0.41              |
| 1:O:202:VAL:HG23 | 1:O:266:LEU:CD2  | 2.50                     | 0.41              |
| 1:P:85:LEU:C     | 1:P:86:LEU:HD22  | 2.45                     | 0.41              |
| 1:R:169:PRO:HG3  | 2:S:146:ILE:CG2  | 2.51                     | 0.41              |
| 4:a:2:ILE:HG23   | 4:a:81:GLY:HA3   | 2.02                     | 0.41              |
| 4:a:3:ILE:O      | 4:a:4:ALA:HB3    | 2.21                     | 0.41              |
| 4:a:118:GLU:HB2  | 4:b:36:GLY:H     | 1.86                     | 0.41              |
| 4:a:128:LYS:HG2  | 4:a:129:ASP:N    | 2.34                     | 0.41              |
| 4:a:177:LYS:NZ   | 5:l:106:ALA:OXT  | 2.53                     | 0.41              |
| 4:b:162:LYS:HE3  | 6:u:186:ARG:CA   | 2.50                     | 0.41              |
| 6:t:96:LYS:HB2   | 7:y:61:ASP:OD2   | 2.20                     | 0.41              |
| 6:t:100:SER:HA   | 7:w:109:SER:HA   | 2.02                     | 0.41              |
| 6:t:103:GLY:HA2  | 7:w:114:ARG:HG3  | 2.02                     | 0.41              |
| 6:v:56:THR:HG23  | 7:y:107:ASP:O    | 2.21                     | 0.41              |
| 7:x:95:GLN:CG    | 7:x:97:ARG:O     | 2.68                     | 0.41              |
| 7:x:101:ASN:OD1  | 7:x:101:ASN:C    | 2.62                     | 0.41              |
| 1:A:213:ASN:O    | 1:A:213:ASN:OD1  | 2.38                     | 0.41              |
| 2:D:11:LEU:O     | 2:D:15:ARG:HD2   | 2.21                     | 0.41              |
| 1:E:230:GLU:HG3  | 1:E:255:LEU:HD11 | 2.03                     | 0.41              |
| 1:F:114:LEU:HD13 | 1:F:166:TYR:HB2  | 2.02                     | 0.41              |
| 1:I:155:ASP:OD1  | 1:I:156:ASP:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:73:GLU:O     | 2:M:1:MET:CG     | 2.68                     | 0.41              |
| 4:a:117:VAL:O    | 4:a:117:VAL:HG22 | 2.21                     | 0.41              |
| 4:a:175:LEU:HD12 | 5:l:1:MET:CE     | 2.51                     | 0.41              |
| 4:b:35:SER:HB3   | 6:t:164:LEU:HD11 | 2.02                     | 0.41              |
| 4:b:119:THR:OG1  | 4:c:39:VAL:CG2   | 2.69                     | 0.41              |
| 4:b:145:ALA:HB3  | 3:q:54:PHE:HA    | 2.02                     | 0.41              |
| 4:d:118:GLU:H    | 4:e:36:GLY:CA    | 2.34                     | 0.41              |
| 6:t:86:PHE:HD2   | 7:y:56:ASN:ND2   | 2.18                     | 0.41              |
| 6:t:101:MET:O    | 7:w:111:SER:N    | 2.54                     | 0.41              |
| 6:t:116:HIS:ND1  | 7:y:55:PHE:CZ    | 2.89                     | 0.41              |
| 6:t:165:ILE:HG23 | 6:t:198:PHE:CD1  | 2.56                     | 0.41              |
| 6:u:46:LYS:HG2   | 6:u:77:GLU:OE1   | 2.20                     | 0.41              |
| 6:v:99:TYR:OH    | 7:x:54:LYS:CG    | 2.69                     | 0.41              |
| 6:v:103:GLY:C    | 7:y:113:SER:C    | 2.88                     | 0.41              |
| 7:w:188:LEU:HD22 | 7:y:188:LEU:HD22 | 2.02                     | 0.41              |
| 7:x:193:GLY:HA2  | 7:y:195:SER:CB   | 2.50                     | 0.41              |
| 1:A:60:GLY:CA    | 2:C:47:TYR:CE1   | 3.03                     | 0.41              |
| 1:K:26:MET:HE3   | 2:M:36:TYR:CE1   | 2.56                     | 0.41              |
| 1:K:68:ASP:OD1   | 2:M:69:ARG:HD2   | 2.21                     | 0.41              |
| 1:P:108:ARG:NH1  | 1:P:113:ASP:OD2  | 2.54                     | 0.41              |
| 4:a:33:ILE:HG22  | 4:a:34:GLU:N     | 2.35                     | 0.41              |
| 4:c:12:VAL:HG23  | 4:c:12:VAL:O     | 2.21                     | 0.41              |
| 4:c:173:GLN:HE22 | 4:c:177:LYS:CE   | 2.34                     | 0.41              |
| 4:d:66:LEU:HB3   | 4:d:93:ILE:HD13  | 2.02                     | 0.41              |
| 4:f:162:LYS:HE3  | 6:t:186:ARG:HB3  | 1.99                     | 0.41              |
| 6:t:103:GLY:N    | 7:w:112:ASP:CG   | 2.70                     | 0.41              |
| 6:v:99:TYR:CE2   | 6:v:101:MET:HE3  | 2.51                     | 0.41              |
| 7:x:60:THR:O     | 7:x:61:ASP:OD1   | 2.37                     | 0.41              |
| 1:B:121:ILE:HG22 | 1:B:122:ASN:O    | 2.21                     | 0.41              |
| 1:B:213:ASN:OD1  | 1:B:213:ASN:O    | 2.39                     | 0.41              |
| 1:H:109:ILE:CG2  | 2:J:136:ARG:HH11 | 2.32                     | 0.41              |
| 1:I:221:ASN:OD1  | 2:M:82:THR:HG23  | 2.21                     | 0.41              |
| 1:O:266:LEU:HB3  | 1:O:278:LEU:HD13 | 2.03                     | 0.41              |
| 4:a:118:GLU:C    | 4:b:36:GLY:O     | 2.63                     | 0.41              |
| 4:d:118:GLU:H    | 4:e:36:GLY:C     | 2.27                     | 0.41              |
| 6:t:103:GLY:O    | 7:w:112:ASP:CG   | 2.64                     | 0.41              |
| 7:w:53:PRO:O     | 7:w:55:PHE:CD2   | 2.74                     | 0.41              |
| 7:x:34:ARG:N     | 7:x:48:GLN:O     | 2.53                     | 0.41              |
| 7:y:66:GLN:HB3   | 7:y:67:GLU:OE1   | 2.21                     | 0.41              |
| 1:B:73:GLU:O     | 2:C:1:MET:CG     | 2.69                     | 0.41              |
| 2:C:8:PRO:HG3    | 2:C:45:MET:CG    | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:36:GLN:HG2   | 1:E:42:LEU:HD23  | 2.02                     | 0.41              |
| 1:E:72:ALA:O     | 1:E:98:ARG:NH2   | 2.51                     | 0.41              |
| 1:F:212:LYS:CE   | 1:O:238:GLY:HA3  | 2.51                     | 0.41              |
| 1:F:268:GLN:O    | 1:F:271:ALA:HB3  | 2.21                     | 0.41              |
| 1:F:278:LEU:HD21 | 1:F:280:MET:HE2  | 2.02                     | 0.41              |
| 1:H:166:TYR:CD1  | 1:I:106:ARG:HD3  | 2.56                     | 0.41              |
| 1:I:19:LEU:O     | 1:I:22:ILE:HG22  | 2.20                     | 0.41              |
| 1:I:204:ILE:CD1  | 1:I:227:LEU:HD22 | 2.50                     | 0.41              |
| 1:K:279:VAL:O    | 1:K:279:VAL:HG23 | 2.21                     | 0.41              |
| 1:L:256:TYR:OH   | 2:S:117:GLY:O    | 2.35                     | 0.41              |
| 1:P:68:ASP:OD1   | 1:P:69:PRO:HD2   | 2.21                     | 0.41              |
| 4:a:92:GLU:HG3   | 4:b:25:LYS:HE2   | 2.03                     | 0.41              |
| 4:a:119:THR:CG2  | 4:b:39:VAL:CG2   | 2.98                     | 0.41              |
| 4:b:39:VAL:CG1   | 6:t:6:TYR:CE2    | 3.04                     | 0.41              |
| 4:c:119:THR:HG23 | 4:d:39:VAL:CG2   | 2.45                     | 0.41              |
| 4:e:121:THR:HB   | 6:v:166:ASN:C    | 2.46                     | 0.41              |
| 4:e:179:VAL:HG21 | 5:i:73:LEU:HD21  | 2.02                     | 0.41              |
| 5:h:37:SER:HA    | 5:h:51:ARG:O     | 2.21                     | 0.41              |
| 5:k:28:TRP:HZ3   | 5:k:39:SER:HG    | 1.62                     | 0.41              |
| 5:l:28:TRP:CZ2   | 5:l:50:GLY:HA2   | 2.56                     | 0.41              |
| 6:t:42:GLY:N     | 7:y:7:LYS:HG3    | 2.35                     | 0.41              |
| 6:t:70:ILE:HD12  | 7:y:57:GLY:HA2   | 2.03                     | 0.41              |
| 6:t:182:LEU:HA   | 6:t:185:ASN:HB2  | 2.03                     | 0.41              |
| 6:v:67:VAL:CG2   | 7:x:56:ASN:O     | 2.68                     | 0.41              |
| 6:v:165:ILE:HG13 | 6:v:208:ILE:N    | 2.36                     | 0.41              |
| 6:v:185:ASN:O    | 6:v:187:LYS:HG2  | 2.21                     | 0.41              |
| 7:w:90:VAL:HG12  | 7:x:75:MET:HE1   | 2.03                     | 0.41              |
| 7:w:190:ILE:H    | 7:x:197:GLY:HA2  | 1.86                     | 0.41              |
| 7:w:193:GLY:HA2  | 7:x:195:SER:CB   | 2.51                     | 0.41              |
| 7:y:62:MET:HE2   | 7:y:118:LEU:HD22 | 2.02                     | 0.41              |
| 7:y:177:ALA:O    | 7:y:181:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:197:LEU:HD12 | 1:A:197:LEU:N    | 2.36                     | 0.41              |
| 1:A:212:LYS:O    | 1:A:213:ASN:OD1  | 2.39                     | 0.41              |
| 1:F:117:ALA:CB   | 1:F:162:LEU:HD11 | 2.51                     | 0.41              |
| 1:H:52:LEU:HD13  | 1:I:49:TYR:CZ    | 2.56                     | 0.41              |
| 2:J:51:VAL:HG23  | 2:J:52:GLU:OE2   | 2.20                     | 0.41              |
| 1:L:198:ILE:HG13 | 1:L:198:ILE:O    | 2.21                     | 0.41              |
| 1:P:114:LEU:HD13 | 1:P:166:TYR:HB2  | 2.03                     | 0.41              |
| 1:P:203:GLU:OE1  | 1:P:294:LEU:HB3  | 2.21                     | 0.41              |
| 4:a:36:GLY:CA    | 4:f:117:VAL:N    | 2.83                     | 0.41              |
| 4:a:128:LYS:HG2  | 4:a:129:ASP:H    | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:c:32:PRO:HA    | 6:t:203:GLN:CG   | 2.51                     | 0.41              |
| 4:f:66:LEU:HB3   | 4:f:93:ILE:HD13  | 2.01                     | 0.41              |
| 6:t:14:ASN:O     | 6:t:14:ASN:CG    | 2.64                     | 0.41              |
| 6:t:105:CYS:O    | 6:t:109:LEU:HG   | 2.21                     | 0.41              |
| 6:u:95:LEU:CD1   | 7:w:59:PRO:HB2   | 2.51                     | 0.41              |
| 6:u:185:ASN:O    | 6:u:187:LYS:HG2  | 2.21                     | 0.41              |
| 6:v:20:LYS:C     | 7:x:7:LYS:HZ1    | 2.17                     | 0.41              |
| 6:v:70:ILE:HD11  | 6:v:101:MET:HE2  | 2.03                     | 0.41              |
| 6:v:100:SER:HA   | 7:y:109:SER:HA   | 2.03                     | 0.41              |
| 6:v:195:GLU:HB2  | 6:v:212:THR:HB   | 2.03                     | 0.41              |
| 7:w:53:PRO:HG2   | 7:w:55:PHE:CZ    | 2.56                     | 0.41              |
| 7:w:215:VAL:HG21 | 7:y:180:MET:HE3  | 2.01                     | 0.41              |
| 7:y:102:TYR:HD1  | 7:y:108:GLY:HA2  | 1.86                     | 0.41              |
| 2:D:6:ALA:O      | 2:D:45:MET:SD    | 2.79                     | 0.40              |
| 1:E:60:GLY:HA3   | 2:G:47:TYR:CE1   | 2.56                     | 0.40              |
| 1:E:128:ARG:HG2  | 1:E:130:TYR:CZ   | 2.56                     | 0.40              |
| 1:E:205:ASP:O    | 1:E:262:VAL:HG22 | 2.21                     | 0.40              |
| 2:G:105:GLU:O    | 2:G:106:PRO:C    | 2.64                     | 0.40              |
| 1:L:81:ALA:HB2   | 1:L:101:ILE:HD11 | 2.03                     | 0.40              |
| 2:M:150:HIS:O    | 2:M:154:GLN:HG3  | 2.21                     | 0.40              |
| 1:P:162:LEU:O    | 1:P:166:TYR:HD1  | 2.03                     | 0.40              |
| 4:b:33:ILE:CG1   | 4:b:34:GLU:H     | 2.34                     | 0.40              |
| 4:b:80:THR:OG1   | 4:b:83:SER:O     | 2.35                     | 0.40              |
| 6:v:165:ILE:HG23 | 6:v:198:PHE:CE1  | 2.57                     | 0.40              |
| 7:w:53:PRO:HG3   | 7:w:62:MET:HE1   | 2.03                     | 0.40              |
| 7:x:52:LYS:HZ3   | 7:x:59:PRO:HB3   | 1.84                     | 0.40              |
| 1:A:21:GLU:HG3   | 2:C:39:LYS:NZ    | 2.36                     | 0.40              |
| 2:D:8:PRO:HG3    | 2:D:45:MET:CG    | 2.51                     | 0.40              |
| 2:J:8:PRO:CG     | 2:J:45:MET:HG3   | 2.50                     | 0.40              |
| 1:L:76:ARG:CZ    | 2:M:4:LEU:HD11   | 2.51                     | 0.40              |
| 2:M:145:ASP:OD1  | 2:M:148:SER:N    | 2.52                     | 0.40              |
| 1:O:186:PHE:CZ   | 1:P:111:LEU:HD12 | 2.56                     | 0.40              |
| 4:a:87:ASN:O     | 4:a:114:VAL:HG23 | 2.21                     | 0.40              |
| 4:a:115:LYS:CB   | 4:b:34:GLU:CB    | 2.99                     | 0.40              |
| 4:e:128:LYS:HB3  | 4:e:138:ASN:OD1  | 2.21                     | 0.40              |
| 5:j:72:LEU:O     | 5:j:73:LEU:HD23  | 2.20                     | 0.40              |
| 6:t:63:LEU:HD12  | 7:y:58:VAL:HG12  | 2.03                     | 0.40              |
| 6:u:66:VAL:HG12  | 7:w:57:GLY:O     | 2.21                     | 0.40              |
| 6:v:99:TYR:C     | 7:y:109:SER:CB   | 2.95                     | 0.40              |
| 7:w:200:HIS:O    | 7:y:187:LYS:HA   | 2.22                     | 0.40              |
| 1:F:232:THR:O    | 1:F:232:THR:HG22 | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:104:VAL:O    | 1:H:106:ARG:N    | 2.54                     | 0.40              |
| 1:K:40:SER:O     | 1:K:44:GLN:NE2   | 2.41                     | 0.40              |
| 1:K:69:PRO:O     | 1:K:98:ARG:HD2   | 2.22                     | 0.40              |
| 2:M:211:ILE:HD11 | 2:M:227:LEU:CB   | 2.50                     | 0.40              |
| 4:a:37:ALA:O     | 4:a:38:ASP:OD1   | 2.39                     | 0.40              |
| 4:b:21:LYS:HB3   | 4:b:51:GLU:HB3   | 2.03                     | 0.40              |
| 4:f:89:ILE:HD12  | 4:f:114:VAL:HG21 | 2.02                     | 0.40              |
| 5:j:51:ARG:HD2   | 5:j:63:PHE:CZ    | 2.56                     | 0.40              |
| 3:n:71:GLY:O     | 3:n:72:TYR:C     | 2.64                     | 0.40              |
| 6:t:98:PRO:HB2   | 7:w:108:GLY:HA3  | 2.04                     | 0.40              |
| 6:u:67:VAL:H     | 7:w:58:VAL:CG2   | 2.34                     | 0.40              |
| 6:v:103:GLY:CA   | 7:y:112:ASP:OD1  | 2.67                     | 0.40              |
| 6:v:149:ILE:HD12 | 6:v:163:ALA:HA   | 2.03                     | 0.40              |
| 7:w:21:GLN:O     | 7:w:25:GLU:HG3   | 2.21                     | 0.40              |
| 7:x:98:SER:OG    | 7:x:110:ALA:HB1  | 2.21                     | 0.40              |
| 7:x:114:ARG:HD2  | 7:x:117:SER:HB2  | 2.02                     | 0.40              |
| 7:y:183:VAL:HA   | 7:y:186:ASP:HB2  | 2.03                     | 0.40              |
| 1:B:12:LYS:HZ3   | 5:i:28:TRP:CD1   | 2.39                     | 0.40              |
| 1:B:280:MET:SD   | 1:B:286:MET:HG3  | 2.61                     | 0.40              |
| 1:E:124:VAL:HG13 | 1:E:151:VAL:HG23 | 2.04                     | 0.40              |
| 1:H:108:ARG:NH1  | 2:J:235:TYR:CD2  | 2.90                     | 0.40              |
| 1:H:111:LEU:HD21 | 1:H:131:VAL:HG21 | 2.02                     | 0.40              |
| 1:H:131:VAL:O    | 1:P:212:LYS:NZ   | 2.54                     | 0.40              |
| 1:I:74:GLY:HA3   | 2:J:1:MET:H2     | 1.86                     | 0.40              |
| 1:P:153:GLY:O    | 1:P:194:ARG:NH1  | 2.50                     | 0.40              |
| 1:Q:107:ALA:HB2  | 2:S:78:CYS:SG    | 2.61                     | 0.40              |
| 4:c:118:GLU:CG   | 6:u:144:PRO:O    | 2.68                     | 0.40              |
| 5:k:34:ASP:O     | 5:k:35:ARG:NH2   | 2.55                     | 0.40              |
| 5:l:85:LEU:HB3   | 5:l:86:PRO:HD3   | 2.04                     | 0.40              |
| 6:t:63:LEU:HD12  | 7:y:59:PRO:O     | 2.20                     | 0.40              |
| 6:t:67:VAL:HG21  | 6:t:86:PHE:HE2   | 1.86                     | 0.40              |
| 6:t:112:LEU:HD21 | 7:y:54:LYS:HG2   | 2.02                     | 0.40              |
| 6:u:66:VAL:HG13  | 6:u:69:GLU:HB2   | 2.04                     | 0.40              |
| 6:v:64:THR:CA    | 7:x:58:VAL:HG21  | 2.51                     | 0.40              |
| 6:v:102:CYS:C    | 7:y:113:SER:CA   | 2.95                     | 0.40              |
| 7:w:99:MET:HE3   | 7:w:102:TYR:HB2  | 2.02                     | 0.40              |
| 7:x:27:VAL:HG12  | 7:x:28:TRP:O     | 2.21                     | 0.40              |
| 7:y:101:ASN:HA   | 7:y:104:VAL:HB   | 2.03                     | 0.40              |
| 2:C:211:ILE:HD11 | 2:C:227:LEU:CB   | 2.51                     | 0.40              |
| 1:F:54:TYR:CE2   | 4:f:152:LYS:HG2  | 2.56                     | 0.40              |
| 1:H:213:ASN:OD1  | 1:H:213:ASN:C    | 2.64                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:214:GLY:O   | 1:O:187:CYS:HB3  | 2.22                     | 0.40              |
| 1:K:69:PRO:HD2  | 2:M:69:ARG:HD2   | 2.03                     | 0.40              |
| 1:L:27:VAL:HG13 | 1:L:32:PRO:HA    | 2.03                     | 0.40              |
| 1:P:207:GLN:HG3 | 1:P:262:VAL:CG2  | 2.51                     | 0.40              |
| 1:Q:70:GLU:OE1  | 2:S:69:ARG:HD2   | 2.21                     | 0.40              |
| 4:a:36:GLY:CA   | 4:f:118:GLU:H    | 2.34                     | 0.40              |
| 4:a:125:SER:HB3 | 6:t:141:LEU:HD13 | 2.03                     | 0.40              |
| 4:c:129:ASP:N   | 4:c:129:ASP:OD1  | 2.45                     | 0.40              |
| 5:i:29:TYR:OH   | 5:i:34:ASP:OD1   | 2.23                     | 0.40              |
| 3:n:11:LEU:HD12 | 3:n:44:GLN:HE21  | 1.86                     | 0.40              |
| 3:p:63:TRP:CE3  | 3:p:67:LEU:HD12  | 2.55                     | 0.40              |
| 6:t:54:SER:HA   | 7:w:111:SER:O    | 2.21                     | 0.40              |
| 6:t:56:THR:OG1  | 7:w:105:GLU:OE1  | 2.40                     | 0.40              |
| 6:t:60:GLY:H    | 6:t:95:LEU:HB2   | 1.87                     | 0.40              |
| 6:t:144:PRO:HG3 | 6:t:148:LEU:HD23 | 2.02                     | 0.40              |
| 6:u:66:VAL:HA   | 6:u:69:GLU:HB2   | 2.03                     | 0.40              |
| 7:w:23:GLU:HB3  | 7:y:24:ARG:NH1   | 2.36                     | 0.40              |
| 7:w:209:LEU:HG  | 7:y:184:ALA:HB1  | 2.03                     | 0.40              |
| 7:x:55:PHE:HD2  | 7:x:60:THR:OG1   | 2.04                     | 0.40              |
| 7:x:66:GLN:HB3  | 7:x:67:GLU:OE1   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 297/299 (99%) | 287 (97%) | 9 (3%)  | 1 (0%)   | 36          | 68  |
| 1   | B     | 297/299 (99%) | 287 (97%) | 10 (3%) | 0        | 100         | 100 |
| 1   | E     | 297/299 (99%) | 286 (96%) | 10 (3%) | 1 (0%)   | 36          | 68  |
| 1   | F     | 297/299 (99%) | 284 (96%) | 13 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 1   | H     | 297/299 (99%) | 286 (96%)  | 10 (3%)  | 1 (0%)   | 36          | 68  |
| 1   | I     | 297/299 (99%) | 284 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 1   | K     | 297/299 (99%) | 285 (96%)  | 11 (4%)  | 1 (0%)   | 36          | 68  |
| 1   | L     | 297/299 (99%) | 280 (94%)  | 15 (5%)  | 2 (1%)   | 18          | 52  |
| 1   | O     | 297/299 (99%) | 283 (95%)  | 13 (4%)  | 1 (0%)   | 36          | 68  |
| 1   | P     | 297/299 (99%) | 286 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 1   | Q     | 297/299 (99%) | 287 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 1   | R     | 297/299 (99%) | 283 (95%)  | 14 (5%)  | 0        | 100         | 100 |
| 2   | C     | 236/238 (99%) | 211 (89%)  | 25 (11%) | 0        | 100         | 100 |
| 2   | D     | 236/238 (99%) | 218 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 2   | G     | 236/238 (99%) | 217 (92%)  | 19 (8%)  | 0        | 100         | 100 |
| 2   | J     | 236/238 (99%) | 217 (92%)  | 19 (8%)  | 0        | 100         | 100 |
| 2   | M     | 236/238 (99%) | 217 (92%)  | 19 (8%)  | 0        | 100         | 100 |
| 2   | S     | 236/238 (99%) | 218 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 3   | X     | 118/125 (94%) | 113 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 3   | n     | 118/125 (94%) | 112 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 3   | o     | 118/125 (94%) | 113 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 3   | p     | 118/125 (94%) | 112 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 3   | q     | 118/125 (94%) | 113 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 3   | r     | 118/125 (94%) | 112 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 4   | a     | 180/191 (94%) | 158 (88%)  | 21 (12%) | 1 (1%)   | 21          | 56  |
| 4   | b     | 180/191 (94%) | 164 (91%)  | 14 (8%)  | 2 (1%)   | 11          | 43  |
| 4   | c     | 180/191 (94%) | 160 (89%)  | 18 (10%) | 2 (1%)   | 11          | 43  |
| 4   | d     | 180/191 (94%) | 165 (92%)  | 13 (7%)  | 2 (1%)   | 11          | 43  |
| 4   | e     | 180/191 (94%) | 159 (88%)  | 20 (11%) | 1 (1%)   | 21          | 56  |
| 4   | f     | 180/191 (94%) | 166 (92%)  | 12 (7%)  | 2 (1%)   | 11          | 43  |
| 5   | h     | 104/106 (98%) | 101 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 5   | i     | 104/106 (98%) | 103 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 5   | j     | 104/106 (98%) | 104 (100%) | 0        | 0        | 100         | 100 |
| 5   | k     | 104/106 (98%) | 102 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 5   | l     | 104/106 (98%) | 104 (100%) | 0        | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | m     | 104/106 (98%)   | 102 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 6   | t     | 227/229 (99%)   | 199 (88%)  | 28 (12%) | 0        | 100         | 100 |
| 6   | u     | 227/229 (99%)   | 204 (90%)  | 23 (10%) | 0        | 100         | 100 |
| 6   | v     | 227/229 (99%)   | 206 (91%)  | 21 (9%)  | 0        | 100         | 100 |
| 7   | w     | 219/221 (99%)   | 193 (88%)  | 26 (12%) | 0        | 100         | 100 |
| 7   | x     | 219/221 (99%)   | 196 (90%)  | 21 (10%) | 2 (1%)   | 14          | 47  |
| 7   | y     | 219/221 (99%)   | 192 (88%)  | 27 (12%) | 0        | 100         | 100 |
| All | All   | 8730/8898 (98%) | 8169 (94%) | 542 (6%) | 19 (0%)  | 44          | 73  |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 105 | ASP  |
| 4   | a     | 116 | ILE  |
| 4   | b     | 116 | ILE  |
| 4   | e     | 116 | ILE  |
| 1   | A     | 105 | ASP  |
| 1   | E     | 105 | ASP  |
| 1   | H     | 105 | ASP  |
| 4   | d     | 116 | ILE  |
| 4   | d     | 117 | VAL  |
| 1   | L     | 277 | PRO  |
| 1   | L     | 278 | LEU  |
| 1   | O     | 278 | LEU  |
| 4   | c     | 116 | ILE  |
| 4   | f     | 116 | ILE  |
| 4   | f     | 117 | VAL  |
| 7   | x     | 110 | ALA  |
| 4   | b     | 117 | VAL  |
| 4   | c     | 32  | PRO  |
| 7   | x     | 49  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | B     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | E     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | F     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | H     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | I     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | K     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | L     | 253/253 (100%) | 251 (99%)  | 2 (1%)   | 73          | 82  |
| 1   | O     | 253/253 (100%) | 252 (100%) | 1 (0%)   | 84          | 86  |
| 1   | P     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | Q     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 1   | R     | 253/253 (100%) | 253 (100%) | 0        | 100         | 100 |
| 2   | C     | 197/197 (100%) | 197 (100%) | 0        | 100         | 100 |
| 2   | D     | 197/197 (100%) | 197 (100%) | 0        | 100         | 100 |
| 2   | G     | 197/197 (100%) | 197 (100%) | 0        | 100         | 100 |
| 2   | J     | 197/197 (100%) | 197 (100%) | 0        | 100         | 100 |
| 2   | M     | 197/197 (100%) | 197 (100%) | 0        | 100         | 100 |
| 2   | S     | 197/197 (100%) | 196 (100%) | 1 (0%)   | 81          | 85  |
| 3   | X     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 3   | n     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 3   | o     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 3   | p     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 3   | q     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 3   | r     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 4   | a     | 144/148 (97%)  | 142 (99%)  | 2 (1%)   | 59          | 77  |
| 4   | b     | 144/148 (97%)  | 143 (99%)  | 1 (1%)   | 76          | 83  |
| 4   | c     | 144/148 (97%)  | 142 (99%)  | 2 (1%)   | 59          | 77  |
| 4   | d     | 144/148 (97%)  | 143 (99%)  | 1 (1%)   | 76          | 83  |
| 4   | e     | 144/148 (97%)  | 142 (99%)  | 2 (1%)   | 59          | 77  |
| 4   | f     | 144/148 (97%)  | 143 (99%)  | 1 (1%)   | 76          | 83  |
| 5   | h     | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 5   | i     | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 5   | j     | 90/90 (100%)    | 89 (99%)    | 1 (1%)   | 65          | 79  |
| 5   | k     | 90/90 (100%)    | 90 (100%)   | 0        | 100         | 100 |
| 5   | l     | 90/90 (100%)    | 89 (99%)    | 1 (1%)   | 65          | 79  |
| 5   | m     | 90/90 (100%)    | 90 (100%)   | 0        | 100         | 100 |
| 6   | t     | 192/192 (100%)  | 192 (100%)  | 0        | 100         | 100 |
| 6   | u     | 192/192 (100%)  | 192 (100%)  | 0        | 100         | 100 |
| 6   | v     | 192/192 (100%)  | 192 (100%)  | 0        | 100         | 100 |
| 7   | w     | 180/180 (100%)  | 180 (100%)  | 0        | 100         | 100 |
| 7   | x     | 180/180 (100%)  | 180 (100%)  | 0        | 100         | 100 |
| 7   | y     | 180/180 (100%)  | 180 (100%)  | 0        | 100         | 100 |
| All | All   | 7326/7380 (99%) | 7311 (100%) | 15 (0%)  | 85          | 89  |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 275 | THR  |
| 1   | L     | 278 | LEU  |
| 1   | O     | 278 | LEU  |
| 2   | S     | 3   | ASN  |
| 4   | a     | 115 | LYS  |
| 4   | a     | 116 | ILE  |
| 4   | b     | 116 | ILE  |
| 4   | c     | 115 | LYS  |
| 4   | c     | 116 | ILE  |
| 4   | d     | 116 | ILE  |
| 4   | e     | 115 | LYS  |
| 4   | e     | 116 | ILE  |
| 4   | f     | 115 | LYS  |
| 5   | j     | 46  | ASN  |
| 5   | l     | 46  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 18  | HIS  |
| 1   | B     | 221 | ASN  |
| 2   | C     | 31  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 77  | HIS  |
| 2   | C     | 112 | HIS  |
| 2   | C     | 154 | GLN  |
| 2   | D     | 77  | HIS  |
| 1   | E     | 36  | GLN  |
| 2   | G     | 31  | ASN  |
| 1   | H     | 132 | ASN  |
| 1   | H     | 268 | GLN  |
| 1   | I     | 207 | GLN  |
| 1   | I     | 239 | ASN  |
| 2   | J     | 31  | ASN  |
| 2   | J     | 99  | GLN  |
| 2   | J     | 139 | GLN  |
| 2   | J     | 170 | GLN  |
| 1   | K     | 284 | GLN  |
| 1   | K     | 289 | ASN  |
| 1   | L     | 18  | HIS  |
| 2   | M     | 77  | HIS  |
| 2   | M     | 99  | GLN  |
| 1   | O     | 161 | GLN  |
| 1   | P     | 18  | HIS  |
| 1   | R     | 18  | HIS  |
| 2   | S     | 99  | GLN  |
| 2   | S     | 112 | HIS  |
| 2   | S     | 139 | GLN  |
| 3   | X     | 16  | GLN  |
| 4   | a     | 138 | ASN  |
| 4   | a     | 173 | GLN  |
| 4   | b     | 101 | HIS  |
| 4   | c     | 158 | ASN  |
| 4   | d     | 101 | HIS  |
| 4   | e     | 158 | ASN  |
| 4   | e     | 173 | GLN  |
| 4   | f     | 31  | ASN  |
| 4   | f     | 101 | HIS  |
| 5   | i     | 97  | GLN  |
| 5   | j     | 46  | ASN  |
| 5   | j     | 97  | GLN  |
| 5   | l     | 46  | ASN  |
| 5   | l     | 97  | GLN  |
| 6   | t     | 172 | ASN  |
| 6   | u     | 94  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | u     | 121 | ASN  |
| 6   | v     | 172 | ASN  |
| 6   | v     | 202 | ASN  |
| 7   | w     | 124 | HIS  |
| 7   | w     | 144 | HIS  |
| 7   | w     | 200 | HIS  |
| 7   | x     | 11  | GLN  |
| 7   | x     | 144 | HIS  |
| 7   | y     | 21  | GLN  |
| 7   | y     | 95  | GLN  |
| 7   | y     | 171 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

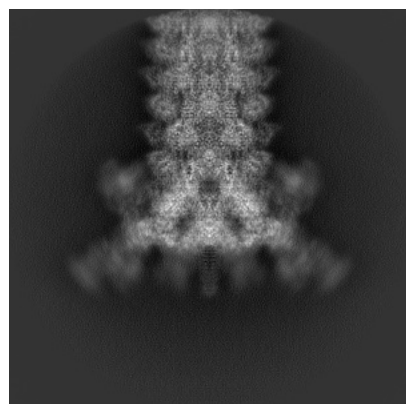
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33802. These allow visual inspection of the internal detail of the map and identification of artifacts.

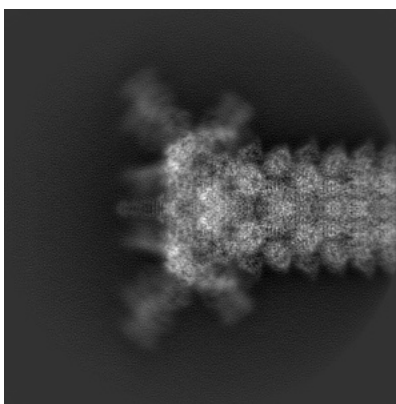
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

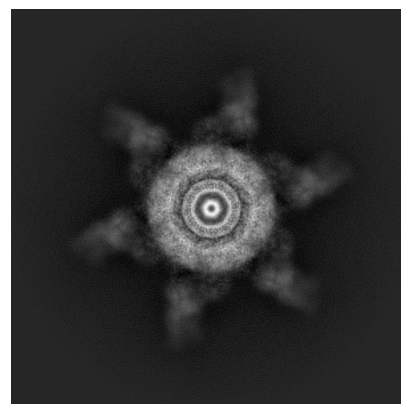
#### 6.1.1 Primary map



X

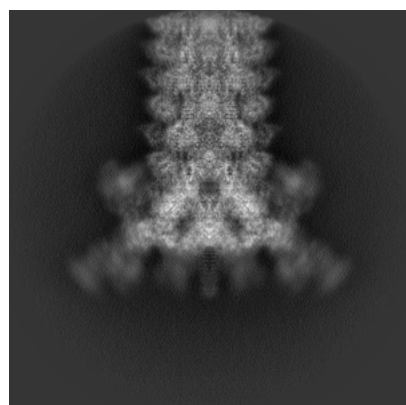


Y

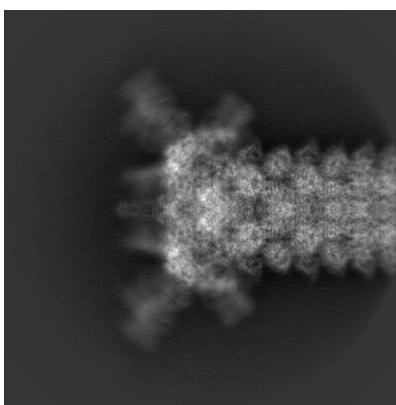


Z

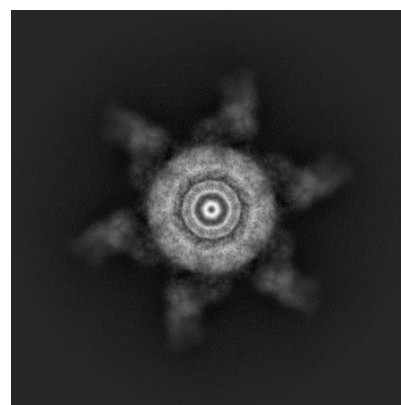
#### 6.1.2 Raw map



X



Y

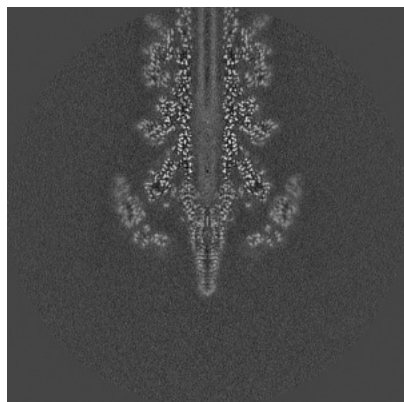


Z

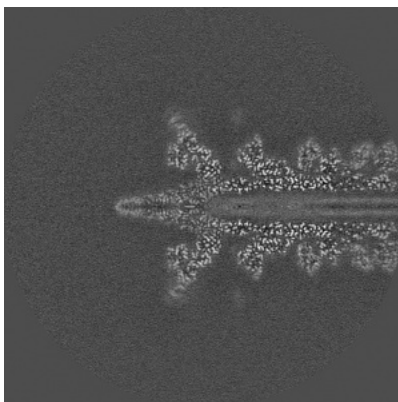
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

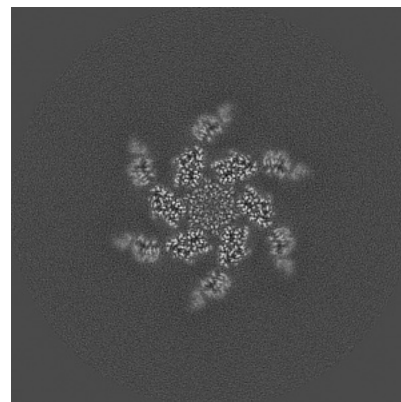
### 6.2.1 Primary map



X Index: 240

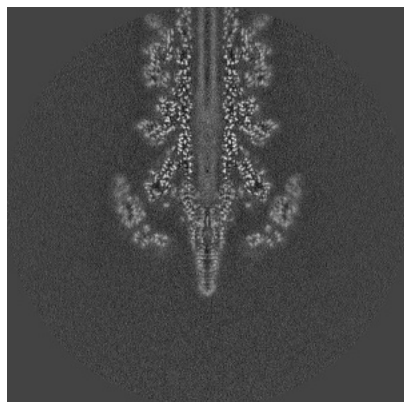


Y Index: 240

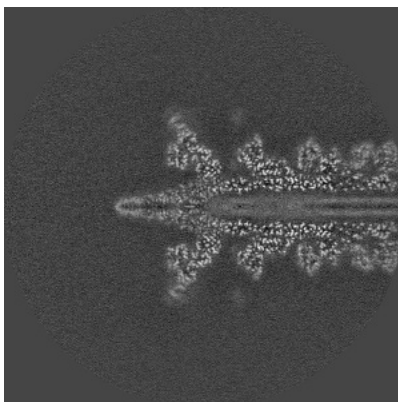


Z Index: 240

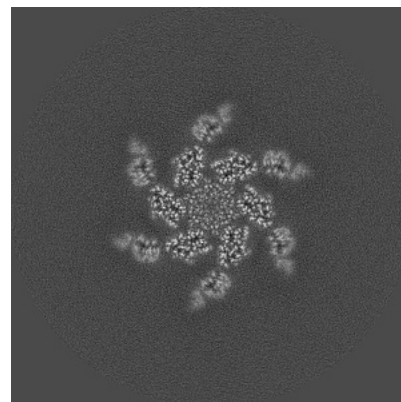
### 6.2.2 Raw map



X Index: 240



Y Index: 240

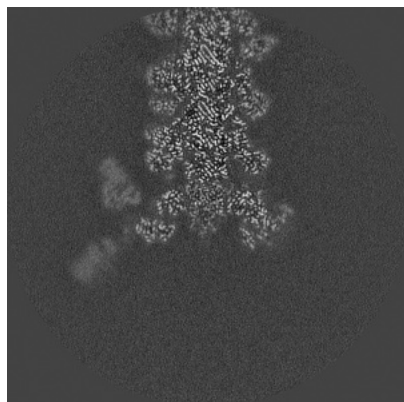


Z Index: 240

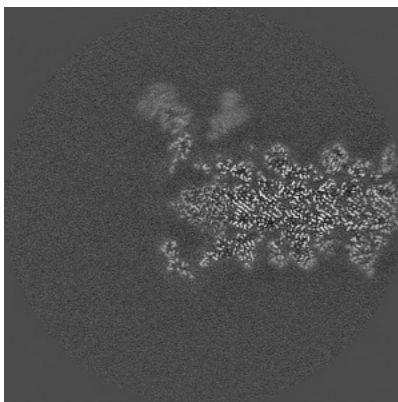
The images above show central slices of the map in three orthogonal directions.

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

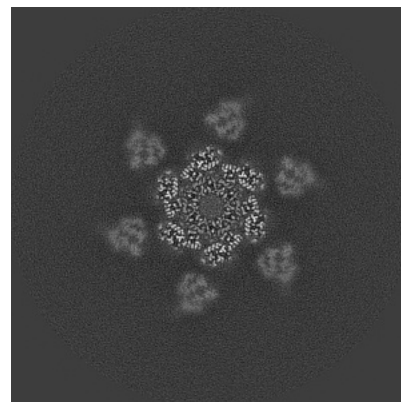
### 6.3.1 Primary map



X Index: 218

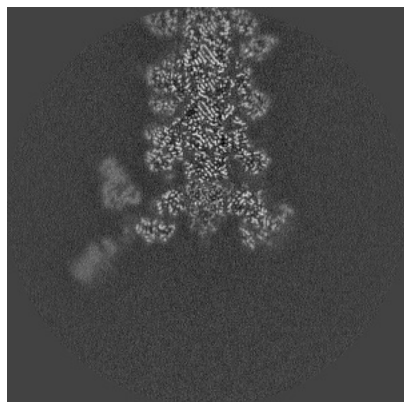


Y Index: 261

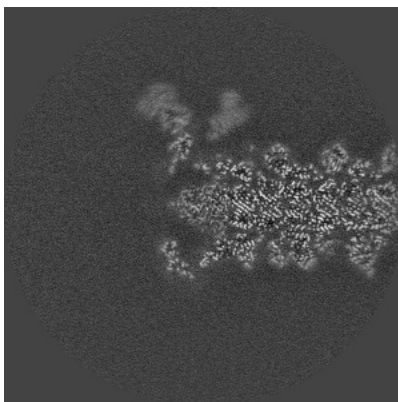


Z Index: 256

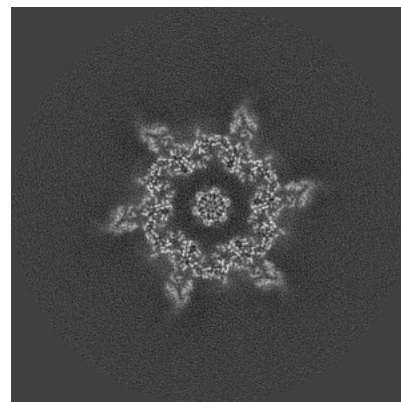
### 6.3.2 Raw map



X Index: 218



Y Index: 261



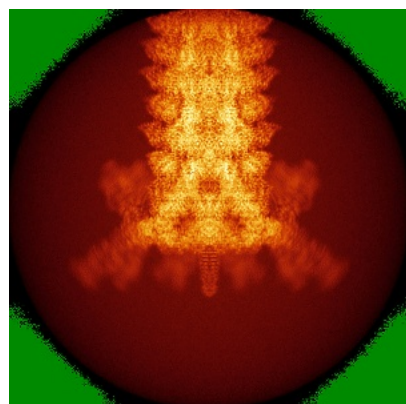
Z Index: 208

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

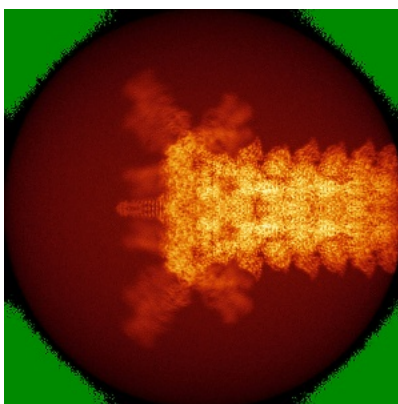


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

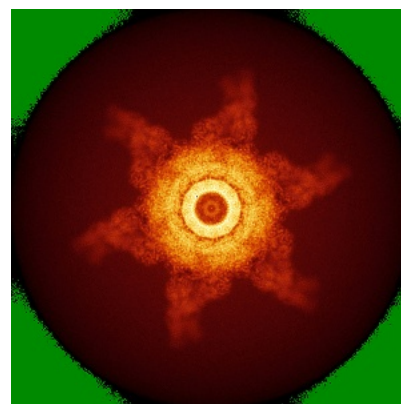
### 6.4.1 Primary map



X

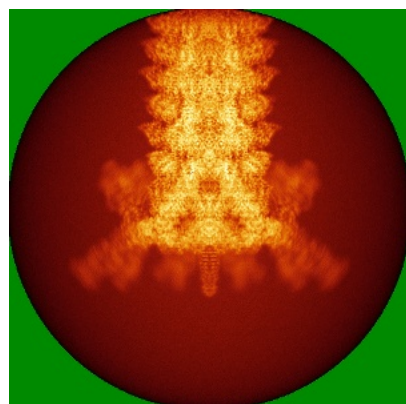


Y

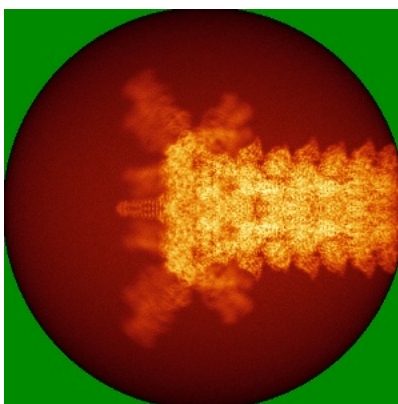


Z

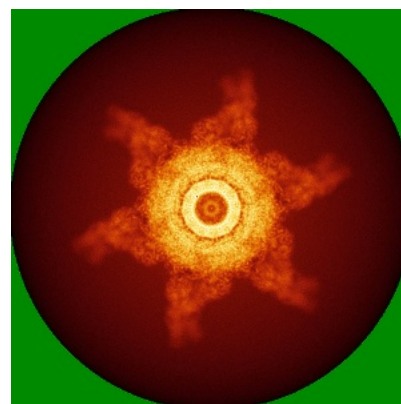
### 6.4.2 Raw map



X



Y

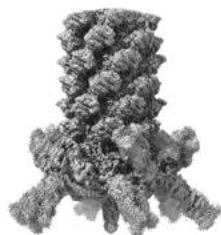


Z

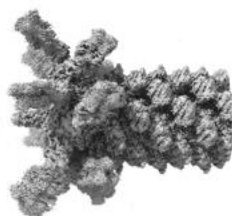
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

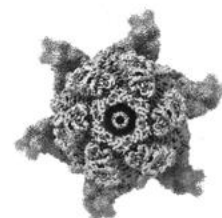
### 6.5.1 Primary map



X



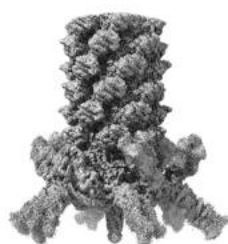
Y



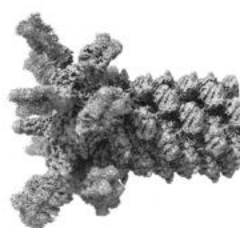
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

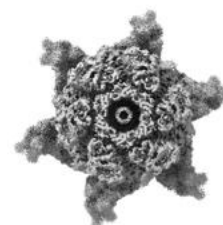
### 6.5.2 Raw map



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.

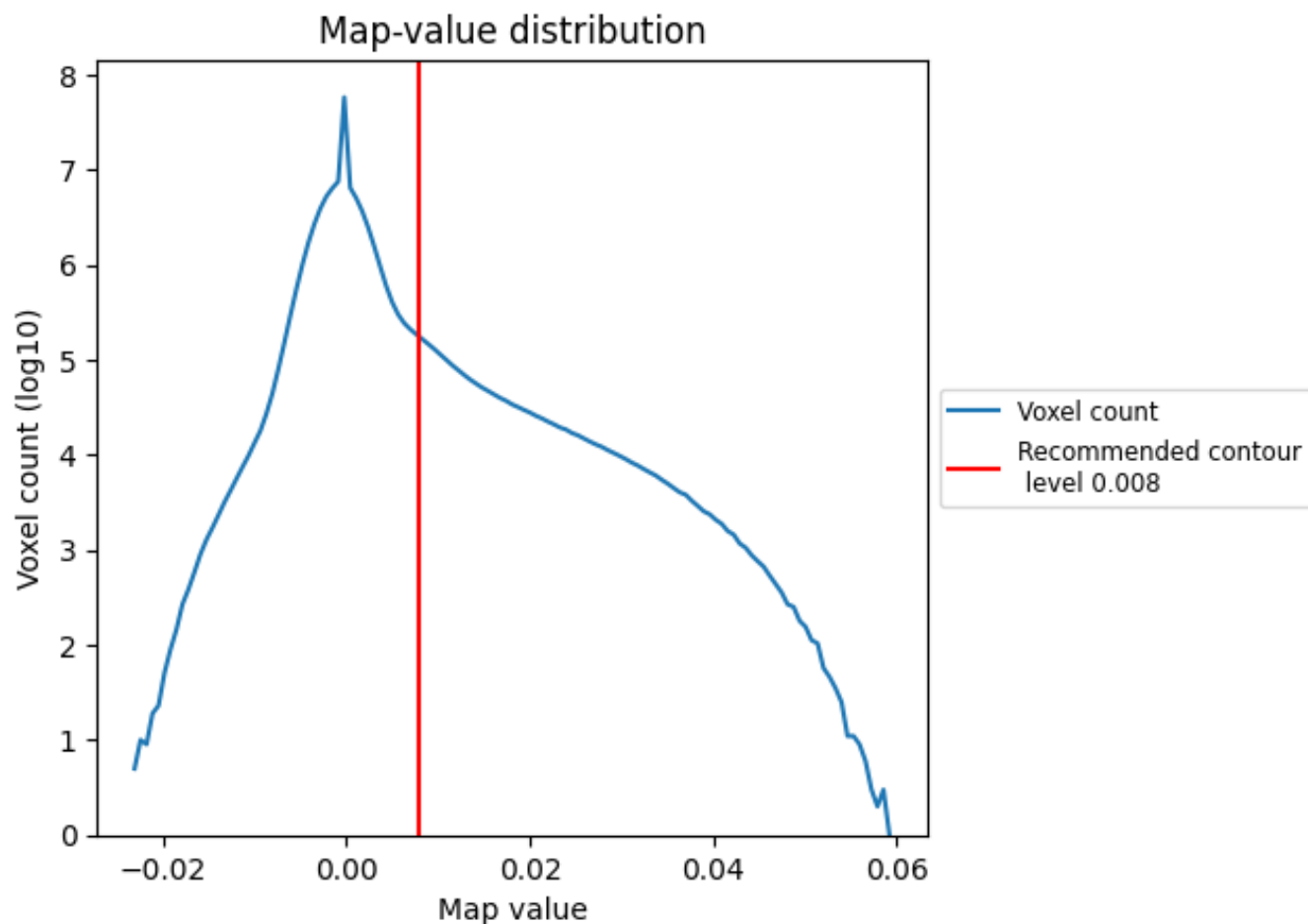
## 6.6 Mask visualisation [i](#)

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.

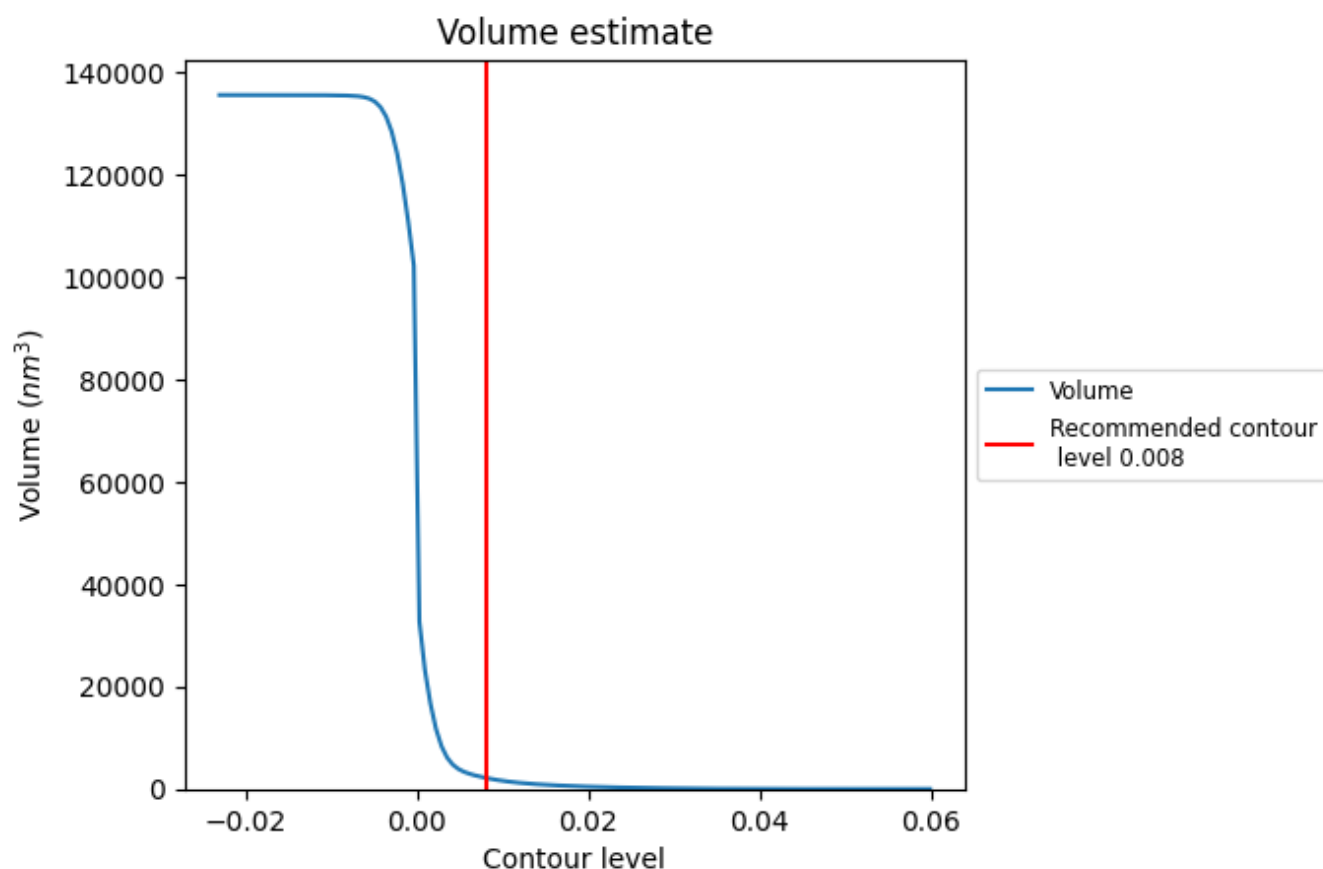
### 7.1 Map-value distribution [i](#)



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.



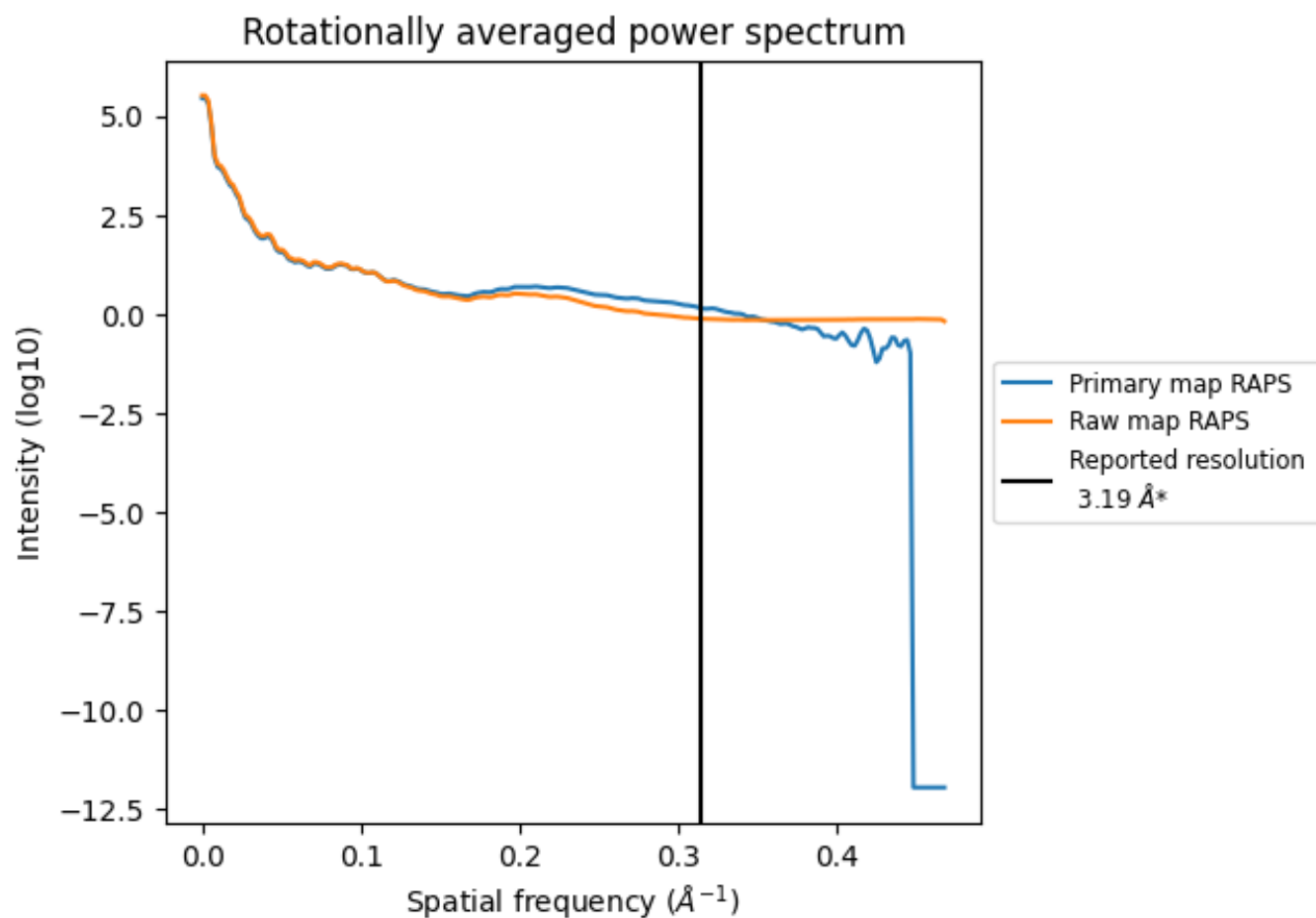
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2164  $\text{nm}^3$ ; this corresponds to an approximate mass of 1955 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 ⓘ

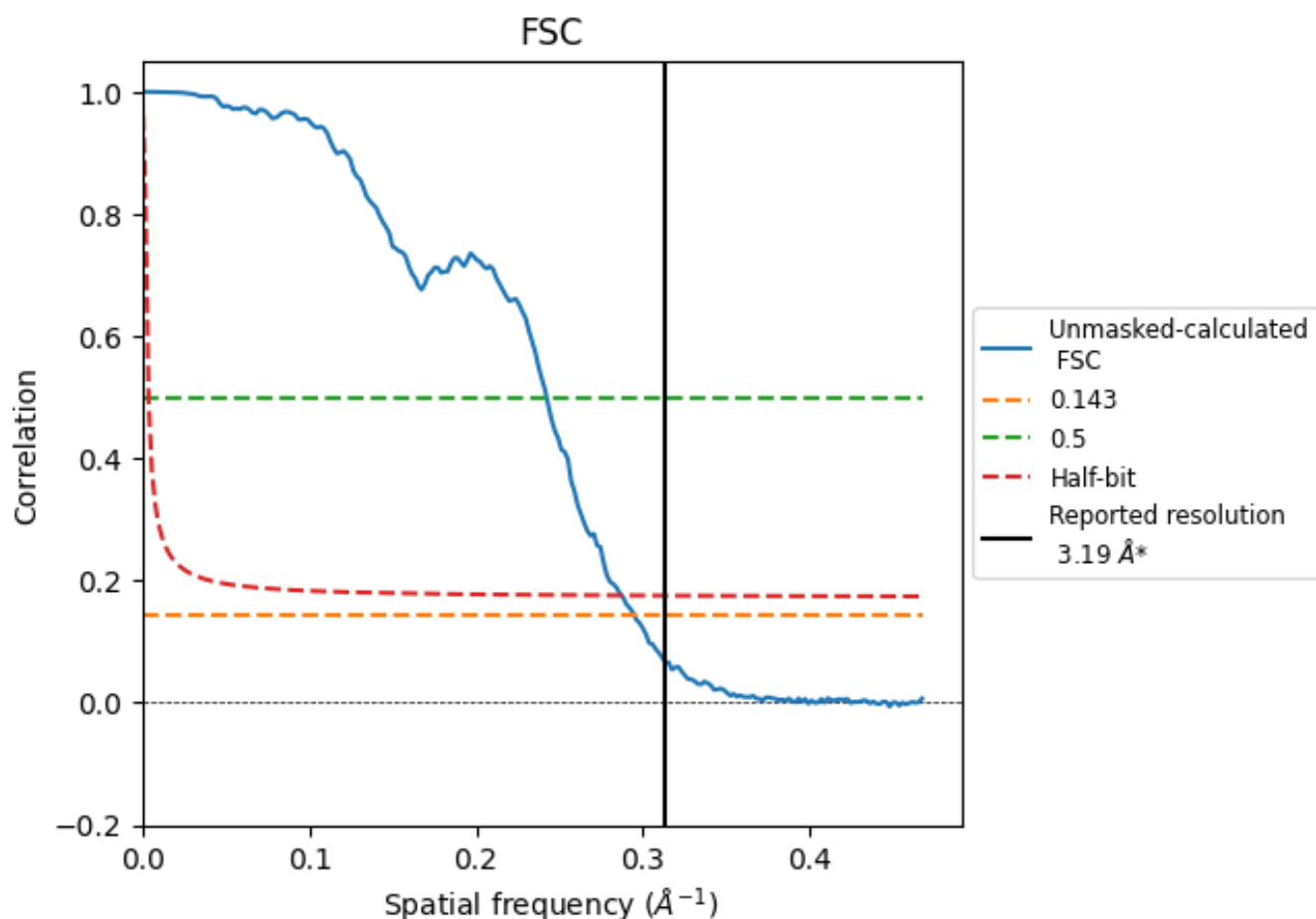


\*Reported resolution corresponds to spatial frequency of 0.313 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.313  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

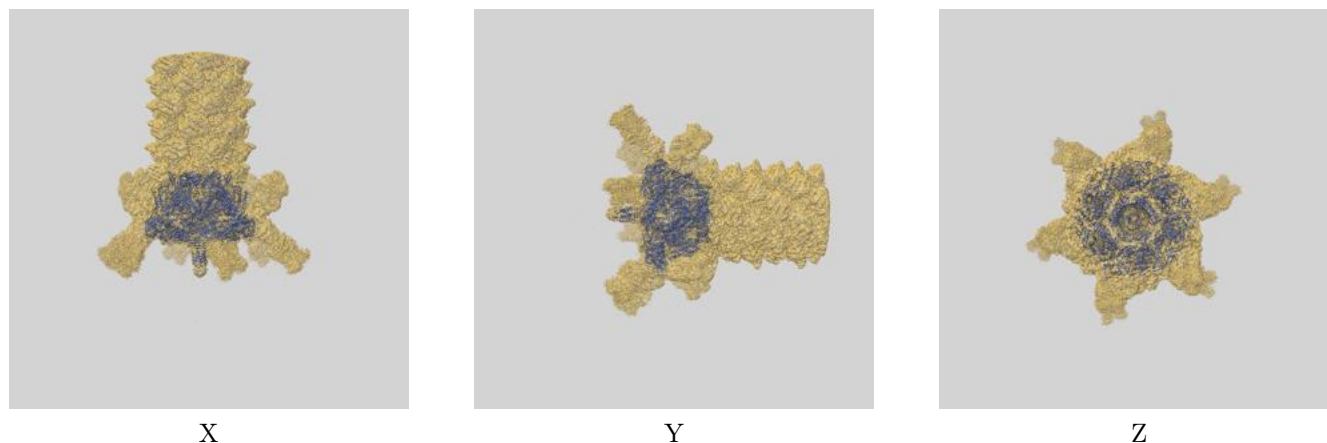
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.19                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.39                               | 4.13 | 3.48     |

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

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

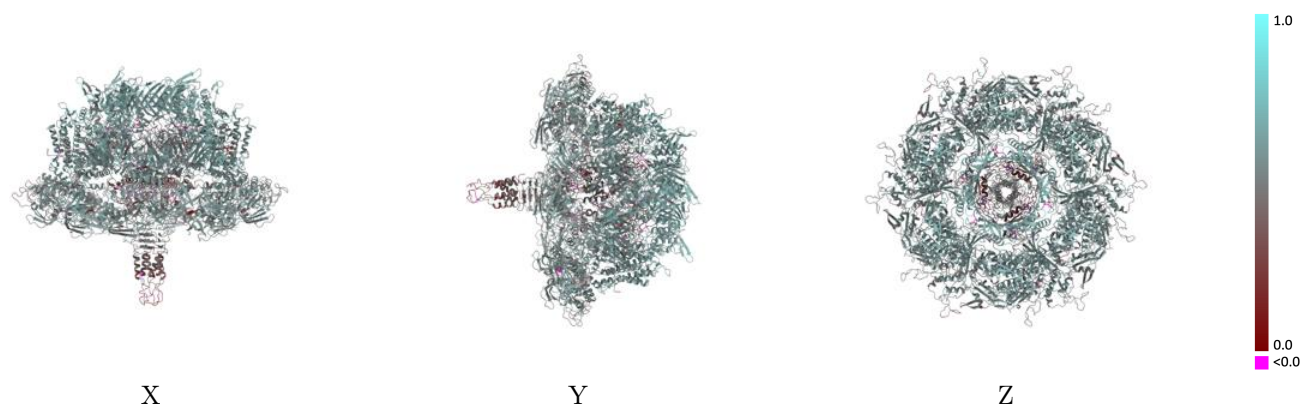
This section contains information regarding the fit between EMDB map EMD-33802 and PDB model 7YFZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



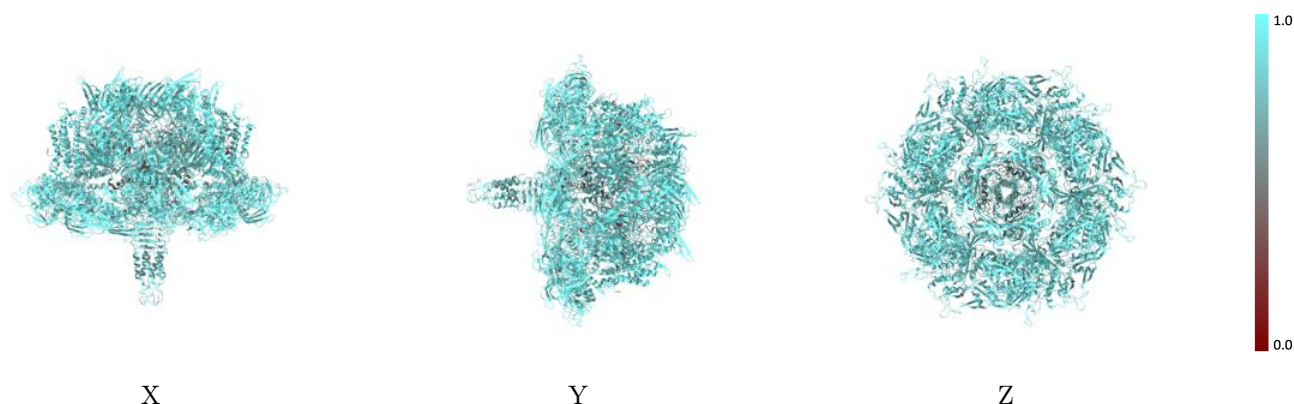
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



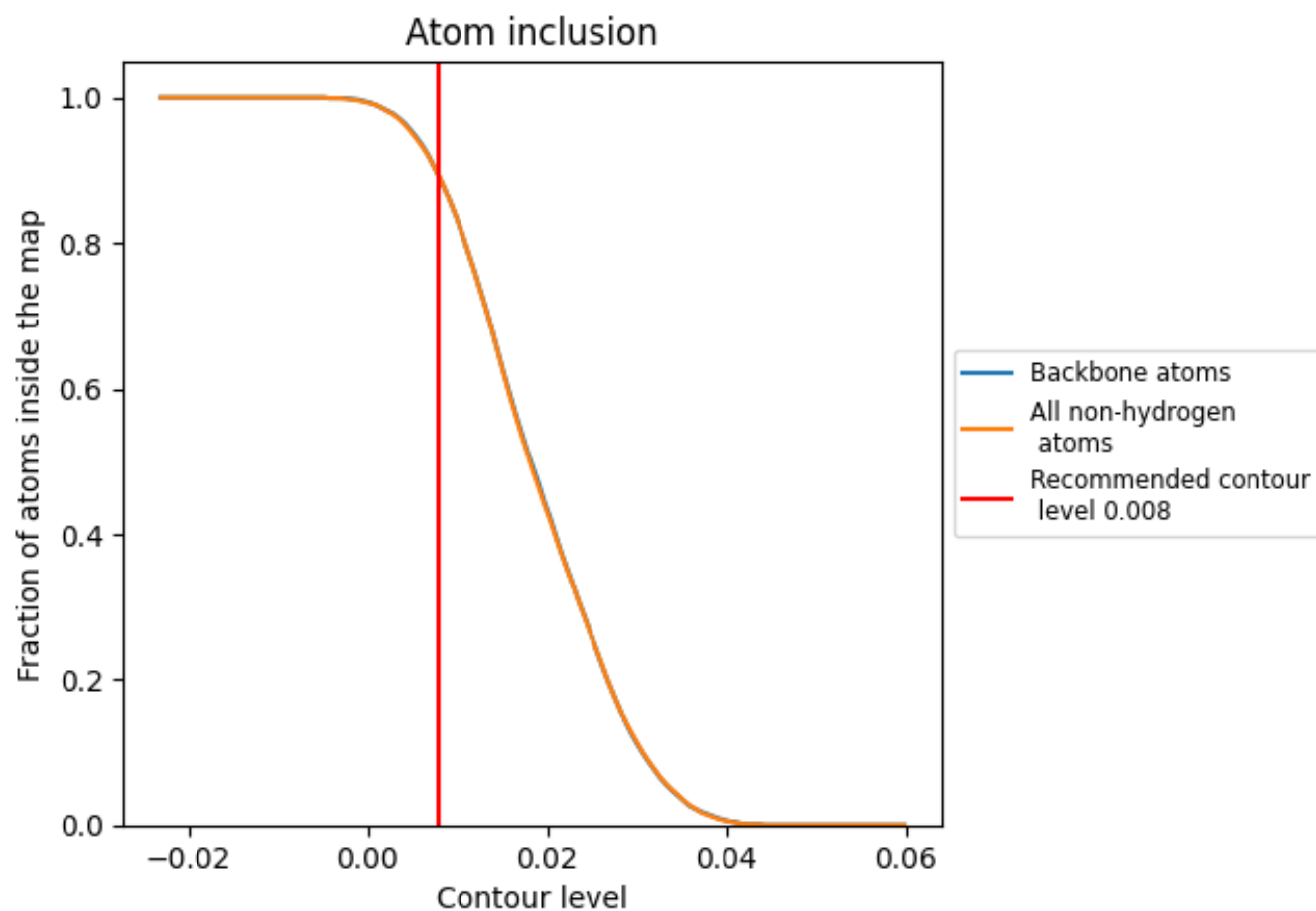
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8920   |  0.5280   |
| A     |  0.9200   |  0.5440   |
| B     |  0.9260   |  0.5460   |
| C     |  0.9170   |  0.5330   |
| D     |  0.9230   |  0.5270   |
| E     |  0.9240   |  0.5430   |
| F     |  0.9180   |  0.5400   |
| G     |  0.9120   |  0.5300   |
| H     |  0.9240   |  0.5430   |
| I     |  0.9290   |  0.5460   |
| J     |  0.9120   |  0.5270   |
| K     |  0.9210   |  0.5480   |
| L     |  0.9140   |  0.5410   |
| M     |  0.9150   |  0.5260   |
| O     |  0.9180  |  0.5450  |
| P     |  0.9220 |  0.5460 |
| Q     |  0.9210 |  0.5400 |
| R     |  0.9280 |  0.5470 |
| S     |  0.9110 |  0.5260 |
| X     |  0.9240 |  0.5850 |
| a     |  0.8820 |  0.5400 |
| b     |  0.8890 |  0.5470 |
| c     |  0.8800 |  0.5420 |
| d     |  0.8870 |  0.5420 |
| e     |  0.8810 |  0.5400 |
| f     |  0.8890 |  0.5470 |
| h     |  0.9200 |  0.5850 |
| i     |  0.9090 |  0.5670 |
| j     |  0.9030 |  0.5650 |
| k     |  0.8990 |  0.5710 |
| l     |  0.9100 |  0.5650 |
| m     |  0.9000 |  0.5730 |
| n     |  0.9240 |  0.5910 |
| o     |  0.9280 |  0.5830 |
| p     |  0.9270 |  0.5880 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| q     |  0.9310 |  0.5840 |
| r     |  0.9220 |  0.5880 |
| t     |  0.7650 |  0.4360 |
| u     |  0.7670 |  0.4400 |
| v     |  0.7640 |  0.4440 |
| w     |  0.7960 |  0.3940 |
| x     |  0.7920 |  0.3920 |
| y     |  0.7950 |  0.3930 |